Classical and quantum mechanics via Lie algebras

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This is the draft of a book. The manuscript has not yet full book quality.
Please refer to the book once it is published.

Until then, we'd appreciate suggestions for improvements; please send them to Arnold.Neumaier@univie.ac.at

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Preface

This book presents classical mechanics, quantum mechanics, and statistical mechanics in an almost completely algebraic setting, thereby introducing mathematicians, physicists, and engineers to the ideas relating classical and quantum mechanics with Lie algebras and Lie groups.

The book should serve as an appetizer, inviting the reader to go more deeply into these fascinating, interdisciplinary fields of science.

Much of the material covered here is not part of standard textbook treatments of classical or quantum mechanics (or is only superficially treated there). For physics students who want to get a broader view of the subject, this book may therefore serve as a useful complement to standard treatments of quantum mechanics.

We motivate everything as far as possible by classical mechanics. This forced an approach to quantum mechanics close to Heisenberg's matrix mechanics, rather than the usual approach dominated by Schrödinger's wave mechanics. Indeed, although both approaches are formally equivalent, only the Heisenberg approach to quantum mechanics has any similarity with classical mechanics; and as we shall see, the similarity is quite close. Indeed, the present book emphasizes the closeness of classical and quantum mechanics, and the material is selected in a way to make this closeness as apparent as possible.

Almost without exception, this book is about precise concepts and exact results in classical mechanics, quantum mechanics, and statistical mechanics. The structural properties of mechanics are discussed independently of computational techniques for obtaining quantitatively correct numbers from the assumptions made. This allows us to focus attention on the simplicity and beauty of theoretical physics, which is often hidden in a jungle of techniques for estimating or calculating quantities of interests. The standard approximation machinery for calculating from first principles explicit thermodynamic properties of materials, or explicit cross sections for high energy experiments can be found in many textbooks and is not repeated here.

Compared with the 2008 version, most of Chapters 2–3 and all of Chapters 14–18 are new; the remaining chapters were slightly improved.

The book originated as course notes from a course given by the first author in fall 2007, written up by the second author, and expanded and polished by combined efforts, resulting in a uniform whole that stands for itself. Parts II and IV are mainly based on earlier work by the first author (including Neumaier [203, 205]); and large parts of Part I were added later. The second author acknowledges support by the Austrian FWF-projects START-project Y-237 and IK 1008-N. Thanks go to Roger Balian, Clemens Elster, Martin Fuchs, Johann Kim, Mihaly Markot, Mike Mowbray, Hermann Schichl, Peter Schodl, and Tapio Schneider, who contributed through their comments on earlier versions of parts of the book.

The audience of the course consisted mainly of mathematics students shortly before finishing their diploma or doctorate degree and a few postgraduates, mostly with only a limited background knowledge in physics.

Thus we assume some mathematical background knowledge, but only a superficial acquaintance with physics, at the level of what is available to readers of the Scientific American, say. It is assumed that the reader has a good command of matrix algebra (including complex numbers and eigenvalues) and knows basic properties of vector spaces, linear algebra, groups, differential equations, topology, and Hilbert spaces. No background in Lie algebras, Lie groups, or differential geometry is assumed. Rudiments of differential geometry would be helpful to expand on our somewhat terse treatment of it in Part V; most material, however, is completely independent of differential geometry.

While we give precise definitions of all mathematical concepts encountered (except in Chapter 4, which is taken verbatim from the theoretical physics FAQ), and an extensive index of concepts and notation, we avoid the deeper use of functional analysis and differential geometry without being mathematically inaccurate, by concentrating on situations that have no special topological difficulties and only need a single chart. But we mention where one would have to be more careful about existence or convergence issues when generalizing to infinite dimensions.

On the physics side, we usually first present the mathematical models for a physical theory before relating these models to reality. This is adequate both for mathematically-minded readers without much physics knowledge and for physicists who know already on a more elementary level how to interpret the basic settings in terms of real life examples.

This is an open-ended book. It should whet the appetite for more, and lead the reader into going deeper into the subject.[1] Thus many topics are discussed far too short for a comprehensive treatment, and often only the surface is scratched. A term has only this many hours, and our time to extend and polish the lectures after they were given was limited, too. We added some material, and would have liked to be more complete in many respects. Nevertheless, we believe that the topics treated are the fundamental ones, whose understanding gives a solid foundation to assess the wealth of material on other topics.

We usually introduce physical concepts by means of informal historical interludes, and only discuss simple physical situations in which the relevant concepts can be illustrated. We refer to the general situation only by means of remarks; however, after reading the book, the reader should be able to go deeper into the original literature that treats these topics in greater physical depth.

Part I is an invitation to quantum mechanics, concentrating on giving motivation and background from history, from classical mechanics, and from simple, highly symmetric quantum systems. The latter are used to introduce the most basic Lie algebras and Lie groups. Part II gives a thorough treatment of the formal part of equilibrium statistical mechanics, viewed in the present context as the common core of classical and quantum

[1] Some general references for further reading: Barut & Raczka [28], Cornwell [68], Gilmore [104], and Sternberg [260], for the general theory of Lie algebras, Lie groups, and their representations from a physics point of view, Wybourne [296] and Fuchs & Schweigert [95] for a more application oriented view of Lie algebras, Kac [145] and Neeb [200] for infinite-dimensional Lie algebras, Papoušek & Aliev [211] for quantum mechanics and spectroscopy, van der Waerden [276] for the history of quantum mechanics, and Weinberg [284] for a (somewhat) Lie algebra oriented treatment of quantum field theory.

mechanics, and discusses the interpretation of the theory in terms of models, statistics and measurements. Part III introduces the basics about Lie algebras and Poisson algebras, with an emphasis on the concepts most relevant to the conceptual side of physics. Part IV discusses the dynamics of nonequilibrium phenomena, i.e., processes where the expectation changes with time, in as far as no fields are involved. This results in a dissipative dynamics. Part V introduces the relevant background from differential geometry and applies it to classical Hamiltonian and Lagrangian mechanics, to a symplectic formulation of quantum mechanics, and to Lie groups. Part VI applies the concepts to the study of quantum oscillators (bosons) and spinning systems (fermions), and to the analysis of empirically observed spectra, concentrating on the mathematical contents of these subjects. The book concludes with numerous references and an index of all concepts and symbols introduced. For a more detailed overview of the topics treated, see Section 1.9.

We hope that you enjoy reading this book!

Wien, April 15, 2011

Arnold Neumaier, Dennis Westra

Part I

An invitation to quantum mechanics

Chapter 1

Motivation

Part I is an invitation to quantum mechanics, concentrating on giving motivation and background from history, from classical mechanics, and from 2-state quantum mechanics.

The first chapter is an introduction and serves as a motivation for the following chapters. We shall go over different areas of physics and give a short glimpse on the mathematical point of view.

The final section of the chapter outlines the content of the whole book.

For the mathematicians most of the folklore vocabulary of physicists may not be familiar, but later on in the book, precise definitions in mathematical language will be given. Therefore, there is no need to understand everything in the first chapter on first reading; we merely introduce informal names for certain concepts from physics and try to convey the impression that these have important applications to reality and that there are many interesting solved and unsolved mathematical problems in many areas of theoretical physics.[1]

1.1 Classical mechanics

Classical mechanics is the part of physics whose development started around the time of Isaac Newton (1642-1727).

It was in the period of Newton, Leibniz, and Galileo that classical mechanics was born, mainly studying planetary motion. Newton wanted to understand why the earth seems to circle around the sun, why the moon seems to circle around the earth, and why apples (and other objects) fall down. By analyzing empirical data, he discovered a formula explaining most of the observed phenomena involving gravity. Newton realized that the laws of physics here on earth are the same as the laws of physics determining the motion of the planets. This was a major philosophical breakthrough.

[1] We encourage readers to investigate for themselves some of the abundant literature to get a better feeling and more understanding than we can offer here.

The motion of a planet is described by its position and velocity at different times. With the laws of Newton it was possible to deduce a set of differential equations involving the positions and velocities of the different constituents of the solar system. Knowing exactly all positions and velocities at a given time, one could in principle deduce the positions and velocities at any other time.

Our solar system is a well-posed initial value problem (IVP). However, an initial error in position and velocities at time $t_0 = 0$ grows exponentially at time $t > 0$ by a factor of $\sim e^{\lambda t}$. The value of λ varies for different initial conditions; its maximum is called the **maximal Lyapunov exponent**. A system with maximal Lyapunov exponent $\lambda = 0$ is called **integrable**. If $\lambda < 0$ the solutions converge to each other and if $\lambda > 0$ the solutions move away from each other. The solar system is apparently not quite integrable: according to numerical simulations, the maximal Lyapunov exponent for our solar system seems to be small but positive, with λ^{-1} being about five million years (Laskar [170, 171], Lissauer [177]).

Frequently, instead of considering separately time-dependent positions and velocities of many objects (e.g., planets, atoms, or particles) in a system, it is more convenient to work with single **trajectories**, paths parameterized by time, in a high-dimensional space called the **phase space** of the system. In the case of the planetary system with N planets, the points in phase space are described by vectors which have $6N$ components grouped into N pairs consisting of three components for position and three components for **momentum**, velocity multiplied by mass, of each particle. One reason that one prefers momentum before velocity is that the total momentum of all particles is **conserved**, i.e., remains constant in time. A deeper reason that will become apparent later is that on the level of position and momentum, the similarity between classical and quantum mechanics is most apparent. For a single particle moving in space, there are three spatial directions to specify its position and three directions to specify the velocity. Hence the phase space of a (free) particle is six-dimensional; for a system of N astronomical bodies, the dimension is $6N$.

Low-dimensional phase spaces are well-understood in general. Newton showed that the configuration of a single planet moving around the sun is stable (in fact, the system is integrable) and motion follows **Kepler's' laws**, which were already known before, thus giving these a theroetical basis. Higher-dimensional phase spaces tend to cause problems. Indeed, for more planets (that is, more than 2 bodies in the system), deviations from elliptic motions are predicted, and the question of stability was open for a long time. The Swedish king Oskar II was willing to reward with a big amount of money the scientist who proved stability of our solar system.

However, Poincaré showed that already three objects (one sun, two planets) cause big problems for a possible stability proof of our solar system and received the prize in 1887. The numerical studies from the end of the last century (quoted above) strongly indicate that the solar system is unstable, though a mathematical proof is missing.

We now turn from celestial mechanics, where phase space is finite-dimensional, to **continuum mechanics**, which has to cope with infinite-dimensional phase spaces. For example, to describe a fluid, one needs to give the distribution of mass and energy and the local ve-

locity for all (infinitely many) points in the fluid. The dynamics is now governed by partial differential equations. In particular, fluid mechanics is dominated by the **Navier–Stokes equations**, which still presents a lot of difficult mathematical problems.

Showing that solutions exist for all times (not only short-time solutions) is one of the Clay Millennium problems (see, e.g., Ladyzhenskaya [166]), and will be rewarded by one million dollars.

The infinitely many dimensions of the phase space cause serious additional problems. The Lyapunov exponents now depend on where the fluid starts in phase space and for fast-flowing fluids, the maximal Lyapunov exponent is much larger than zero in most regions of phase space. This results in a phenomenon called **turbulence**, well-known from the behavior of water. The notion of turbulence is still not well understood mathematically. Surprisingly enough, the problems encountered with turbulence are of the same kind as the problems encountered in quantum field theories (QFT's) – one of the many instances where a problem in classical mechanics has an analogue in quantum physics.

Another area of continuum mechanics is **elasticity theory**, where solids are treated as continuous, nearly rigid objects, which deform slightly under external forces. The rigidity assumption is easily verified empirically; try to swim in metal at room temperature.... Due to the rigidity assumption the behavior is much better understood mathematically than in the fluid counterpart.

The configuration of a solid is close to equilibrium and the deviations from the equilibrium position are strongly suppressed (this *is* rigidity). Hence the rigidity assumption implies that linear Taylor approximations work well since the remaining terms of the Taylor series are small, and the Lyapunov exponent is zero.

Elasticity theory is widely applied in engineering practice. Modern bridges and high rise buildings would be impossible without the finite element analyses which determine their stability and their vibration modes. In fact, the calculations are done in finite-dimensional discretizations, where much of the physics is reducible to linear algebra. Indeed, all continuum theories are (and have to be) handled computationally in approximations with only finitely many degrees of freedom; in most areas very successfully. The mathematical difficulties are often related to establishing a valid continuum limit.

1.2 Relativity theory

In the period between 1900 and 1920, classical mechanics was enriched with **special relativity theory** (SRT) and **general relativity theory** (GRT). In SRT and GRT, space and time merge into a four-dimensional manifold, called space-time.

In SRT, space-time is flat. Distances in space and time are measured with the Minkowski metric, an indefinite metric (discussed in more detail in Section 3.13) which turns space-time a pseudo-Riemannian manifold. Different observers (in SRT) all see the same speed of light. But they see the same distances only when measured with the Minkowski metric –

not with the Euclidean spatial or temporal metric (which also holds for the orthogonality mentioned above). It follows that spatial separation and temporal separation between localized systems (for example a chicken laying an egg and an atom splitting) are different for different observers! But the difference is observable only when the two systems move at widely different velocities, hence Newton couldn't have noticed this deviation from his theory.

In classical mechanics, time is absolute in the sense that there exists a global time up to time shifts; the time difference between two events is the same in every coordinate system. The symmetries of classical space-time is thus the group generated by time-translations, space translations and rotations. This group is the Galilean group. Due to the experimental fact that the speed of light in vacuum is the same for all observers led Einstein to the conclusion that time is not absolute and that the Galilean group should be enlarged with transformations that rotate space and time coordinates into each other. The result was the theory of special relativity. Due to special relativistic effects in the quantum theory, the world indeed looks different; for example, without special relativity, gold would be white, and mercury would be solid at room temperature Norrby [208].

SRT is only valid if observers move at fixed velocities with respect to each other. To handle observers whose relative velocities may vary requires the more general but also more complex GRT. The metric now depends on the space-time point; it becomes a nondegenerate symmetric bilinear form on the space-time manifold. The transformations (diffeomorphisms) relating the metric in one patch to the metric in another patch cannot change the signature. Hence the signature is the same for all observers.

The changing metric has the effect that in GRT, space-time is no longer flat, but has curvature. That means that freely moving objects do not follow real straight lines – in fact the notion of what straight means is blurred. The trajectory that an object in a free fall, where no forces are exerted on the object, will follow is called a **geodesic**. The geodesics are determined by the geometry by means of a second-order differential equation. The preferred direction of time on a curved space-time is now no longer fixed, or as mathematicians say 'canonical', but is determined by the observer: The geodesic along the observers' 4-momentum vector defines the world line of the observer (e.g., a measuring instrument) and with it its time; the space-like surfaces orthogonal to the points on the world line define the observer's 3-dimensional space at each moment. When the observer also defines a set of spatial coordinates around its position, and a measure of time (along the observers' geodesic), one can say that a chart around the observer has been chosen.

When time becomes an observer dependent quantity, so becomes energy. Local energy conservation is still well defined, described by a conservation law for the resulting differential equations. The differential equations are covariant, meaning that they make sense in any coordinate system. For a large system in general relativity, the definition of a total energy which is conserved, i.e., time-independent, is however problematic, and well-defined only if the system satisfies appropriate boundary conditions such as asymptotic flatness, believed to hold for the universe at large. Finally, if the system is dissipative, there is energy loss, and the local conservation law is no longer valid. Not even the rate of energy loss is well defined. Dissipative general relativity has not yet found its final mathematical form.

1.3 Statistical mechanics and thermodynamics

Thermodynamics describes ordinary matter on the level of ordinary experience. Loosely speaking, it is the theory of the quantitative relations between volume and pressure, temperature and heat, and how this characterizes different substances in their different phases – as solid, fluid, or gas. **Statistical mechanics** is the part of physics that derives the macroscopic properties of matter – which themselves are primarily described by thermodynamics – from microscopic principles.

An important ingredient in classical statistical mechanics is a **phase space density** ρ playing the role of a measure to calculate probabilities; the expectation value of a function f is given by

$$\langle f \rangle := \int \rho f, \tag{1.1}$$

where the integral indicates integration with respect to the so-called Liouville measure in phase space.

In the quantum version of statistical mechanics the density ρ gets replaced by a linear operator ρ on Hilbert space called the **density matrix**, the functions become linear operators, and we have again (1.1), except that the integral is now interpreted as the **quantum integral**,

$$\int f = \operatorname{tr} f, \tag{1.2}$$

where $\operatorname{tr} f$ denotes the trace of a trace class operator.

We shall see that the algebraic properties of the classical integral and the quantum integral are so similar that using the same name and symbol is justified.

A deeper justification for the quantum integral becomes visible if we introduce the **Lie product**[2]

$$f \angle g := \begin{cases} \{g, f\} & \text{in the classical case,} \\ \frac{i}{\hbar}[f, g] & \text{in the quantum case,} \end{cases} \tag{1.3}$$

unifying the classical **Poisson bracket**

$$\{f, g\} := \partial_q f \cdot \partial_p g - \partial_q g \cdot \partial_p f$$

on the algebra $\mathbb{E} = C^\infty(\Omega)$ of smooth functions on phase space $\Omega = \mathbb{R}^{3N} \times \mathbb{R}^{3N}$, and the quantum **commutator**

$$[f, g] := fg - gf$$

on the algebra $\mathbb{E} = \operatorname{Lin} C^\infty(\mathbb{R}^{3N})$ of linear operators on the space of smooth functions on configuration space. (Here $i = \sqrt{-1}$ – complex numbers will figure prominently in this book! –, and $\hbar$ is **Planck's constant** in the form introduced by Dirac [74]. Planck had used instead the constant $h = 2\pi\hbar$ which caused many additional factors of 2π in formulas discovered later.) The Lie product is in both cases an antisymmetric bilinear map from $\mathbb{E} \times \mathbb{E}$ to $\mathbb{E}$ and satisfies the **Jacobi identity**; see Chapter 11 for precise definitions.

[2] The symbol $\angle$, frequently used in the following, is interpreted as a stylized capital letter L and should be read as "Lie".

In the classical case, the fact that integration and differentiation are inverse operations implies that the integral of a derivative of a function vanishing at infinity is zero. The traditional definition of the Poisson bracket therefore implies that, for functions f, g vanishing at infinity,

$$\int f \angle g = 0. \tag{1.4}$$

Remarkably, in the quantum case, (1.4) is valid for Hilbert–Schmidt operators f, g since then $\operatorname{tr} fg = \operatorname{tr} gf$, so that $\int f \angle g = \operatorname{tr} \frac{i}{\hbar}[f, g] = \frac{i}{\hbar}(\operatorname{tr} fg - \operatorname{tr} gf) = 0$. Thus the quantum integral behaves just like the Liouville integral!

Thus we see that there is a very close parallel between the classical and the quantum case. Indeed, statistical mechanics is the area where classical mechanics and quantum mechanics meet most closely, and hence an area of central interest for our book. This field, growing out of the desire to seek a more fundamental understanding of thermodynamics, was developed especially during the industrial revolution in England. Maxwell wrote many papers on a mathematical foundation of thermodynamics. With the establishment of a molecular world view the thermodynamical machinery slowly got replaced by statistical mechanics, where the macroscopic properties like heat capacity, entropy, temperature were explained through considerations of the statistical properties of a big population of particles. The first definite treatise on statistical thermodynamics is by Gibbs [102][3] who also invented much of the modern mathematical notation in physics, especially the notation for vector analysis.

Quantum mechanics and classical mechanics look almost the same when viewed in the context of statistical mechanics; indeed, Gibbs' account of statistical mechanics had to be altered very little after quantum mechanics revolutionized the whole of science. In this course, we shall always emphasize the closeness of classical and quantum reasoning, and put things in a way to make this closeness as apparent as possible.

1.4 Hamiltonian mechanics

Understanding statistical physics requires the setting of **Hamiltonian mechanics**, which exists both in a classical and a quantum version.

Much of classical mechanics can be understood in both a Hamiltonian formulation and a Lagrangian formulation; cf. Chapter 18. In the Hamiltonian formulation, the basic object is the **Hamiltonian** function H on the phase space Ω, which gives the value of the energy at an arbitrary point of phase space. Specifying H essentially amounts to specifying the physical system under consideration. Often the phase space Ω is the **cotangent bundle** T^*M of a manifold M. In the Lagrangian formulation, the main object is a **Lagrangian function** L on the **tangent bundle** TM of a manifold M. The Lagrangian is thus not a function on phase space, and has no simple physical interpretation, but in some sense, it plays a more fundamental role than the Hamiltonian since it survives the transition to the currently most fundamental physical theory, quantum field theory. The physics point of view on quantum field theory is expounded in many books, perhaps explained

[3] Today, this book from 1902 is still easily readable.

most thoroughly in the volumes by Weinberg [284]. For an introduction to quantum field theory from a mathematician's point of view, see Zeidler [299]; this book draws connections to many topics of contemporary mathematics, and points out basic unresolved marthematical issues in quantum field theory. Both books together provide complementary perspectives on the subject.

The passage between the Hamiltonian and the Lagrangian formulation is straightforward in simple cases but may cause problems, especially in so-called **gauge theories** (pronounced in English transcription as *gaidge*). Gauge theories are outside the scope of this book; the curious reader is referred to the vast literature.

In the Hamiltonian formulation the time-dependence of a function f on the phase space is determined by the **classical Heisenberg equation**

$$\frac{df}{dt} = H\angle f = \{f, H\} \ , \tag{1.5}$$

where H is the Hamiltonian function defined above. Important to note is that the Hamiltonian function determines the time-evolution. If we can solve these differential equations, this defines an operator $U(s,t)$ that maps objects at a time s to corresponding objects at a time t.

Clearly, the composition of the operators gives $U(s,s')U(s',t) = U(s,t)$. If the Hamiltonian is independent of time (this amounts to assuming that there are no external forces acting on the system) the maps U form a so-called one-parameter group, since one can write

$$U(s,t) = e^{(t-s)\mathrm{ad}_H} \ ,$$

with the associated **Hamiltonian vector field** ad_H, which is determined by H. The vector field ad_H generates shifts in time. In terms of ad_H, the multiplication is given by

$$e^{t\mathrm{ad}_H} e^{s\mathrm{ad}_H} = e^{(t+s)\mathrm{ad}_H} \ ,$$

and the inverse is given by

$$U(r,s)^{-1} = U(s,r) \, , \quad (e^{t\mathrm{ad}_H})^{-1} = e^{-t\mathrm{ad}_H} \ .$$

From a mathematical point of view, the physical Hamiltonian is just one of many Hamiltonian functions that can be used in the above discussion. Given another Hamiltonian function H' we get another Hamiltonian vector field $\mathrm{ad}_{H'}$, another one-parameter group, and a "time" parameter t with a different physical interpretation (if one exists). For example, if H' is a component of the momentum vector (or the angular momentum vector) then t corresponds to a translation (or rotation) in the corresponding coordinate direction by a distance (or angle) t. Combining these groups for all H', where the initial value problem determined by $\mathrm{ad}_{H'}$ is well posed, we get an infinite-dimensional Lie group. (See Sections 11.3 and 17.7 for a definition of Lie groups.) Thus, classical mechanics can be understood in terms of infinite-dimensional groups!

To avoid technical complications, we shall however mainly be concerned with the cases where we can simplify the system such that the groups are finite-dimensional. In the

present case, to obtain a finite-dimensional group one either picks a nice subgroup (this involves understanding the symmetries of the system) or one makes a partial discretization of phase space.

Most of our discussions will be restricted to conservative systems, which can be described by Hamiltonians. However, these only describe systems which can be regarded as isolated from the environment, apart from influences that can be specified as external forces. Many real life systems (and strictly speaking all systems with the exception of the universe as a whole) interact with the environment – indeed, if it were not so, they would be unobservable!

Ignoring the environment is possible in so-called reduced descriptions, where only the variables of the system under consideration are kept. This usually results in differential equations which are dissipative. In a **dissipative system**, the energy dissipates, which means that some energy is lost into the unmodelled environment. Due to the energy loss, going back in time is not well defined in infinite-dimensional spaces; the initial value problem is solvable only in the forward time direction. Hence we can not find an inverse for the translation operators $U(s,t)$, and these are defined only for $s \leq t$. Therefore, in the most general case of interest, the dissipative infinitesimal generators do not generate a group, but only a semigroup. A well-known example is heat propagation, described by the heat equation. Its solution forward in time is a well-posed initial value problem, whereas the solution backward in time suffers from uncontrollable instability. Actually, many dissipative systems are not even described by a Hamiltonian dynamics, but the semigroup property of the flow they generate still remains valid.

1.5 Quantum mechanics

The historical point of view on quantum mechanics is that it is a deformation of classical mechanics obtained by a process called quantization. The deformation parameter is Planck's constant $\hbar$.

Since in daily life we do not really see so much of quantum physics, one requires that the so-called **correspondence principle** holds. The correspondence principle states that the formulas of quantum physics should turn into corresponding formulas of classical mechanics in the limit when $\hbar \to 0$. This limit is called the **classical limit**. However, $\hbar$ is a constant of Nature and not a parameter that can be changed in experiments; thus this 'limit' must be properly interpreted. The **action** of a physical system is a certain functional S that gives rise to equations of motion and is measured in units of $\hbar$. The right way to think of the classical limit is therefore the limit when the dimensionless quotient $S/\hbar$ becomes arbitrarily large. The classical limit therefore amounts to considering the limiting case of very large S. Thus classical mechanics appears as the limit of quantum mechanics when all values of the action involved are huge when measured in units of $\hbar$, which is the case when the systems are sufficiently large.

Keeping only the linear orders of $\hbar$ one obtains so-called **semiclassical approximations**, which is intermediate between quantum mechanics and the classical limit, and often can be

used for quite small systems.

The value of Planck's constant is approximately $6.6 \cdot 10^{-34} Js$; its smallness is the reason why we do not encounter quantum phenomena on our length and time scales that often.

A nice gedanken experiment, which goes under the name **Schrödinger's cat**, illustrates – though in a philosophically questionable way – quantum mechanics in terms of daily-life physics. In short the experiment goes as follows. Suppose we have put a cat in a box and in the same box we have a single radioactive nucleus. The state of the nucleus is determined by the laws of quantum physics; the nucleus can disintegrate but we don't know when. The process of disintegration is described by a probability distribution that is dictated by the laws of quantum mechanics. Now suppose we link to the nucleus a detector and a gun; if the nucleus disintegrates, the gun, which is aimed at the cat, goes off and kills the cat. The state of the cat, dead or alive, is now given by a quantum mechanical probability distribution. But common sense expects the cat to be either dead or alive. . . .

This sort of quantum weirdness is often propagated in the literature about quantum mechanics for the general public. But those who want to get a thorough understanding of quantum physics should try to forget all that weird stuff, which is only due to an inadequate visualization of what quantum mechanics is about. The science of quantum mechanics is very orderly and free from paradoxes, if everything is expressed in the proper – mathematical – language.

Many quantum observations, for example scattering processes, exhibit a stochastic character, so probabilities are frequent in quantum mechanics. Probabilities in quantum mechnaics are usually introduced in terms of an abstract concept without an intuitive meaning, that of the wave function. In contrast, in this book, we shall hardly make use of wave functions, since our goal is to emphasize a view that shows how classical mechanics and quantum mechanics are very alike. Rather than postulating probabilities as fundamental, as in the usual approach, we derive the probabilistic view in Chapter 10 in a manner exhibiting the conditions under which this view is appropriate. Therefore, from the point of view of this book, the wave function is only a mathematical artifice to perform certain calculations which result in physics of interest. Nevertheless we give here a short introduction so that readers can easily make the connection to the standard presentation.

The **wave function** of a single particle is a complex-valued function of space and time coordinates that is square-integrable over the space coordinates for all time t. For example, the Uranium nucleus in the gedanken experiment described above is described by such a wave function.

In quantum chemistry, the square absolute value of the wave function of an electron is interpreted (apart from a constant factor) as its charge density. One usually normalizes the wave function to have total weight 1; then the squared absolute value of the wave function integrates to one, and can be viewed as a probability distribution in space. It is the distribution governing the random quantum response of an array of detectors placed at various position in space (when this is feasible to do). In the Copenhagen interpretation of quantum mechanics (a semiclassical view interpreting quantum aspects of a system

with classical measurement equipment), one regards it as the distribution for "finding" the particle in the position where such a detctor responds.

In particular, in case of a single particle, the probability density for observing a detector response at x is $|\psi(x)|^2$. Physicists and chemists occasionally view a scaled version of the probability distribution $|\psi|$ as a charge density. The justification is that in a population of a great number of particles that are all subject to the same Schrödinger equation, the particles will distribute themselves more or less according to the probability distribution of a single particle.

In a first course on quantum mechanics one postulates the **time-dependent Schrödinger equation**

$$i\hbar \frac{d}{dt}\psi = H\psi \tag{1.6}$$

for a single particle described by the wave function ψ, where H is the Hamiltonian – now an operator. The Schrödinger equation describes the dynamics of the wave function and thus of the particle. Given a solution ψ to the Schrödinger equation, normalized to satisfy $\psi^*\psi = 1$ (where ψ^* is the adjoint linear functional, in finite dimensions the conjugate transpose), one obtains a density operator $\rho = \psi\psi^*$, which is a Hermitian, positive semidefinite rank-one operator of trace $\operatorname{tr}\rho = \psi^*\psi = 1$. This type of density operator characterizes so-called **pure states**; the nomenclature coincides here with that of the mathematical theory of **C*-algebras**.

In quantum mechanics, the classical functions are replaced by corresponding operators defined on a dense subspace of a suitable separable Hilbert space. For example, the momentum in the x-direction of a particle described by a wave function $\psi(x)$ can be described by the operator $-i\hbar\partial_x$. As we shall see, this process of **quantization** has interesting connections to the representation theory of Lie algebras. Using the correspondence between classical functions and operators one deduces the Hamiltonian for an electron of the hydrogen atom, the basis for an explanation of atomic physics and the periodic system of elements.

The hydrogen atom is the quantum version of the 2-body problem of Newton and is the simplest of a large class of problems for which one can explicitly get the solutions of the Schrödinger equation – it is integrable in a sense paralleling the classical notion. Unfortunately, integrable systems are not very frequent; they seem to exist only for problems with finitely many degrees of freedom, for quantum fields living on a 2-dimensional space-time, and for noninteracting theories in higher dimensions. (Whether there are exactly solvable interacting local 4-dimensional field theories is an unsolved problem.) Nevertheless, the hydrogen atom and other integrable systems are very important since one can study in these simple models the features which in some approximate way still hold for more complicated physical systems.

1.6 Quantum field theory

In N-particle quantum mechanics, the Hamiltonian is a second-order differential operator with respect to the spatial coordinates. According to the present state of knowledge, the fundamental description of nature is, however, given not in terms of particles but in terms of fields. The quantum mechanics of fields is called **quantum field theory**; the Hamiltonian is now an expression composed of field operators rather than differential operators. While nonrelativistic quantum mechanics may be treated equivalently as N-particle mechanics or as nonrelativistic quantum field theory, the relativistic quantum mechanics of more than one particle (see, e.g., the survey by Keister & Polyzou [148]) is somewhat clumsy, and one uses almost exclusively relativistic quantum field theory for the description of multiple relativistic particles.

Although very important in physics, the mathematical theory of quantum fields is well developed only in the case of space-time dimensions < 4. While this covers important applications such as quantum wires or nanotubes (which have only one or two important spatial dimensions), it does not cover the most important case – the 4-dimensional space-time we live in. For example, quantum electrodynamics (QED), the most accurate of all quantum theories, exists only in the form of perturbative expansions (or other approximation schemes) and provides mathematically well-defined coefficients of a series in the fine structure constant α (whose experimental value is about 1/137), which is believed to be divergent Dyson [76]. The first few terms provide approximations to α-dependent numbers like the **magnetic moment** $g(\alpha)$ of the electron, which match experimental data to 12 digit accuracy, or the **Lamb shift** $\Delta E_{\text{Lamb}}(\alpha)$ of hydrogen, whose explanation in 1947 by Julian Schwinger ushered in the era of quantum field theory. However, the value of a divergent asymptotic series at a finite value of α is mathematically ill-defined; no consistent definition of functions such as $g(\alpha)$ is known to which the series would be asymptotic.

Finding a mathematically consistent theory of a class of 4-dimensional quantum field theories (quantum Yang–Mills gauge theory with a compact simple, nonabelian gauge group, believed to be the most accessible case) is another of the Clay Millennium problems whose solution is worth a million dollars.

In this book, we shall say very little about quantum field theory.

1.7 The Schrödinger picture

For conservative systems, the Hamiltonian is a self-adjoint linear operator. We assume that the quantum system is confined to a large box; a frequently employed artifice in quantum mechanics, which in a rigorous treatment must be removed later by going to the so-called **thermodynamic limit** where the box contains an arbitrarily large ball. Under this circumstance the spectrum of the Hamiltonian is discrete. The eigenvalues of the Hamiltonian correspond to energy levels, but only energy differences are observable (e.g., as spectral lines), and one generally shifts the Hamiltonian operator such that the lowest

eigenvalue is zero. By the **spectral theorem**, the eigenvalues

$$0 = E_0 \leq E_1 \leq E_2 \leq ...$$

are real, and we can find a set of eigenvectors ψ_k, normalized to satisfy $\psi_k^* \psi_k = 1$, such that

$$H\psi_k = E_k \psi_k$$

and

$$H = \sum E_k \psi_k \psi_k^* \,. \tag{1.7}$$

ψ_0 is called a **ground state**, the E_k are the **energy levels**, and $E_1 = E_1 - E_0 \geq 0$ is called the **energy gap**. The energy gap is positive iff[4] the smallest eigenvalue is simple, i.e., iff the ground state is unique up to a **phase**, a constant factor of absolute value 1. The eigenvectors are the solutions of the **time-independent Schrödinger equation**

$$H\psi = E\psi, \tag{1.8}$$

and the ground state is the solution of minimal energy E_0. With our normalization of energies, $E_0 = 0$ and hence $H\psi_0 = 0$, implying that the ground state is a time-independent solution of the time-dependent Schrödinger equation (1.6). The other eigenvectors ψ_k lead to time-dependent solutions $\psi_k(t) = e^{itE_k/\hbar}\psi_k$, which oscillate with the angular frequency $\omega_k = E_k/\hbar$. This gives Planck's basic relation

$$E = \hbar\omega \tag{1.9}$$

relating energy and angular frequency. (In terms of the ordinary frequency $\nu = \omega/2\pi$ and Planck's original constant $h = 2\pi\hbar$, this reads $E = h\nu$.) The completeness of the spectrum and the superposition principle now implies that for a **nondegenerate spectrum** (where all energy levels are distinct),

$$\psi(t) = \sum \alpha_k e^{i\omega_k t}\psi_k$$

is the general solution of the time-dependent Schrödinger equation. (In the degenerate case, a more complicated confluent formula is available.) Thus the time-dependent Schrödinger equation is solvable in terms of the time-independent Schrödinger equation, or equivalently with the spectral analysis of the Hamiltonian. This is the reason why spectra are in the center of attention in quantum mechanics. The relation to observed spectral lines, which gave rise to the name spectrum for the list of eigenvalues, is discussed in Chapter 23.

The spectral decomposition (1.7) also provides the connection to quantum statistical mechanics. A thorough discussion of equilibrium statistical mechanics emphasizing the quantum-classical correspondence will be given in Part II. Here we only scratch the surface. Under sufficiently idealized conditions, a thermal quantum system is represented as a so-called **canonical ensemble**, characterized by a density operator of the form

$$\rho = e^{-\beta H}, \quad \beta = (\kappa T)^{-1} \,,$$

[4] **iff** is the mathematician's abbreviation for "if and only if".

with T the temperature and $\hbar$ the **Boltzmann constant**, a tiny constant with approximate value $1.38 \cdot 10^{-23} J/K$. Hence we get

$$\rho = \sum e^{-\beta E_k} \psi_k \psi_k^* = \psi_0 \psi_0^* + e^{-\beta E_1} \psi_1 \psi_1^* + \dots \tag{1.10}$$

At room temperature, $T \approx 300K$, hence $\beta \sim 5 \cdot 10^{20} J^{-1}$. Therefore, if the energy gap $E_1 - E_0$ is not too small, it is enough to keep a single term, and we find that $\rho \approx \psi_0 \psi_0^*$. Thus the system is approximately in the ground state.

The fact that the ground state is the most relevant state is the basis for fields like **quantum chemistry**: For the calculation of electron configuration and the corresponding energies of molecules at fixed positions of the nuclei, it suffices to know the ground state. An exception is to be made for laser chemistry where a few excited states become relevant. To compute the ground state, one must solve (1.8) for the electron wave function ψ_0, which, because of the minimality condition, is a global optimization problem in an infinite-dimensional space. The **Hartree–Fock method** and their generalizations are used to solve these in some discretization, and the various solution techniques are routinely available in modern quantum chemistry packages.

Applying the Schrödinger equation to the pure state $\rho = \psi\psi^*$ and noting that $H^* = H$, one finds that

$$i\hbar \frac{d\rho}{dt} = i\hbar(\dot{\psi}\psi^* + \psi\dot{\psi}^*) = (i\hbar\dot{\psi})\psi^* - \psi(i\hbar\dot{\psi})^* = H\psi\psi^* - \psi(H\psi)^* = H\rho - \rho H,$$

giving the **quantum Liouville equation**

$$\frac{d\rho}{dt} = \frac{1}{i\hbar}(H\rho - \rho H) = \frac{1}{i\hbar}[H, \rho]\,. \tag{1.11}$$

1.8 The Heisenberg picture

In the beginning of quantum mechanics there were two independent formulations; the **Heisenberg picture** (discovered in 1925 by Heisenberg), and the **Schrödinger picture** (discovered in 1926 by Schrödinger). Although the formulations seemed very different at first, they were quickly shown to be completely equivalent.

In the Schrödinger picture, the physical configuration is described by a time-dependent state vector in a Hilbert space, and the observables are time-independent operators on this Hilbert space. In the Heisenberg picture this is the other way around; the vector is time-independent and the observables are time-dependent operators.

The connection between the two pictures comes from noting that everything in physics that is **objective** in the sense that it can be verified repeatedly is computable from expectation values (here representing averages over repeated observations), and that the time-dependent expectations

$$\langle f \rangle_t = \int \rho(t) f = \int f \rho(t) \tag{1.12}$$

(remember that the quantum integral (1.2) is a trace!) in the Schrödinger picture can be alternatively written in the Heisenberg picture as

$$\langle f\rangle_t = \int \rho f(t) = \int f(t)\rho\,. \tag{1.13}$$

The traditional view of classical mechanics corresponds to the Heisenberg picture – the observables depend on time and the density is time-independent. However, both pictures can be used in classical mechanics, too.

To transform the Heisenberg picture description to the Schrödinger picture, we note that the Heisenberg expectations (1.13) satisfy

$$\frac{d\langle f\rangle_t}{dt} = \int \rho \dot{f}(t) = \int \rho\{f(t), H\} = \langle\{f, H\}\rangle_t\,,$$

giving the differential equation

$$\frac{d\langle f\rangle_t}{dt} = \langle\{f, H\}\rangle_t \tag{1.14}$$

for the expectations. An equivalent description in the Schrödinger picture expresses the same dynamical law using the Schrödinger expectations (1.12). To deduce the dynamics of $\rho(t)$ we need the following formula which can be justified for concrete Poisson brackets with integration by parts,

$$\int\{f, g\}h = \int f\{g, h\}\,; \tag{1.15}$$

cf. (1.19) below. Using this, we find as consistency condition that $\frac{d}{dt}\langle f\rangle_t = \int f\dot{\rho}(t)$ and $\langle\{f, H\}\rangle_t = \int\{f, H\}\rho(t) = \int f\{H, \rho(t)\}$ must agree for all f. This dictates the **classical Liouville equation**

$$\dot{\rho}(t) = \{H, \rho(t)\}\,. \tag{1.16}$$

In the quantum case, the Heisenberg and Schrödinger formulations are equivalent if the dynamics of $f(t)$ is given by the **quantum Heisenberg equation**

$$i\hbar\frac{d}{dt}f(t) = [H, f(t)]\,.$$

To check this, one may proceed in the same way as we did for the classical case above. Using the Lie product notation (1.3), the dynamics for expectations takes the form

$$\frac{d}{dt}\langle f\rangle = \langle H\angle f\rangle,$$

the Heisenberg equation becomes

$$\frac{d}{dt}f = H\angle f, \tag{1.17}$$

and the Liouville equation becomes

$$\dot{\rho}(t) = \rho(t)\angle H. \tag{1.18}$$

(Note that here H appears in the opposite order!) These formulas hold whether we consider classical or quantum mechanics.

We find the remarkable result that these equations look identical whether we consider classical or quantum mechanics; moreover, they are linear in f although they encode all the intricacies of nonlinear classical or quantum dynamics. Thus, **on the statistical level, classical and quantum mechanics look formally simple and identical in structure**. The only difference lies in the definition of the Lie product and the integral.

The connection is in fact much deeper; we shall see that classical mechanics and quantum mechanics are two applications of the same mathematical formalism. At the present stage, we get additional hints for this by noting that, as we shall see later, both the classical and the quantum Lie product satisfies the **Jacobi identity**

$$f\angle(g\angle h) + g\angle(h\angle f) + h\angle(f\angle g) = 0,$$

hence define a Lie algebra structure; cf. Section 11.1. They also satisfy the **Leibniz identity**

$$g\angle fh = (g\angle f)h + f(g\angle h)$$

characteristic of a Poisson algebra; cf. Section 12.1. Integrating the Leibniz identity and using (1.4) gives $0 = \int g\angle fh = \int((g\angle f)h + f(g\angle h)) = -\int(f\angle g)h + \int f(g\angle h)$, hence the **integration by parts** formula

$$\int f(g\angle h) = \int(f\angle g)h. \tag{1.19}$$

Readers having some background in Lie algebras will recognize (1.19) as the property that $\int fg$ defines a bilinear form with the properties characteristic for the Killing form of a Lie algebra – again both in the classical and the quantum case. Finally, the Poisson algebra of quantities carries both in the classical case and in the quantum case an intrinsic real structure given by an involutive mapping $*$ satisfying $f^{**} = f$ and natural compatibility relations with the algebraic operations: f^* is the complex conjugate in the classical case, and the adjoint in the quantum case.

Thus the common structure of classical mechanics and quantum mechanics is encoded in the algebraic structure of a Poisson $*$-algebra. This algebraic structure is built up in the course of the book, and then exploited to analyze one of the characteristic quantum features of nature – the spectral lines visible in light emanating from the sun, or from some chemical compound brought into the flame of a Bunsen burner.

1.9 Outline of the book

The goal of this book is to introduce the ideas relating quantum mechanics, Lie algebras and Lie groups, motivating everything as far as possible by classical mechanics. We shall mostly be concerned with systems described by a finite-dimensional phase space; the infinite-dimensional case is too difficult for a presentation at the level of this book. However, we present the concepts in such a way that they are valid even in infinite dimensions, and select the material so that it provides some insight into the infinite-dimensional case.

Chapter 2 discusses the mathematics and physics of the 2-level system, the simplest quantum system. It describes a number of important physical situations: Systems having only two energetically accessible energy eigenstates (e.g., 2-level atoms), the spin of a single particle such as an electron or a silver atom, the two polarization degrees of freedom of light, the isospin symmetry between proton and neutron, and the qubit, the smallest unit of quantum information theory. From a mathematical point of view, this is essentially the theory of the Lie group SU(2) and its Lie algebra su(2); therefore we introduce along the way basic concepts for matrix groups and their Lie algebras.

Chapter 3 discusses the mathematics of the most important symmetries found in our universe, and their associated Lie groups and Lie algebras: The rotation group and the group of rigid motions in physical space $\mathbb{R}^3$, the Heisenberg groups describing systems of point particles, the Galilei group and the Poincare group describing the symmetry of Newtonian and Minkowski space-time, the Lorentz group describing basic features of the theory of relativity, and some more groups describing the hydrogen atom, the periodic system of elements, a model for nuclei, and quarks. Currently, parts of this chapter are only very sketchy.

Chapter 4 currently contain a number of sections quoted verbatim from the Theoretical Physics FAQ at `http://www.mat.univie.ac.at/~neum/physfaq/physics-faq.html`; the material there must be integrated into the other chapters of the book (mostly into Chapter 3), a task still to be done..

Chapter 5 discusses systems of classical oscillators, starting with ordinary differential equations modeling nonlinearly coupled, damped oscillators, and introducing some notions from classical mechanics – the Hamiltonian (energy), the notion of conservative and dissipative dynamics, and the notion of phase space. We then look in more detail into the single oscillator case, the classical anharmonic oscillator, and show that the phase space dynamics can be represented both in terms of Hamilton's equations, or in terms of Poisson brackets and the classical Heisenberg equation of motion. Since the Poisson bracket satisfies the Jacobi identity, this gives the first link to Lie algebras. Considering the special case of harmonic oscillators, we show that they naturally arise from eigenmodes of linear partial differential equations describing important classical fields: The Maxwell equations for beams of light and gamma rays, the Schrödinger equation and the Klein–Gordon equation for nonrelativistic and relativistic beams of alpha rays, respectively, and the Dirac equation for beams of beta rays.

Chapter 6.5 relates the dynamics of arbitrary systems to those of oscillators by coupling the latter to the system, and exploring the resulting frequency spectrum. The observation that experimental spectra often have a pronounced discrete structure (analyzed in more detail in Chapter 11) is found to be explained by the fact that the discrete spectrum of a quantum Hamiltonian is directly related to the observed spectrum via the quantum Heisenberg equation of motion. Indeed, the observed spectral lines have frequencies corresponding to differences of eigenvalues of the Hamiltonian, multiplied by Planck's constant. This naturally explains the Rydberg–Ritz combination principle that had been established about 30 years before the birth of modern quantum theory. An excursion into the early history of quantum mechanics paints a colorful picture of this exciting time when the modern world

view got its nearly definite shape. We then discuss general properties of the spectrum of a system consisting of several particles, and how it reflects the bound state and scattering structure of the multiparticle dynamics. Finally, we show how black body radiation, the phenomenon whose explanation (by Planck) initiated the quantum era, is related to the spectrum via elementary statistical mechanics.

Part II discusses statistical mechanics from an algebraic perspective, concentrating on thermal equilibrium but discussing basic things in a more general framework. A treatment of equilibrium statistical mechanics and the kinematic part of nonequilibrium statistical mechanics is given. From a single basic assumption (Definition 9.1.1) the full structure of phenomenological thermodynamics and of statistical mechanics is derived, except for the third law which requires an additional quantization assumption.

Chapter 7 gives a description of standard phenomenological equilibrium thermodynamics for single-phase systems in the absence of chemical reactions and electromagnetic fields. Section 7.1 states the assumptions needed in an axiomatic way that allows an easy comparison with the statistical mechanics approach discussed in later chapters, and derives the basic formulas for the thermodynamic observables. Section 7.2 then discusses the three fundamental laws of thermodynamics; their implications are discussed in the remainder of the chapter. In particular, we derive the conventional formulas that express the thermodynamic observables in terms of the Helmholtz and Gibbs potentials and the associated extremal principles.

Chapter 8 introduces the technical machinery of statistical mechanics, Gibbs states and the partition function, in a uniform way common to classical mechanics and quantum mechanics. Section 8.1 introduces the algebra of quantities and their basic realizations in classical and quantum mechanics. Section 8.2 defines Gibbs states, their partition functions, and the related KMS condition, and illustrates the concepts by means of the canonical ensemble and harmonic oscillators. The abstract properties of Gibbs states are studied in Section 8.3, using the Kubo product and the Gibbs-Bogoliubov inequality. These are the basis of approximation methods, starting with mean field theory, and we indicate the connections. However, since approximation methods are treated abundantly in common texts, we discuss elsewhere in the present book only exact results. The final Section 8.4 discusses limit resolutions for the values of quantities, and the associated uncertainty relations.

Chapter 9 rederives the laws of thermodynamics from statistical mechanics, thus putting the phenomenological discussion of Chapter 7 on more basic foundations. Section 9.1 defines thermal states and discusses their relevance for global, local, and microlocal equilibrium. Section 9.2 deduces the existence of an equation of state and connects the results to the phenomenological exposition in Section 7.1. Section 9.3 proves the first law of thermodynamics. In Section 9.4, we compare thermal states with arbitrary Gibbs states and deduce the extremal principles of the second law. Section 9.5 shows that the third law is related to a simple quantization condition for the entropy and relates it to the time-independent Schrödinger equation.

In Chapter 10 we discuss in more detail the relation between mathematical models of physical systems and reality. Through a discussion of the meaning of uncertainty, statistics, and probability, the abstract setting introduced in the previous chapters is given both a

deterministic and a statistical interpretation. Section 10.1 discusses questions relating to different thermal models constructed on the basis of the same Euclidean $*$-algebra by selecting different lists of extensive quantities. Section 10.2 discusses the hierarchy of equilibrium descriptions and how they relate to each other. Section 10.3 reviews the role of statistics in the algebraic approach to statistical mechanics. Section 10.4 gives an operational meaning to classical instruments for measuring the value of uncertain quantities, and to statistical instruments whose measurement results are only statistically correlated to properties of the measured system. Section 10.5 extends the discussion to quantum systems, and discusses the deterministic and statistical features of quantum mechanics. Section 10.6 relates the subject to information theory, and recovers the usual interpretation of the value of the entropy as a measure of unobservable internal complexity (lack of information). The final Section 10.7 discusses the extent to which an interpretation in terms of subjective probability makes sense, and clarifies the relations with the maximum entropy principle.

Part III introduces the basics about Lie algebras and Lie groups, with an emphasis on the concepts most relevant to the conceptual side of physics.

Chapter 11 introduces Lie algebras. We introduce in Section 11.1 the basic definitions and tools for verifying the Jacobi identity, and establish the latter for the Poisson bracket of a single harmonic oscillator and in Section 11.2 for algebras of derivations in associative algebras. Noncommutative associative algebras give rise to Lie algebras in a different way – via commutators, discussed in Section 11.3. The fact that linear operators on a vector space form a Lie algebra brings quantum mechanics into the picture. Differential equations in associative algebras defining exponentials naturally produce Lie groups and the exponential map, which relates Lie groups and Lie algebras. In Section 11.4, we discuss classical groups and their Lie algebras. Taking as the vector space the space of n-dimensional column vectors gives as basic examples the Lie algebra of $n \times n$ matrices and its most important Lie subalgebras, the orthogonal, symplectic, and unitary Lie algebras. Many finite-dimensional Lie groups arise as groups of square invertible matrices, and we discuss the most important families, in particular the unitary, orthogonal, and symplectic groups. We then discuss Heisenberg algebras and Heisenberg groups and their relation to the Poisson bracket of harmonic oscillators via the canonical commutation relations. The product law in Heisenberg groups is given by the famous Weyl relations, which are an exactly representable case of the Baker–Campbell–Hausdorff formula valid for many other Lie groups, in particular for arbitrary finite-dimensional ones. We end the Chapter with a treatment of the slightly richer structure of a Lie $*$-algebra usually encountered in the mechanical applications. In traditional terms, Lie $*$-algebras are equivalent to complexifications of real Lie algebras, but the $*$-formulation is often more suitable for discussing physics.

Chapter 12 brings more physics into play by introducing Poisson algebras, the algebras in which it is possible to define Hamiltonian mechanics. Poisson algebras abstract the algebraic features of both Poisson brackets and commutators, and hence serve as a unifying tool relating classical and quantum mechanics. After defining the basic concepts in Section 12.1, we discuss in Section 12.2 rotating rigid bodies, in Section 12.3 the concept of angular momentum, and the commutative Poisson algebra of smooth functions of angular momentum. It is directly related to the group SO(3) of 3-dimensional rotations and the corresponding

Lie algebra so(3) of infinitesimal rotations, which is generated by the components of the angular momentum. In particular, we obtain in Section 12.4 the Euler equations for a spinning rigid body from a Hamiltonian quadratic in the angular momentum. This example shows how the quantities of a classical Poisson algebra are naturally interpreted as physical observables. The angular momentum Poisson algebra is a simple instance of Lie–Poisson algebras, a class of commutative Poisson algebras canonically associated with any Lie algebra and constructed in Section 12.5. The Poisson bracket for the harmonic oscillator is another instance, arising in this way from the Heisenberg algebra. Thus Hamiltonian mechanics on Lie–Poisson algebras generalizes the classical anharmonic oscillator, and gives for so(3) the dynamics of spinning rigid bodies. Sections on classical symplectic mechanics and its application to the dynamics of molecules and an outlook to quantum field theory conclude the chapter.

Chapter 13 introduces representations of Lie algebras and Lie groups in associative algebras and in Poisson algebras. A general physical system can be characterized in terms of a Poisson representation of the kinematical Lie algebra of distinguished quantities of interest, a Hamiltonian, a distinguished Hermitian quantity in the Poisson algebra defining the dynamics, and a state defining a particular system at a particular time. We also introduce Lie algebra and Lie group representations in associative algebras, which relate Lie algebras and Lie groups of matrices or linear operators to abstract Lie algebras and Lie groups. These linear representations turn out to be most important for understanding the spectrum of quantum systems, as discussed later in Section 23.6. We then discuss unitary representations of the Poincare group, the basis for relativistic quantum field theory. An overview over semisimple Lie algebras and their classification concludes the chapter.

Part IV discusses the dynamics of nonequilibrium phenomena, i.e., processes where the expectation changes with time, in as far as no fields are involved. This part is still in a preliminary, somewhat sketchy form. It also lacks references (both to historical origins, the literature on the subject) and subject indexing, and must also better connected with the earlier parts.

Chapter 14 discusses general Markov processes, i.e., abstract (classical or quantum) stochastic processes without memory. It will also contain the basic features of quantum dynamical semigroups and the associated Lindblad dynamics.

Chapter 15 discusses stochastic differential equations and associated diffusion processes, and their deterministic limits – dissipative Hamiltonian systems.

Chapter 16 discusses collective processes described by a master equation, and their most prominent application – stirred chemical reactions.

Part V gives an introduction to differential geometry from an algebraic perspective.

Chapter 17 starts with an introduction to basic concepts of differential geometry. We define (smooth, infinitely often differentiable) manifolds and the associatated algebra of scalar fields. Its derivations define vector fields, which form important examples of Lie

algebras. The exterior calculus on alternating forms is developped. Finally, Lie groups are interpreted as manifolds.

Chapter 18 discusses the construction of Poisson algebras related to manifolds, and associated Poisson manifolds, the arena for the most general classical dynamics. We show how classical symplectic mechanics (in flat phase space) and constrained Hamiltonian mechanics fit into the general abstract picture. We end the chapter with a discussion of the Lagrangian approach to classical mechanics.

Chapter 19 is about Hamiltonian quantum mechanics. We discuss a classical symplectic framework for the Schrodinger equation. This is then generalized to a framework for quantum-classical dynamics, including important models such as the Born-Oppenheimer approximation for the quantum motion of molecules. A section on deformation quantization relates classical and quantum descriptions of a system, and the Wigner transform makes the connection quantitiatively useful in the special case of a canonical system with finitely many degrees of freedom.

Part VI applies these concepts to the study of the dominant kinds of elementary motion in a bound system, vibrations (described by oscillators, Poisson representations of the Heisenberg group), rotations (described by a spinning top, Poisson representations of the rotation group), and their interaction. On the quantum level, quantum oscillators are always bosonic systems, while spinning systems may be bosonic or fermionic depending on whether or not the spin is integral. The analysis of experimental spectra, concentrating on the mathematical contents of the subject, concludes our discussion.

Chapter 20 is a study of harmonic oscillators (bosons, elementary vibrations), both from the classical and the quantum point of view. We introduce raising and lowering operators in the symplectic Poisson algebra, and show that the classical case is the limit $\hbar \to 0$ of the quantum harmonic oscillator. The representation theory of the single-mode Heisenberg algebra is particularly simple since by the Stone–von Neumann theorem, all unitary representations are equivalent. We find that the quantum spectrum of a harmonic oscillator is discrete and consists of the classical frequency (multiplied by $\hbar$) and its nonnegative integral multiples (overtones, excited states). For discussing the representation where the harmonic oscillator Hamiltonian is diagonal, we introduce Dirac's bra-ket notation, and deduce the basic properties of the bosonic Fock spaces, first for a single harmonic oscillator and then for a system of finitely many harmonic modes. We then introduce coherent states, an overcomplete basis representation in which not only the Heisenberg algebra, but the action of the Heisenberg group is explicitly visible. The coherent state representation is particularly relevant for the study of quantum optics, but we only indicate its connection to the modes of the electromagnetic field.

Chapter 21 discusses spinning systems, again from the classical and the quantum perspective. Starting with the Lie-Poisson algebra for the rotation group and a Hamiltonian quadratic in the angular momentum, we obtain the Euler equations for the classical spinning top. The quantum version can be obtained by looking for canonical anticommutation relations, which naturally produce the Lie algebra of a spinning top. As for oscillators, the canonical anticommutation relations have a unique irreducible unitary representation,

which corresponds to a spin 1/2 representation of the rotation group. The multimode version gives rise to fermionic Fock spaces; in contrast to the bosonic case, these are finite-dimensional when the number of modes is finite. In particular, the single mode fermionic Fock space is 2-dimensional. Many constructions for bosons and fermions only differ in the signs of certain terms, such as commutators versus anticommutators. For example, quadratic expressions in bosonic or fermionic Fock spaces form Lie algebras, which give natural representations of the universal covering groups of the Lie algebras $so(n)$ in the fermionic case and $sp(2n, \mathbb{R})$ in the bosonic case, the so-called spin groups and metaplectic groups, respectively. In fact, the analogies apart from sign lead to a common generalization of bosonic and fermionic objects in form of super Lie algebras, which are, however, outside the scope of the book. Apart from the Fock representation, the rotation group has a unique irreducible unitary representation of each finite dimension. We derive these spinor representations by restriction of corresponding nonunitary representations of the general linear group $GL(2, \mathbb{C})$ on homogeneous polynomials in two variables, and find corresponding spin coherent states.

Chapter 22 discusses highest weight representations, providing tools for classifying many irreducible representations of interest. The basic ingredient is a triangular decomposition, which exists for all finite-dimensional semisimple Lie algebras, but also in other cases of interest such as the oscillator algebra, the Heisenberg algebra with the harmonic oscillator Hamiltonian adjoined. We look at detail at 4-dimensional Lie algebras with a nontrivial triangular decomposition (among them the oscillator algebra and $so(3)$), which behave almost like the oscillator algebra. As a result, the analysis leading to Fock spaces generalizes without problems, and we are able to classify all irreducible unitary representations of the rotation group.

Chapter 23 applies the Lie theoretic structure to the analysis of quantum spectra. After a short history of some aspects of spectroscopy, we look at the spectrum of bound systems of particles. We show how to obtain from a measured spectrum the spectrum of the associated Hamiltonian, and discuss qualitative results on vibrations (giving discrete spectra) and chemical reactions (giving continuous spectra) that come from the consideration of simple systems and the consideration of approximate symmetries. The latter are shown to result in a clustering of spectral values. The structure of the clusters is determined by how the irreducible representations of a dynamical Lie algebra split when the algebra is reduced to a subalgebra of generating symmetries. The clustering can also occur in a hierarchical fashion with fine splitting and hyperfine splitting, corresponding to a chain of subgroups. As an example, we discuss the spectrum of the hydrogen atom.

The material presented should be complemented (in a later version of the book) by two further parts, one covering quantum field theory, and the other on nonequilibrium statistical mechanics, deriving space-time dependent thermodynamics from quantum field theory.

Chapter 2

The simplest quantum system

The simplest quantum system is a 2-level system. It describes a number of different situations important in practice: Systems having only two energetically accessible energy eigenstates (e.g., 2-level atoms), the spin of a single particle such as an electron or a silver atom, the two polarization degrees of freedom of light, the isospin symmetry between proton and neutron, and the qubit, the smallest unit of quantum information theory.

The observable quantities of a 2-level system are 2×2 matrices. Matrices and their infinite-dimensional generalizations – linear operators – are the bread and butter of quantum mechanics.

In mathematics and physics, symmetries are described in terms of Lie groups and Lie algebras. An understanding of these concepts is fundamental to appreciate the unity of modern physics.

This chapter introduces some basic concepts for matrix groups and their Lie algebras, concentrating on the case of 2×2 matrices and their physical interpretation. In the next chapter we introduce in an elementary way a number of other Lie groups and Lie algebras that are important for physics, by means of concrete matrix representations, and relate them to concrete physics. A general, more abstract treatment of Lie groups and Lie algebras is given later in Chapter 11.

We assume that the reader already has a good command of matrix algebra (including complex numbers and eigenvalues) and knows basic properties of vector spaces, linear algebra, limits, and power series (quickly reviewed in Section 2.1).

The beginning is just matrix calculus with some new terminology, but the subject soon takes on a life of its own.... Readers who see matrix groups for the first time may want to skip forward to the sections with more physical content to get a better idea of how matrix group are used in physics, before reading the chapter in a linear order.

2.1 Matrices, relativity and quantum theory

The early 20th century initiated two revolutions in physics that changed the nature of the mathematical tools used to describe physics. Both revolutions gave matrices a prominent place in understanding the new physics.

The transition from the old, Newtonian world view to the new, relativistic conception of the world culminated in the realization that Nature is governed by symmetries that can be descibed in terms of the Lorentz group, a group of 4×4-matrices that mathematicians refer to by the symbolic name $SO(1,3)$ or $SL(2,\mathbb{C})$. Since then, many other symmetry groups have found uses in physics. Indeed, symmetry considerations and the associated group theory have become a unifying theme and one of the most powerful tools in modern physics.

Independently of the theory of relativity, an increasing number of quantum phenomena defying an explanation in terms of classical physics were noticed, beginning in 1900, when Max Planck [219] successfully used a quantization condition for his analysis of black body radiation. After 25 years of groping in the dark to make classical sense of these quantum phenomena, Werner Heisenberg [123] laid in 1925 the mathematical foundations of modern quantum mechanics. The key was the insight that basic physical quantities such as the components of position and momentum should be represented in terms of matrices (in this case infinite arrays of numbers) rather than by single numbers as in classical mechanics. Since then, matrices and linear operators, their infinite-dimensional generalizations, form the cornerstone of quantum mechanics.

Therefore, the language of matrices is an indispensible foundation for a deeper understanding of modern physics. To fix the notation and to remind the reader, we begin by repeating some definitions and properties of matrices and related concepts. Thorough treatments (from complementary points of views) are given in Lax [172] and Horn & Johnson [127].

$\mathbb{K}$ denotes a field, usually the field $\mathbb{R}$ of real numbers or the field $\mathbb{C}$ of complex numbers. Then $\mathbb{K}^n$ denotes the space of column vectors x of length n with entries $x_k \in \mathbb{K}$ ($k = 1, \ldots, n$), and $\mathbb{K}^{m\times n}$ denotes the vector space of all $m \times n$ matrices A with entries $A_{jk} \in \mathbb{K}$ ($j = 1, \ldots, m$; $k = 1, \ldots, n$). We identify 1×1 matrices with the entry they contain, and column vectors with matrices having a single column; thus $\mathbb{K}^{1\times 1} = \mathbb{K}$ and $\mathbb{K}^{m\times 1} = \mathbb{K}^m$. The **zero matrix** of any size (with all entries zero) is denoted by 0, or by 0_n if it is square and its size $n \times n$ is emphasized. The **identity matrix** of any size is denoted by 1, or by 1_n if its size $n \times n$ is emphasized; multiples of the identity are identified with the corresponding elements of $\mathbb{K}$. The **transpose** of the matrix $A \in \mathbb{K}^{m\times n}$ is the matrix $A^T \in \mathbb{K}^{n\times m}$ with entries $(A^T)_{jk} := A_{kj}$; the transpose of the column vector $x \in \mathbb{K}^n$ is the row vector $x^T \in \mathbb{K}^{1\times n}$. The matrix A is called **symmetric** if $A^T = A$. The **conjugate transpose** of the matrix $A \in \mathbb{C}^{m\times n}$ is the matrix $A^* \in \mathbb{C}^{n\times m}$ with entries $(A^*)_{jk} := \overline{A}_{kj}$, where $\overline{\lambda} = \lambda^*$ denotes the complex conjugate of $\lambda \in \mathbb{C}$. The matrix A is called **Hermitian** if $A^* = A$.

The **product** of the $m \times n$ matrix A and the $n \times r$ matrix B is the $m \times r$ matrix AB with

entries $(AB)_{jk} = \sum_{l=1}^{m} A_{jl}B_{lk}$. The product is associative, $(AB)C = A(BC)$, and distributive, $A(B+C) = AB+AC$, $(A+B)C = AB+AC$, but in general not commutative. For a square matrix $A \in \mathbb{K}^{n\times n}$, the number $\operatorname{tr} A := \sum_{k=1}^{n} A_{kk}$ is the **trace** of A, and $\det A$ denotes the **determinant** of A. The trace of a product is generally written without parentheses. The trace is a linear operation, and for $A, B \in \mathbb{K}^{n\times n}$, we have

$$\operatorname{tr} A^T = \operatorname{tr} A, \quad \operatorname{tr} A^* = (\operatorname{tr} A)^*, \quad \operatorname{tr} AB = \operatorname{tr} BA,$$

$$\det A^T = \det A, \quad \det A^* = (\det A)^*, \quad \det(AB) = \det A \det B.$$

The determinant $\det(\lambda - A)$ of a real or complex $n \times n$ matrix A factors into a product of n linear factors $\lambda - \lambda_k$ with complex numbers λ_k called the **eigenvalues** of A; they are are unique up to ordering. The trace is the sum of the eigenvalues, and the determinant is their product. All eigenvalues of a Hermitian matrix are real numbers. The real or complex $n \times n$ matrix A is called **positive semidefinite** (**positive semidefinite**) if $x^*Ax \geq 0$ for all $x \in \mathbb{C}^n$ (resp. $x^*Ax > 0$ for all nonzero $x \in \mathbb{C}^n$). The eigenvalues of a positive semidefinite (positive definite) matrix have nonnegative (positive) real part.

$|x| = \sqrt{x^Tx}$ is the **length** of the vector $x \in \mathbb{R}^n$. $|\psi| = \sqrt{\psi^*\psi}$ is the **norm** of the vector $\psi \in \mathbb{C}^n$. For any real or complex matrix A, the matrix A^*A is Hermitian and positive semidefinite; the square roots of the (real and nonnegative) eigenvalues of A^*A are called the **singular values** of A. The maximal singular value of A is called the **spectral norm** $\|A\|$ of A. For $A, B \in \mathbb{C}^{n\times n}$ and $\alpha, \beta \in \mathbb{C}$, we have

$$\|\alpha A + \beta B\| \leq |\alpha|\|A\| + |\beta|\|B\|, \quad \|AB\| \leq \|A\|\,\|B\|,$$

and

$$|A\psi| \leq \|A\|\,|\psi| \quad \text{for } \psi \in \mathbb{C}^n.$$

Matrix functions of a real or complex square matrix A are defined by power series with real or complex coefficients. If a power series in x has convergence radius r then the series with x replaced by a square matrix A converges for $\|A\| < r$. Any two matrix functions of the same matrix A commute. If A has the eigenvalues λ_k then the matrix function $f(A)$ has the eigenvalues $f(\lambda_k)$. Identities for power series involving only a single variable x remain valid when x is replaced by a square matrix; moreover, $f(A^T) = f(A)^T$ and $f(A^*) = f(A)^*$. In particular, the **matrix exponential**

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k$$

is defined for all real or complex square matrices A, and satisfies for $s, t \in \mathbb{C}$ the relations

$$e^{sA}e^{tA} = e^{(s+t)A}, \quad (e^{sA})^t = e^{stA}. \tag{2.1}$$

On the other hand, e^{A+B} is in general distinct from e^Ae^B; however, $e^{A+B} = e^ae^B$ if A and B **commute**, i.e., $AB = BA$. We also note the formula

$$\det e^A = e^{\operatorname{tr} A}, \tag{2.2}$$

which follows from $\det e^A = \prod e^{\lambda_k} = e^{\sum \lambda_k} = e^{\operatorname{tr} A}$.

2.2 Continuous motions and matrix groups

A basic fact about square real and complex matrices is that they can often be interpreted in terms of motions in the underlying vector space on which they act. This gives them an intuitive meaning that makes it easy to interpret even very abstract applications. Since motions can be combined and reversed they carry a natural group structure that gives rise to the concept of a matrix group. Different matrix groups characterize different forms of permitted motions. Matrix groups are important examples of so-called **Lie groups**, defined in Section 17.7. Indeed, by the **theorem of Ado** (Ado [2]), every finite-dimensional Lie group is isomorphic to a matrix group.

A **matrix group** over $\mathbb{K}$ is a nonempty, closed set $\mathbb{G}$ of invertible matrices from $\mathbb{K}^{n\times n}$ with the property that the product of any two matrices from $\mathbb{G}$ and the inverse of a matrix from $\mathbb{G}$ are in $\mathbb{G}$. In particular, $1 \in \mathbb{G}$, and the limit of any convergent sequence of elements $U_l \in \mathbb{G}$ $(l = 1, 2, 3, \ldots)$ is again in $\mathbb{G}$. If $\mathbb{K} = \mathbb{R}$ (or $\mathbb{K} = \mathbb{C}$) then $\mathbb{G}$ is called a **real** (or **complex**) matrix group. The matrix group $\mathbb{G}$ is called **abelian** if all its elements commute, i.e., if $UV = VU$ for all $U, V \in \mathbb{G}$.

Let $\mathbb{G}$ be a real or complex matrix group. A $\mathbb{G}$**-motion** (by $V \in \mathbb{G}$) is an arbitrarily often differentiable map $U : [0, 1] \to \mathbb{G}$ such that $U(0) = 1$ (and $U(1) = V$). If the group consists of $n \times n$ matrices, the $\mathbb{G}$-motion moves a vector $x_0 \in \mathbb{K}$ from $x(0) = x_0$ to $x(1) = Vx_0$, sweeping out a path $x(t) = U(t)x_0$ for $t \in [0, 1]$. It is natural to interpret t as a time coordinate in suitable units of time.

2.2.1 Examples. We shall meet a large number of examples in this and the next chapter, progressing from the matrix groups easiest to define to the ones most useful in physics. We begin by naming the smallest and largest matrix groups of a given size.

(i) The set $\mathrm{Id}(n)$ consisting only of the $n \times n$ identity matrix is a matrix group, called a **trivial group**.

(ii) The set $L(n, \mathbb{K}) = GL(n, \mathbb{K})$ of all invertible $n \times n$ matrices with entries in $\mathbb{K}$ is a matrix group, called a **general linear group** over $\mathbb{K}$. In particular, $L(1, \mathbb{K})$ is the **multiplicative group** $\mathbb{K}^\times := \mathbb{K} \setminus \{0\}$ of the field $\mathbb{K}$.

We now illustrate the geometric inplications of the definitions by means of the complex plane and the motions corresponding to $\mathbb{C}^\times$ and some of its subgroups.

The first subgroup of $\mathbb{C}^\times$ of geometric interest is the group $\mathbb{R}^\times_+$ of positive real numbers. An $\mathbb{R}^\times_+$-motion stretches or compresses all vectors from the origin to a nonzero complex number by a time-varying factor. Such a stretching or compression is called a **dilatation** or **dilation**; thus $\mathbb{R}^\times_+$ is the group of dilatations (with respect to the origin) of the complex plane. It is well-known that the real multiplicative group and the real additive group $\mathbb{R}$ of translations along the real axis are isomorphic: Vie the exponential function, one can associate to every translation by $f \in \mathbb{R}$ a dilatation $U = e^f \in \mathbb{R}^\times_+$, and conversely, find for every dilatation $U \in \mathbb{R}^\times_+$ a unique $f = \log U \in \mathbb{R}$ such that $U = e^f$. In particular, a

uniform stretch (or compression) is obtained by the exponential motion $U(t) = e^{tf}$ when $f > 0$ (resp. $f < 0$).

The subgroup $L(1, \mathbb{R}) = \mathbb{R}^\times$ of all nonzero real numbers contains dilations, the reflections at zero given by multiplication with -1, and their products, given by arbitrary negative real numbers.

Another important subgroup is the group consisting of all complex numbers with absolute value one, forming the unit circle in the complex plane. This group is the smallest of the unitary groups defined in Section 2.8, and is therefore generally denoted by $U(1)$[1]. Using the Euler relation $e^{i\varphi} = \cos\varphi + i\sin\varphi$, one can again represent arbitrary group elements $U \in U(1)$ as exponential $U = e^{i\varphi}$ of a purely imaginary element $f = i\varphi$. As group elements acting by multiplication on the complex plane, the elements of $U(1)$ correspond to rotations around zero. Indeed, $U = e^{i\varphi}$ is a rotation by the angle φ. In particular, a uniform rotational motion progresses by equal angles in equal time intervals, hence is given by the exponential motion $U(t) = \cos(t\varphi) + i\sin(t\varphi) = e^{i\varphi t}$.

Since rotations by integral multiples of 2π have no net effect, the representation $U = e^{i\varphi}$ does not define φ uniquely; hence imaginary elements f differing by a multiple of $2\pi i$ give the same group element $U = e^f$. Thus while the two groups behave the same locally, there is a global topological difference. This also shows in the fact that, as a manifold, $U(1)$ is compact, while $\mathbb{R}_+^\times$ is noncompact.

2.3 Infinitesimal motions and matrix Lie algebras

The matrix

$$U'(0) := \frac{d}{dt}U(t)\Big|_{t=0}$$

is called the **infinitesimal motion** of the $\mathbb{G}$-motion $U : [0,1] \to \mathbb{G}$. Thus f is the infinitesimal motion of $U : [0,1] \to \mathbb{G}$ iff, for small t,

$$U(t) = 1 + tf + O(t^2).$$

Here the **Landau symbol** $O(t^2)$ denotes an expression in t whose norm is bounded for small t by a constant multiple of t^2 (which may be different in each occurrence of the Landau symbol). The **Lie algebra** of (or associated with) the real or complex matrix group $\mathbb{G}$ is the set $\log\mathbb{G}$ of all infinitesimal motions of $\mathbb{G}$-motions.

The following fundamental theorem gives basic properties of the Lie algebra $\log\mathbb{G}$ and describes the effect that a coordinate transformation in form of a $\mathbb{G}$-motion has on Lie algebra elements.

2.3.1 Theorem.
(i) The Lie algebra $\mathbb{L} := \log\mathbb{G}$ of any real or complex matrix group $\mathbb{G}$ is a vector space

[1]The reader should not confuse the occurrences of $U(1)$ as group with those of $U(1)$ as the final group element of a motion $U : [0,1] \to \mathbb{G}$.

containing with any two matrices f, g their ***commutator***

$$[f, g] := fg - gf.$$

(ii) For every $U \in \mathbb{G}$,

$$\mathrm{Ad}_U f := UfU^{-1} \quad \text{for } f \in \mathbb{L} \tag{2.3}$$

defines a linear mapping $\mathrm{Ad}_U : \mathbb{L} \to \mathbb{L}$, called the ***adjoint mapping*** *of U.*

(iii) Every adjoint mapping is a Lie algebra **automorphism**, *i.e.,*

$$\mathrm{Ad}_U[f, g] = [\mathrm{Ad}_U f, \mathrm{Ad}_U g] \quad \text{for } f, g \in \mathbb{L}. \tag{2.4}$$

Proof. Let $\mathbb{G}$ be a matrix group over $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$, and $\alpha, \beta \in \mathbb{K}$. If $f, g \in \mathbb{L}$ then there are $\mathbb{G}$-motions $V_1(t) = 1 + tf + O(t^2)$ and $V_2(t) = 1 + tg + O(t^2)$. The product $V(t) := V_1(\alpha t)V_2(\beta t)$ is a $\mathbb{G}$-motion with $V(t) = (1+\alpha tf)(1+\beta tg)+O(t^2) = 1+t(\alpha f+\beta g)+O(t^2)$, so that $\alpha f + \beta g \in \log \mathbb{G}$. Therefore $\mathbb{L}$ is a vector space over $\mathbb{K}$.

Let $U \in \mathbb{G}$. Then $W(t) := UV(t)U^{-1}$ is a $\mathbb{G}$-motion with $W(t) = U(1 + tf)U^{-1} + O(t^2) = 1 + tUfU^{-1} + O(t^2)$, whence $UfU^{-1} \in \mathbb{L}$. Therefore Ad_U maps $\mathbb{L}$ into itself. The linearity of the adjoint mapping is straightforward.

In particular, since $V_2(t)^{-1} = (1+tg)^{-1}+O(t^2) = 1-tg+O(t^2)$, the Lie algebra $\mathbb{L}$ contains $\mathrm{Ad}_{V_2(t)}f - f = V_2(t)fV_2(t)^{-1} - f = (1+tg)f(1-tg) - f+O(t^2) = t[g, f]+O(t^2)$. Dividing by t and letting t go to zero, we see that the commutator $[g, f]$ is also in $\mathbb{L}$.

Finally, the property (2.4) is again straightforward. □

The above property (i) motivates to define in general a **matrix Lie algebra** over $\mathbb{K}$ to be a subspace $\mathbb{L}$ of $\mathbb{K}^{n\times n}$ closed under commutation. The matrix Lie algebra $\mathbb{L}$ is called **abelian** if all its elements commute, i.e., if $[f, g] = 0$ for all $f, g \in \mathbb{L}$. A subset of a matrix Lie algebra $\mathbb{L}$ closed under commutation is again a matrix Lie algebra, and is called a **Lie subalgebra** of $\mathbb{L}$.

2.3.2 Examples. We shall meet a large number of examples in this and the next chapter, progressing from the matrix Lie algebras easiest to define to the ones most useful in physics. We begin by naming the smallest and largest matrix Lie algebras of a given size.

(i) The set $\mathrm{id}(n)$ consisting only of the $n \times n$ zero matrix is a matrix Lie algebra, called a **trivial Lie algebra**. Clearly, if $\mathbb{K}$ is the real or complex field, $\mathrm{id}(n)$ is the Lie algebra of the trivial group $\mathrm{Id}(n)$.

(ii) $l(n, \mathbb{K}) = gl(n, \mathbb{K}) = \mathbb{K}^{n\times n}$ is a matrix Lie algebra, called a **general linear Lie algebra** over $\mathbb{K}$. If $\mathbb{K}$ is the real or complex field, $l(n, \mathbb{K})$ is the Lie algebra of the general linear group $L(n, \mathbb{K})$ since for every $f \in l(n, \mathbb{K})$, the mapping U defined by $U(t) = e^{tf}$ is an $L(n, \mathbb{K})$-motion with infinitesimal motion f.

We are mainly interested in matrix groups whose associated Lie algebra has interesting properties. However, there are important matrix groups with a trivial infinitesimal structure. A matrix group is called **discrete** if its Lie algebra is trivial. Discrete matrix groups that play an important role for the description of symmetris of molecules and crystals. For example, a **permutation group** is a group $\mathbb{G}$ of bijective mappings of a finite set X. If the members of X are the atoms of a molecule with given chemical structure, its **symmetry group** $\mathbb{G}$ consits of the permutations that preserve the chemical nature of the atoms and the chemical bonds between them; for example, the benzene ring has a dihedral symmetry group with 12 elements. Assocoated with each permutation group is a finite group of $n \times n$ **permutation matrices** $U \in \mathbb{R}^{n\times n}$, where n is the size of X, and $U_{jk} = 1$ iff, in a fixed ordering of the elements of X, the jth element is permuted to the kth element, $U_{jk} = 0$ otherwise. The representation theory of these discrete matrix groups gives important information about the chemical properties of symmetric molecules. In this book, we shall meet discrete groups only in passing; for a deeper treatment we refer to Cornwell [68], Cotton [69], Kim [150], or Weyl [286].

2.4 Uniform motions and the matrix exponential

We now generalize the construction of uniform rotations in $U(1)$ to arbitrary real or complex matrix groups.

Let $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$, and $f \in \mathbb{K}^{n\times n}$. Because of (2.1), the set of $\exp(tf) = e^{tf}$ with $t \in \mathbb{R}$ is a matrix group, called the **one-parameter group** with **infinitesimal generator** f. The infinitesimal generator is determined only up to a nonzero scalar multiple. Because of the property (2.1) and the analogy to uniform rotations in the complex plane, $\mathbb{G}$-motions of the form $U(t) = e^{tf}$ are called **uniform motions**. Since $U(t) = 1 + tf + O(t^2)$, the infinitesimal generator of a uniform motion belongs to the Lie algebra $\log \mathbb{G}$. In view of

$$\frac{d}{dt}e^{tf} = fe^{tf} = e^{tf}f$$

and the unique solvability of the intitial-value problems for ordinary differential equations in finite-dimensional spaces, uniform $\mathbb{G}$-motions are characterized by the property

$$U(1) = 0, \quad \frac{d}{dt}U(t) = fU(t)$$

for some $f \in \log \mathbb{G}$, which is the infinitesimal generator.

The set of limits of sequences of products $U_1^{k_1} \cdot \ldots \cdot U_s^{k_s}$ of an arbitrary number $s \geq 0$ of arbitrary powers $U_j^{k_j}$ of arbitrary elements U_j $(j = 1, \ldots, s)$ from a set S is a matrix group, called the group **generated** by S. If $\mathbb{L}$ is a matrix Lie algebra, $\exp \mathbb{L}$ denotes the group generated by the exponentials e^f with $f \in \mathbb{L}$. Whether the exponentials themselves form a group depends on the Lie algebra $\mathbb{L}$.; see

By joining and inverting paths, it is easy to see that the set $\mathbb{G}_0$ consisting of all $V \in \mathbb{G}$ for which a motion by V exists is a matrix group, called the **connected subgroup** of $\mathbb{G}$. The

matrix group $\mathbb{G}$ is called **connected** if $\mathbb{G}_0 = \mathbb{G}$. Clearly, the group generated by a set of elements form $\mathbb{G}_0$ is contained $\mathbf{G}_0$. A matrix group $\mathbb{G}$ and its connected subgroup $\mathbb{G}_0$ have the same associated Lie algebra. Moreover, due to the existence of uniform motions, $\exp \mathbb{L}$ is connected. Thus one often concentrates in physics on connected groups.

The **dimension** of a real or complex matrix group $\mathbb{G}$ is the dimension of the associated Lie algebra $\log \mathbb{G}$, considered as a real vector spece. Finite groups are 0-dimensional. The only connected 0-dimensional matrix groups are the groups $\mathrm{Id}(n)$. The connected 1-dimensional group are just the one-parameter groups.

2.4.1 Theorem.
(i) Let $\mathbb{G}$ be a matrix group. Then the exponentials e^f with $f \in \log \mathbb{G}$ belong to $\mathbb{G}$ and generate its connected subgroup $\mathbb{G}_0$; thus, $\exp \log \mathbb{G} = \mathbb{G}_0$.

(ii) Let $\mathbb{L}$ be a matrix Lie algebra. Then $\log \exp \mathbb{L} = \mathbb{L}$.

Proof. (i) This is one of the few places where we need explicit analysis to establish a limit. To show that $e^f \in \mathbb{G}$, we need to represent e^f as a limit of group elements. We construct these by noting that a uniform motion can be considered as a composition of many identical tiny, almost infinitesimal motions. The eigenvalues of the matrices $e^{f/k}$ have the form $e^{\lambda/k}$ with eigenvalues λ of f. For any fixed $c > \|f\|$, the exponentials $e^{\lambda/k}$ can be bounded in absolute value by $e^{c/k}$ since $|\lambda| \le \|f\| < c$. Therefore the $E_k := e^{f/k}$ satisfy

$$\|E_k\| \le e^{c/k}.$$

We know already that there is some $\mathbb{G}$-motion $U : [0,1] \to \mathbb{G}$ with infinitesimal motion $f \in \mathbb{L} := \log \mathbb{G}$. We now put $U_k := U(1/k)$ and show that

$$e^f = \lim_{k\to\infty} U_k^k. \tag{2.5}$$

Since $\|U(t)\| = \|1 + tf + O(t^2)\| = 1 + t\|f\| + O(t^2) \le 1 + ct \le e^{ct}$ for sufficiently small $t > 0$, we have

$$\|U_k\| \le e^{c/k}$$

for sufficiently large k. Since the Taylor expansions of $U(t)$ and e^{tf} agree up to first order, we have $U(t) - e^{tf} = O(t^2)$; hence there is a constant $C > 0$ such that

$$\|U_k - E_k\| = \|U(1/k) - e^{f/k}\| \le C/k^2$$

for sufficiently large k. Now

$$\begin{aligned}
\|U_k^k - e^f\| &= \|U_k^k - E_k^k\| = \Big\| \sum_{j=1}^k E_k^{j-1}(U_k - E_k)E_k^{k-j} \Big\| \\
&\le \sum_{j=1}^k \|E_k\|^{j-1}\|U_k - E_k\|\|E_k\|^{k-j} \\
&\le \sum_{j=1}^k e^{(j-1)c/k} C/k^2 e^{(k-j)c/k} = \sum_{j=1}^k C e^{(k-1)c/k}/k^2 \le Ce^c/k,
\end{aligned}$$

which tends to zero as $k \to \infty$. This establishes the limit (2.5) and proves that $e^f \in \mathbb{G}$.

Since every e^f with $f \in \mathbb{L}$ is part of a uniform motion, it is in $\mathbb{G}_0$. hence the group generated by these exponentials is contained in $\mathbb{G}_0$.

(ii) $\square$

The theorem implies that connected matrix groups are characterized completely by their Lie algebras. Since Lie algebras are vector spaces, their structure can be studied with the help of linear algebra, while most matrix groups are intrinsically nonlinear. This explains the importance of Lie algebras in the study of connected groups.

2.5 Volume preservation and special linear groups

The oriented volume is preserved iff the determinant is one. The unoriented volume is preserved iff the determinant has absolute value one.

If $\mathbb{G}$ is a matrix group then the set $S\mathbb{G}$ consisting of all elements in $\mathbb{G}$ with determinant one is a matrix group. Indeed, if $U, V \in S\mathbb{G}$ then $\det(UV) = \det U \det V = 1$ and $\det U^{-1} = (\det U)^{-1} = 1$, so that $UV, U^{-1} \in S\mathbb{G}$. In particular, the **special linear group** $SL(n, \mathbb{K})$ consisting of all $n \times n$ matrices with entries in $\mathbb{K}$ and determinant one is a matrix group.

The center of $SL(n, \mathbb{C})$ is the group $\mathbb{Z}_n = \{\lambda \in \mathbb{C} \mid \lambda^n = 1\}$ of nth roots of unity, and the quotients $PSL(n, \mathbb{C}) = SL(n, \mathbb{C})/\mathbb{Z}_n$ form a family of simple Lie groups. The group $PSL(2, \mathbb{C}) = SL(2, \mathbb{C})/\mathbb{Z}_2$ is isomorphic to the restricted Lorentz group defined in Section 3.13.

If $\mathbb{L}$ is a matrix Lie algebra then the set $s\mathbb{L}$ consisting of all elements in $\mathbb{L}$ with zero trace is a matrix Lie algebra. Indeed, if $f, g \in s\mathbb{L}$ then $\operatorname{tr}[f, g] = \operatorname{tr} fg - \operatorname{tr} gf = 0$, so that $[f, g] \in s\mathbb{L}$. In particular, the **special linear Lie algebra** $sl(n, \mathbb{K})$ consisting of all $n \times n$ matrices with entries in $\mathbb{K}$ and zero trace is a matrix Lie algebra. Since

$$\det(1 + tf + O(t^2)) = 1 + \operatorname{tr} tf + O(t)^2 \,,$$

the trace of infinitesimal generators of $S\mathbb{G}$ vanishes; conversely, the property (2.2) implies that the exponentials of elements of $s\mathbb{L}$ have determinant one, hence belong to $S\mathbb{G}$. Therefore $s\mathbb{L}$ is the Lie algebra corresponding to the matrix group $S\mathbb{G}$.

We consider the algebraic properties of the special linear group $SL(2, \mathbb{C})$ and its Lie algebra $sl(2, \mathbb{C})$ in some detail, since the group $SL(2, \mathbb{C})$, its subgroups, and the Lie algebra $sl(2, \mathbb{C})$ and its Lie subalgebras play a very important role in physics. $SL(2, \mathbb{C})$ and/or $sl(2, \mathbb{C})$ are implicitly present even in applications not mentioning Lie groups or Lie algebras explicitly: In special relativity, $SL(2, \mathbb{C})$ appears because of its relation to the Lorentz group. The Dirac equation for electrons and positrons (see Section 5.5) uses properties of Pauli matrices (or their cousins, the Dirac matrices), whose relation to $SL(2, \mathbb{R})$ is now established.

3-vectors and 4-vectors. As traditional in physics, we usually use fat letters to write column vectors $\mathbf{a}$ with three components a_1, a_2, a_3. Depending on the context, these three components may be real or complex numbers, matrices, linear operators, or elements from an arbitrary associative algebra $\mathbb{A}$. We write $\mathbb{A}^3$ for the set of all vectors with three components from $\mathbb{A}$. The **inner product** of $\mathbf{a}, \mathbf{b} \in \mathbb{A}^3$ is the element

$$\mathbf{a} \cdot \mathbf{b} := \mathbf{a}^T \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3 \in \mathbb{A};$$

clearly $\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a}$. We write

$$\mathbf{a}^2 := \mathbf{a} \cdot \mathbf{a} = a_1^2 + a_2^2 + a_3^2.$$

The **length** of a vector $\mathbf{a} \in \mathbb{C}^3$ is

$$|\mathbf{a}| := \sqrt{\mathbf{a}^* \mathbf{a}} = \sqrt{|a_1|^2 + |a_2|^2 + |a_3|^2},$$

so $\mathbf{a}^2 = |\mathbf{a}|^2$ if $\mathbf{a} \in \mathbb{R}^3$.

We write $\mathbb{A}^{1,3}$ for the set of vectors p with four components $p_0, p_1, p_2, p_3 \in \mathbb{A}$, arranged as

$$\mathbf{p} = \begin{pmatrix} p_0 \\ \mathbf{p} \end{pmatrix}, \quad p_0 \in \mathbb{A}, \ \mathbf{p} \in \mathbb{A}^3.$$

Using the traditional terminology from relativity theory, we call such vectors p **4-vectors**, and call p_0 the **time part** and $\mathbf{p}$ the **space part** of p. The **Minkowski inner product** of $p, q \in \mathbb{A}^{1,3}$ is the element

$$p \cdot q := p_0 q_0 - \mathbf{p} \cdot \mathbf{q} = p_0 q_0 - p_1 q_1 - p_2 q_2 - p_3 q_3, \tag{2.6}$$

and

$$p^2 := p \cdot p = p_0^2 - \mathbf{p}^2.$$

Note that p^2 may be negative!

Pauli matrices. With these preparations, we define the **Pauli matrices**

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.7}$$

Assembling the last three in the **Pauli vector**

$$\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)^T \in l(2, \mathbb{C})^3,$$

we write for any $\mathbf{p} \in \mathbb{R}^3$

$$\mathbf{p} \cdot \boldsymbol{\sigma} := p_1 \sigma_1 + p_2 \sigma_2 + p_3 \sigma_3 = \begin{pmatrix} p_3 & p_1 + i p_2 \\ p_1 - i p_2 & -p_3 \end{pmatrix}. \tag{2.8}$$

This matrix has zero trace, hence belongs to $sl(2, \mathbb{C})$, and it is easily seen that every element of $sl(2, \mathbb{C})$ can be written uniquely in this form. Similarly, each complex 2×2-matrix can

be written as a complex linear combination of all four Pauli matrices. Defining the **Pauli 4-vectors**

$$\sigma_\pm := \begin{pmatrix} \sigma_0 \\ \pm\boldsymbol{\sigma} \end{pmatrix} \in l(2,\mathbb{C})^{1,3},$$

we may write the general element of $l(2,\mathbb{C})$ as

$$p\cdot\sigma_\pm = p_0\sigma_0 \mp \mathbf{p}\cdot\boldsymbol{\sigma} = \begin{pmatrix} p_0 \mp p_3 & \mp p_1 \mp ip_2 \\ \mp p_1 \pm ip_2 & p_0 \pm p_3 \end{pmatrix}, \quad \text{for some } p = \begin{pmatrix} p_0 \\ \mathbf{p} \end{pmatrix} \in \mathbb{C}^{1,3}. \tag{2.9}$$

We note that, for $p, q \in \mathbb{C}^{1,3}$,

$$(p\cdot\sigma_-)(q\cdot\sigma_+) = p\cdot q\sigma_0\,,$$

$$\det(p\cdot\sigma_\pm) = p^2.$$

Clifford algebras. (2.10) also implies the anti-commutation rule

$$[\mathbf{p}\cdot\boldsymbol{\sigma}, \mathbf{q}\cdot\boldsymbol{\sigma}]_+ = 2\mathbf{p}\cdot\mathbf{q}\sigma_0\,.$$

Here

$$[f,g]_+ := fg + gf$$

denotes the **anticommutator** of f and g.

$$[\sigma_k, \sigma_l]_+ = 2\delta_{kl}\sigma_0 \quad \text{for } k,l = 1,2,3\,.$$

2.6 The vector product, quaternions, and $SL(2,\mathbb{C})$

The vector product. The structure of the Lie algebra $sl(2,\mathbb{C})$ is intimately tied up with the vector product in $\mathbb{R}^3$.

The **vector product** of $\mathbf{a}, \mathbf{b} \in \mathbb{A}^3$ is the vector

$$\mathbf{a}\times\mathbf{b} := \begin{pmatrix} a_2b_3 - a_3b_2 \\ a_3b_1 - a_1b_3 \\ a_1b_2 - a_2b_1 \end{pmatrix} \in \mathbb{A}^3,$$

One easily checks that

$$\mathbf{a}\times\mathbf{b} = -\mathbf{b}\times\mathbf{a},$$

and the determinant formula for the bfitriple product

$$(\mathbf{a}\times\mathbf{b})\cdot\mathbf{c} = \mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \det(\mathbf{a},\mathbf{b},\mathbf{c}) := \det\begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix},$$

The most common case is that all three components are real or complex vectors. In this case, the following rules, which will be used in the following without comment, hold.

$$\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}) = \mathbf{b}\cdot(\mathbf{c}\times\mathbf{a}) = \mathbf{c}\cdot(\mathbf{a}\times\mathbf{b}),$$

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) = (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{b}\cdot\mathbf{c})(\mathbf{a}\cdot\mathbf{d}),$$

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b}),$$

$$(\mathbf{a}\times\mathbf{b})\times\mathbf{c} = \mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{a}(\mathbf{b}\cdot\mathbf{c}),$$

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = (\mathbf{a}\times\mathbf{b})\times\mathbf{c} + \mathbf{b}\times(\mathbf{a}\times\mathbf{c}),$$

$$(\mathbf{a}\times\mathbf{c})\times(\mathbf{b}\times\mathbf{c}) = \det(\mathbf{a},\mathbf{b},\mathbf{c})\mathbf{c}.$$

Indeed, each property follows by a simple computation either directly or from the previous property.

A simple calculation with (2.8) verifies the product formula

$$(\mathbf{p}\cdot\boldsymbol{\sigma})(\mathbf{p}\cdot\boldsymbol{\sigma}) = (\mathbf{p}\cdot\mathbf{q})\sigma_0 + i(\mathbf{p}\times\mathbf{q})\cdot\boldsymbol{\sigma}, \tag{2.10}$$

from which we obtain the commutation rule

$$[\mathbf{p}\cdot\boldsymbol{\sigma},\mathbf{q}\cdot\boldsymbol{\sigma}] = 2i\mathbf{p}\times\mathbf{q}\cdot\boldsymbol{\sigma}$$

and the trace formula

$$\operatorname{tr}(\mathbf{p}\cdot\boldsymbol{\sigma})(\mathbf{q}\cdot\boldsymbol{\sigma}) = 2\mathbf{p}\cdot\mathbf{q}.$$

Although measurements usually involve real numbers only, the need for complex matrices in physics is undisputable.

Less familiar than complex numbers are the quaternions, obtained by extending the complex number system by adjoining a further square root. This is possible without introducing zero divisors by renouncing the commutative law of multiplication (which is lost for matrices anyway). After their discovery by William Hamilton in 1843 (cf. Hamilton [120]), quaternions had an important role to play in physics because of their usefulness in describing rotations. But with the introduction of the vector product by Gibbs [101] in 1881, quaternions declined in popularity and later almost disappeared from physics. However, they were kept alive in mathematics, and found new and important applications in modern computational geometry, where they are the method of choice for working with rotational motion and describe time-dependent rotations, and in astrodynamics, where they are used for spacecraft attitude control systems.

In the context of Lie groups, quaternions and matrices whose coefficients are quaternions still play a significant role in the classification of real simple Lie groups and associated symmetric spaces; see., e.g., Chevalley [61], Gilmore [104], or Helgason [124].

The Pauli matrices satisfy the product rule

$$(a\cdot\sigma)(b\cdot\sigma) = a\cdot b + i(a\times b)\cdot\sigma \quad \text{for } a,b\in\mathbb{C}^3. \tag{2.11}$$

(2.11) shows that the vector space $\mathbb{Q}'$ of complex 2×2 matrices of the form $a_0 + ia\cdot\sigma$ ($a_0\in\mathbb{R}$, $a\in\mathbb{R}^3$) is an algebra. Indeed, if we embed $\mathbb{C}$ into $\mathbb{R}^{2\times 2}$ using the imaginary unit $i = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ (which satisfies $i^2=-1$), we can write the quaternions (3.41) as

$$\mathbf{i} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\sigma_3, \quad \mathbf{j} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_2, \quad \mathbf{k} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = i\sigma_1,$$

which exhibits the isomorphism. $\mathbb{Q}'$ can also be desribed as the set of complex 2×2 matrices U satisfying $U_{22} = U_{11}^*$ and $U_{21} = -U_{12}^*$, and the matrices in $\mathbb{Q}'$ of determinant 1 are just the unitary 2×2 matrices, hence form the Lie group $U(2)$. This proves that $U(2)$ is isomorphic to a double covering of the group $SO(3)$. An explicit isomorphism is given by

$$(r_0 + ir\cdot\sigma)(x\cdot\sigma)(r_0+ir\cdot\sigma)^* = (Q[r]x)\cdot\sigma, \quad r_0 = \sqrt{1-r^2}. \tag{2.12}$$

$$a^TQb = \frac{1}{2}\operatorname{tr}(a\cdot\sigma)U(b\cdot\sigma)U^*,$$

$$U = \frac{1+\sigma\cdot Q\sigma}{2\sqrt{1+\operatorname{tr}Q}}$$

2.6.1 Theorem. *The set $\mathbb{Q}$ of quaternions is a* ***skew field****, i.e., an associative algebra in which every nonzero element has an inverse. We have*

$$U(r_0,\mathbf{r}) + U(s_0,\mathbf{s}) = U(r_0+s_0, \mathbf{r}+\mathbf{s}), \tag{2.13}$$

$$\lambda U(r_0,\mathbf{r}) = U(\lambda r_0, \lambda\mathbf{r}), \tag{2.14}$$

$$U(r_0,\mathbf{r})^T = U(r_0,-\mathbf{r}), \tag{2.15}$$

$$U(r_0,\mathbf{r})U(s_0,\mathbf{s}) = U(r_0s_0 - r\cdot\mathbf{s},\ s_0\mathbf{r}+r_0\mathbf{s}+\mathbf{r}\times\mathbf{s}), \tag{2.16}$$

$$U(r_0,\mathbf{r})^{-1} = \frac{1}{r_0^2+\mathbf{r}^2}U(r_0,-\mathbf{r}) \quad \text{if } r_0^2+\mathbf{r}^2\neq 0. \tag{2.17}$$

Proof. (2.13)–(2.15) are trivial, and (2.16) follows by direct computation, using Specializing (2.16) to $s_0 = r_0, \mathbf{s} = -\mathbf{r}$ gives

$$U(r_0,\mathbf{r})U(r_0,-\mathbf{r}) = U(r_0^2+\mathbf{r}^2, 0) = (r_0^2+\mathbf{r}^2)1, \tag{2.18}$$

which implies (2.17). Therefore $\mathbb{Q}$ is a vector space closed under multiplication, and every nonzero element in $\mathbb{Q}$ has an inverse. Since matrix multiplication is associative, $\mathbb{Q}$ is a skew field. □

In the standard treatment, quaternions are treated like complex numbers, as objects of the form

$$\mathbf{q}(r_0,\mathbf{r}) = r_0 1 + r_1\mathbf{i} + r_2\mathbf{j} + r_3\mathbf{k}$$

with special unit quaternions $1,\mathbf{i},\mathbf{j},\mathbf{k}$. The correspondence is given by the identification

$$\mathbf{i} = \sigma_1, \quad \mathbf{j} = \sigma_2, \quad \mathbf{k} = -\sigma_3 \tag{2.19}$$

in terms of which $\mathbf{q}(r_0,\mathbf{r}) = U(r_0,\mathbf{r})$.

2.7 The Hamiltonian form of a Lie algebra

In the Hamiltonian form, one takes Hermitian matrices and uses the Lie product i/hbar[f,g], to match things with quantum mechanical usage. Expressed in terms of commutators, as usual, the structure constants (e.g., for su(2)-so(3)) become purely imaginary, although the Lie algebra is real.

In the applications, distinguished generators typically are Hermitian and represent important real-valued observables. Therefore they tend to replace the matrix A by iA. This is one of the reasons why the structure constants for real algebras appear in the physics literature with an i when written in terms of commutators.

Every one-parameter group is isomorphic to either $L(1,\mathbb{R})$ or $U(1)$. Two connected matrix groups are called **locally isomorphic** if their associated Lie algebras are isomorphic. For example, $L(1,\mathbb{R})$ and $U(1)$ are locally isomorphic but not isomorphic.

Generators, commutation relations, and structure constants

Introduce the vector $\mathbf{L}$ of generators for $SL(2,\mathbb{C})$ and its commutation relations.

The components of the vector product satisfy

$$(\mathbf{a}\times\mathbf{b})_j = a_{j+1}b_{j-1} - a_{j-1}b_{j+1} \quad \text{(indices } j = 1,2,3 \bmod 3).$$

We may express this as in terms of the **Levi–Cività symbol**, defined by

$$\epsilon_{jkl} = \begin{cases} 1 & \text{if } jkl \text{ is an even permutation of } 123\,, \\ -1 & \text{if } jkl \text{ is an odd permutation of } 123\,, \\ 0 & \text{otherwise.} \end{cases} \tag{2.20}$$

Thus ϵ_{jkl} is completely antisymmetric in the indices j,k,l and $1 \le j,k,l \le 3$.

The Pauli matrices (2.7) satisfy (componentwise version of (2.10))

$$\sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k\,,$$

$$\operatorname{tr}\sigma_i = 0\,, \quad \operatorname{tr}\sigma_i\sigma_j = 2\delta_{ij}\,, \quad \operatorname{tr}[\sigma_i,\sigma_j]\sigma_k = 4i\epsilon_{ijk}\,.$$

The Pauli matrices satisfy

$$[\sigma_k,\sigma_l] = 2i\sum_{m=1}^{3}\epsilon_{klm}\sigma_m \quad \text{for } k,l = 1,2,3\,.$$

The summation above contains only one nonzero term. For example, $[\sigma_1,\sigma_2] = 2i\sigma_3$, and all other Lie products can be found using a cyclic permutation.

2.8 Atomic energy levels and unitary groups

In the terminology to be systematically developed in Chapter 8, the **quantities** are the elements of the algebra $\mathbb{E} = \mathbb{C}^{N\times N}$ of square complex $N \times N$ matrices, the **constants** are the multiples of the identity matrix. The **Hamiltonian** H represents the **energy** and is a diagonal matrix $H = \mathrm{Diag}(E_1, \ldots, E_N)$ whose diagonal entries E_k are the **energy levels** of the system. In the **nondegenerate** case (the only case considered in this section), all E_k are distinct, and the diagonal matrices comprise all functions of H. Quantities represented by arbitrary nondiagonal matrices are less easy to interpret. However, an important class of quantities are the matrices of the form $P = \psi\psi^*$, where ψ is a vector of norm 1; they satisfy $P^2 = P = P^*$ and are the quantities observed in binary measurements such as detector clicks; see Section 10.5. The **states** of the N-level system are the linear mappings that map a quantity $f \in \mathbb{E}$ to its **value** $\langle f\rangle = \mathrm{tr}\,\rho f$, where $\rho \in \mathbb{E}$ is a positive semidefinite Hermitian matrix with trace one, called the **density matrix** of the state. (Frequently, one talks somewhat sloppily of the "state" ρ.) The diagonal entries $p_k := \rho_{kk}$ represent the probability for obtaining a response in a binary test for the kth quantum level; the off-diagonal entries ρ_{jk} represent deviations from a classical mixture of quantum levels.

The standard basis consisting of the N **unit vectors** $|k\rangle$ with a one in component k and zeros in all other component corresponds to the N levels of the quantum systems.

Extra structure of a **Euclidean $*$-algebra**, important for the applications; see Section : The **conjugate** f^* of f is given by conjugate transposition, and the **integral** $\int g = \mathrm{tr}\, g$ is the **trace**, the sum of the diagonal entries or, equivalently, the sum of the eigenvalues.

Closely related to n-level quantum systems are the unitary groups and their Lie algebras.

A matrix $U \in \mathbb{C}^{n\times n}$ is called **unitary** if $U^*U = 1$, equivalently, if U is invertible and $U^{-1} = U^*$. The set $U(n)$ of all unitary $n \times n$ matrices is a matrix group, called a (full) **unitary group**. Indeed, if $U, V \in U(n$ then $(UV)^*UV = V^*U^*UV = V^*V = 1$ and $(U^{-1})^*U^{-1} = (U^*)^*U^1 = UU^{-1} = 1$, so that $UV, U^{-1} \in U(n)$. The unitary $n \times n$ matrices with determinant one form a matrix group $SU(n)$, called a **special unitary group**.

$U(n)$ acts on the matrices of fixed trace and determinant by mapping ρ to

$$U\{\rho\} := U\rho U^*.$$

Show preservation of semidefiniteness, trace and determinant. $UV\{\rho\} = U\{V\{\rho\}\}$.

A matrix $A \in \mathbb{C}^{n\times n}$ is called **antihermitian** if $A^* = -A$. The set $u(n)$ of all antihermitian $n\times n$ matrices is a matrix Lie algebra, called a **unitary Lie algebra**. Indeed, if $f, g \in u(n)$ then $[f, g]^* = (fg - gf)^* = (g^*f^* - f^*g^* = (-g)(-f) - (-f)(-g) = -(fg - gf) = -[f, g]$, hence $[f, g] \in u(n)$. The Lie algebra of infinitesimal generators of $U(n)$ is $u(n)$. Indeed, if $U(t) = 1+tf+O(t^2)$ is unitary, we have $1 = U(t)U(t)^* = (1+tf+O(t^2))(1+tf+O(t)^2)^* = 1+t(f+f^*)+O(t)^2$, implying that f is antihermitian. The antihermitian $n \times n$ matrices with trace zero form a Lie algebra $su(n)$, called a **special unitary Lie algebra**. $su(n)$ is the Lie algebra of the matrix group $SU(n)$.

2.9 Qubits and Bloch sphere

The smallest quantum systems have two levels only and are called **qubits**; they play an fundamental role in quantum information theory and quantum computing; cf. Nielsen & Chuang [207].

We have

$$(p \cdot \sigma_\pm)^* = \overline{p} \cdot \sigma_\pm \,,$$

so that $p \cdot \sigma_\pm$ is Hermitian if and only if the components of p are real, and antihermitian if and only if the components of p are purely imaginary. Therefore

$$u(2) = \{ip \cdot \sigma_\pm \mid p \in \mathbb{R}^{1,3}\} \,,$$

and letting p take complex values we get the whole of $l(2, \mathbb{C})$.

Similarly, the matrices $i\sigma_0, i\sigma_1, i\sigma_2, i\sigma_3$ form a basis of the Lie algebra $u(2)$, considered as a real vector space; indeed, any Hermitian 2×2 matrix can be written in a unique way as $p \cdot \sigma_+$ for some $p \in \mathbb{R}^{1,3}$.

We obtain $su(2)$ for p real and $p_0 = 0$.

The Lie algebras $u(2)$ and $su(2)$. The matrices $i\sigma_1, i\sigma_2, i\sigma_3$ form a basis for the Lie algebra $su(2)$, considered as a real vector space; indeed, any traceless and Hermitian 2×2 matrix can be written in a unique way as $\mathbf{p} \cdot \boldsymbol{\sigma}$ for some $\mathbf{p} \in \mathbb{R}^3$. Clearly, $i\sigma_0$ spans the center of the Lie algebra $u(2)$. As a consequence, we can write $u(2) \cong \mathbb{R} \oplus su(2)$.

The Lie group $U(2)$. In the case $n = 2$ it is a nice exercise to show that each special unitary matrix U can be written as

$$U = \begin{pmatrix} x & y \\ -\overline{y} & \overline{x} \end{pmatrix} \,, \quad x, y \in \mathbb{C} \,,\ |x|^2 + |y|^2 = 1 \,.$$

Writing $x = a + ib$ and $y = c + id$ for $a, b, c, d \in \mathbb{R}$ we see that $a^2 + b^2 + c^2 + d^2 = 1$. This implies that there is a one-to-one correspondence between $SU(2)$ and the set of points on the unit sphere S^3 in $\mathbb{R}^4$. Thus $SU(2)$ is as a manifold homeomorphic to S^3. (The manifold point of view of matrix groups may be used to give a definition of abstract Lie groups; see .)

We now show that $SU(2)$ is a real manifold that is isomorphic to the three sphere S^3. We do this by finding an explicit parametrization of $SU(3)$ in terms of two complex numbers x and y satisfying $|x|^2 + |y|^2 = 1$, which defines the three-sphere.

We write an element $g \in SU(2)$ as

$$g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \,.$$

Writing out the equation $g^*g = 1$ and $\det g = 1$ one finds the following equations:

$$\begin{aligned} |a|^2 + |c|^2 &= 1\,, \qquad & |b|^2 + |d|^2 &= 1\,, \\ \overline{a}b + \overline{c}d &= 0\,, \qquad & ad - bc &= 1\,. \end{aligned}$$

We first assume $b = 0$ and find then that $ad = 1$ and $\overline{c}d = 0$, implying that $c = 0$ and U is diagonal with $a = \overline{d}$. Next we suppose $b \neq 0$ and use $a = -c\overline{d}/\overline{b}$ to deduce that $|b| = |c|$ and $|a| = |d|$; we thus have $b \neq 0 \Leftrightarrow c \neq 0$. We also see that we can use the ansatz

$$\begin{aligned} a &= e^{i\alpha}\cos\theta\,, \qquad & b &= e^{i\beta}\sin\theta\,, \\ c &= -e^{i\gamma}\sin\theta\,, \qquad & d &= e^{i\delta}\cos\theta\,. \end{aligned}$$

Using again $a = -c\overline{d}/\overline{b}$ we see $\alpha + \delta = \beta + \gamma$ and writing out $ad - bc = 1$ we find $\alpha = -\delta$ and $\beta = -\gamma$. We thus see $a = \overline{d}$ and $b = -\overline{c}$. Hence the most general element of $SU(2)$ can be written as

$$g(x, y) = \begin{pmatrix} x & y \\ -\overline{y} & \overline{x} \end{pmatrix}\,, \quad \text{with} \quad |x|^2 + |y|^2 = 1\,.$$

The map $S^3 \to SU(2)$ mapping (x, y) to $g(x, y)$ is clearly injective, and from the above analysis bijective. Furthermore the map is smooth. Hence we conclude that $SU(2) \cong S^3$ as a real manifold.

2.10 Polarized light and beam transformations

Qubits are closely related to the polarization of light. Since polarization phenomena show the basic principles of quantum mechanics in a clean and transparent way, we use polarization to derive the basic equations of quantum mechanics, the Liouville equation and the Schrödinger equation, thus giving them an easily understandable meaning.

Polarized light was discovered by Christiaan Huygens [132] in 1690. The transformation behavior of beams of completely polarized light was first described by Etienne-Louis Malus[180] in 1809 (who coined the name "polarization"), and that of partially polarized light by George Stokes [262] in 1852. The transverse nature of polarization was discovered by Augustin Fresnel [93] in 1866, and the description in terms of (what is now called) the Bloch sphere by Henri Poincare [221] in 1892.

It is instructive to read Stokes' 1852 paper [262] in the light of modern quantum mechanics. One finds there all quantum phenomena for modern qubits, explained in classical terms!

Splitting polarized monochromatic beams into two beams with different, but orthogonal polarization corresponds to writing a wave functions as superposition of preferred basis vectors. Mixtures are defined (in Stokes' paragraph 9) as arising from "groups of independent polarized streams" and give rise to partially polarized beams. What is now called the polarization matrix is represented by Stokes with four real parameters comprising, in today's terms, the Stokes vector, or, equivlently, the polarization matrix. Stokes asserts (in his paragraph 16) the impossibility of recovering from a mixture of several distinct pure

states any information about these states beyond what is encoded in the Stokes vector (i.e., the polarization matrix). The latter can be linearly decomposed in many essentially distinct ways into a sum of pure states, but all these decompositions are optically indistinguishable.

If one interprets the normalized polarization matrix as density matrix of a qubit, a polarized monochromatic beam of classical light behaves exactly like a modern qubit, which shares all the features mentioned. Polarized light is therefore the simplest quantum phenomenon, and the only one that was understood quantitatively already before the birth of quantum mechanics in 1900.

Experiments with polarization filters are easy to perform; probably they are already known from school. Since polarization is a macroscopic phenomenon, the counterintuitive features of quantum mechanics irritating the untrained intuition are still absent. But polarization was recognized as a quantum phenomenon only when quantum mechanics was already fully developed. Norbert Wiener [291] 1930 exhibited a description in terms of the Pauli matrices and wrote: "It is the conviction of the author that this analogy" between classical optics and quantum mechanics "is not merely an accident, but is due to a deep-lying connection between the two theories". This is indeed the case; see, e.g., Neumaier [206].

The mathematics of polarization. A beam of polarized light of fixed frequency is characterized by a state, described equivalently by the **Stokes vector**, a real 4-dimensional vector

$$S = (S_0, S_1, S_2, S_3)^T = \begin{pmatrix} S_0 \\ \mathbf{S} \end{pmatrix} \in \mathbb{R}^{1,3}$$

with

$$S_0 \geq |\mathbf{S}|, \tag{2.21}$$

or by a **polarization matrix** (also called **coherence matrix**) a complex positive semidefinite Hermitian 2×2 matrix C. These are related by

$$C = \frac{1}{2} \begin{pmatrix} S_0 + S_3 & S1 + iS_2 \\ S_1 - iS_2 & S_0 - S_3 \end{pmatrix} = \frac{1}{2} S \cdot \sigma_- = \frac{1}{2}(S_0 \sigma_0 + \mathbf{S} \cdot \boldsymbol{\sigma})$$

in terms of the Pauli matrices (2.7). (In the literature, the signs and order of the components may differ.)

The trace $\operatorname{tr} C = S_0$ of the polarization matrix is the **intensity** of the beam. If $S_0 = 0$, the beam is **dark** and contains no light. Otherwise, one may normalize the intensity by dividing the polarization matrix by S_0, resulting in a **density matrix** of trace one,

$$\rho = C / \operatorname{tr} C = \frac{1}{2} r \cdot \sigma_-, \quad r = S/S_0 = \begin{pmatrix} 1 \\ \mathbf{r} \end{pmatrix};$$

it contains the intensity-independent information about the beam. The intensity-independent quotient

$$d := |\mathbf{r}| = |\mathbf{S}|/S_0 \in [0, 1]$$

is called the **degree of polarization**, and allows the determinant of the polarization matrix to be written as $\det C = \frac{1}{4}(S_0^2 - \mathbf{S}^2) = \frac{1}{4} S_0^2 (1 - d^2)$.

The extremal case $d = 0$ characterizes **unpolarized light**, which therefore has a polarization matrix $C = \frac{1}{2}S_0\sigma_0$. At the other extreme, a fully polarized beam (a pure polarization state) has $d = 1$; it corresponds to a so-called **pure** polarization state. Since $d = 1$ characterizes singular polarization matrices, a pure polarization state can be written in the form $C = \psi\psi^*$ with a **state vector** ψ determined up to a phase. In this case, the intensity of the beam is $S_0 = |\psi|^2 = \psi^*\psi$. In particular, a normalized state vector has norm $|\psi| = \sqrt{\psi^*\psi} = 1$.

Beam transformations. Optical instruments may transform beams by letting them pass through a filter. A linear, non-mixing (not depolarizing) **filter** is characterized by a complex 2×2 **Jones matrix** U. (In the literature, many authors call U^* the Jones matrix.) The instrument transforms an in-going beam in the state C into an out-going beam in the state $C' = UCU^*$. If the instrument is lossless, the intensities of the in-going and the out-going beam are identical. This is the case if and only if the Jones matrix U is unitary.

A linear, mixing (depolarizing) filter transforms C instead into a sum of several terms of the form UCU^*. It is therefore described by a **completely positive** linear map on the space of 2×2 matrices, or a corresponding real 4×4 matrix acting linearly on the Stokes vector, called the **Müller matrix**. For definitions and details, see, e.g., Aiello et al. [3] and Benatti & Floreanini [30].

The Liouville equation. Passage through inhomogeneous media can be modelled by means of slices consisting of many very thin filters with Jones matrices close to the identity.

The Schrödinger equation. If Δt is the time needed to pass through one slice and $\psi(t)$ denotes the pure state at time t then $\psi(t + \Delta t) = U(t, \Delta t)\psi(t)$, where $U(t, \cdot)$ is a $L(2, \mathbb{C})$-motion parameterized by the transition time Δt. We therefore introduce its infinitesimal generator

$$H(t) := i\hbar\partial U(t, \Delta t)/\partial\Delta t)\Big|_{\Delta t=0},$$

called the **Hamiltonian** of the filter. Thus we have

$$U(t) = 1 - \frac{i\Delta t}{\hbar}H(t) + O(\Delta t^2) \tag{2.22}$$

In the lossless case, $U(t) = U(t, \Delta t)$ is unitary, which implies that $H(t)$ is Hermitian.

A linear, non-mixing (not depolarizing) instrument with Jones matrix U transforms an in-going beam in the pure state with state vector ψ into an out-going beam in a pure state with state vector $\psi' = U\psi$. (2.22) implies

$$i\hbar\frac{d}{dt}\psi(t) \approx \frac{i\hbar}{\Delta t}(\psi(t + \Delta t) - \psi(t)) = \frac{i\hbar}{\Delta t}(U(t) - 1)\psi(t).$$

In a continuum limit we thus recover the time-dependent **Schrödinger equation**

$$i\hbar\frac{d}{dt}\psi(t) = H(t)\psi(t).$$

2.11 Spin and spin coherent states

In this section, we discuss the **spinor representations** of $L(2,\mathbb{C})$, see also STERNBERG [260]. By restricting to the unitary matrices we get unitary representations of the group $SU(2)$. As we shall see later in Section 22.3, these representations comprise all irreducible unitary representations of $SU(2)$.

For $0 \leq s \in \frac{1}{2}\mathbb{Z}$ (the factor $\frac{1}{2}$ appears here for historical reasons only) we denote with $\mathbb{P}_s$ the complex vector space of all homogeneous polynomials of degree $2s$ in $z = (z_1, z_2) \in \mathbb{C}^2$. The space $\mathbb{P}_s$ has dimension $2s+1$ since the monomials $z_1^k z_2^{2s-k}$ $(k = 0, 1, \ldots, 2s)$ form a basis of $\mathbb{P}_s$. The group $L(2,\mathbb{C})$ of invertible complex 2×2 matrices acts on $\mathbb{C}^2$ in the natural way. On $\mathbb{P}_s$ we get a representation of $L(2,\mathbb{C})$ by means of the formula

$$(U(g)\psi)(z) := \psi(g^{-1}z) \quad \text{for } g \in L(2,\mathbb{C})\,. \tag{2.23}$$

Then indeed $U(g)U(h)\psi(z) = U(h)h\psi(g^{-1}z) = \psi(h^{-1}g^{-1}z) = \psi((gh)^{-1}z) = U(gh)\psi(z)$. Taking infinitesimal group elements, we find that the Lie algebra $l(2,\mathbb{C})$ acts on $\mathbb{P}_s$ by means of the representation J defined by

$$(J(f)\psi)(z) = -(fz)\cdot\nabla\psi(z)\,, \quad \text{for } f \in l(2,\mathbb{C})\,. \tag{2.24}$$

Note that this is again a homogeneous polynomial of degree $2s+1$.

In nonrelativistic quantum mechanics, an elementary particle with **spin** s is described by an element of the space $L^2(\mathbb{R}^3, \mathbb{P}_s)$ of square integrable mappings from $\mathbb{R}^3$ to $\mathbb{P}_s$. The Hamiltonian for a particle with spin s in a magnetic field $\mathbf{B} \in \mathbb{R}^3$ is given in terms of the Pauli matrices by

$$H = -\mathbf{B}\cdot\boldsymbol{\sigma} = -\begin{pmatrix} B_3 & B_1 + iB_2 \\ B_1 - iB_2 & -B_3 \end{pmatrix}\,, \tag{2.25}$$

where the action of H is given by (2.24). The dynamics is described by the Schrödinger equation

$$i\hbar\dot{\psi} = H\psi\,. \tag{2.26}$$

The unitary case. By restricting in (2.9) to real-valued p, we represent $u(2)$. The resulting representation turns out to be unitary. To give $\mathbb{P}_s$ the appropriate Hilbert space structure, we define on the unit disk

$$D = \{z \in \mathbb{C}^2 \mid z^* z \leq 1\}$$

of $\mathbb{C}^2$ the measure Dz by

$$\int Dz f(z^*, z) = \int_D dz^2 f(z^*, z)\,. \tag{2.27}$$

Explicitly we thus have $Dz = dz_1 d\bar{z}_1 dz_2 d\bar{z}_2$, so that for example

$$\int Dz \bar{z}_1^k z_1^l \bar{z}_2^m z_2^n \;=\; 4\pi^2 \delta_{kl}\delta_{mn} \int_{0\leq x^2+y^2\leq 1} x^{2k+1} y^{2m+1} dx dy$$

$$
\begin{aligned}
&= \pi^2 \delta_{kl}\delta_{mn} \int_{0\le s+t\le 1} s^k t^m \, ds\, dt \\
&= \frac{\pi^2 k! m!}{(k+m+2)!}\delta_{kl}\delta_{mn}\,,
\end{aligned}
$$

where in the last step we used

$$
\int_0^1 x^a (1-x)^b \, dx = \frac{a!b!}{(a+b+1)!}\,.
$$

2.11.1 Proposition. *Dz is an $SU(2)$ invariant measure satisfying*

$$
\int Dz (z^* x)^{2s} (z^T y)^{2s} = \gamma_s (x^T y)^{2s}, \quad 0 \le s \in \frac{1}{2}\mathbb{Z}, \tag{2.28}
$$

where

$$
\gamma_s = \pi^2/(2s+1)(2s+2). \tag{2.29}
$$

Proof. Under a change of integration $z' = gz$ we have $dz_1' d\bar{z}_1' = \det g dz_1 d\bar{z}_1 = dz_1 d\bar{z}_1$. Hence if we use for $g \in SU(2)$ the substitution $z = gz'$, then the integral in (2.28) transforms into the same integral with $(x', y') = (\bar{U}x, Uy)$ in place of (x, y). Thus it is invariant under $SU(2)$ and depends therefore only on $x^T y$. Indeed, we can always rotate x such that $x = (x_1, 0)$ and then clearly the right-hand side is a polynomial with terms $x_1^{2s} y_1^m y_2^{2s-m}$, which is only invariant under the diagonal $U(1)$-subgroup if $m = 2s$. Hence the right-hand side of (2.28) is fixed up to the constant γ_s, which is found by looking at the special case $x = y = \binom{1}{0}$:

$$
\gamma_s = \int Dz\, (z_1^*)^{2s} z_1^{2s} = \int_D dz^2 |z_1|^{4s} = \frac{\pi^2 (2s)!}{(2s+2)!} = \frac{\pi^2}{(2s+1)(2s+2)}\,. \tag{2.30}
$$

□

We make $\mathbb{P}_s$ into a Hilbert space by giving it the inner product

$$
\phi^* \psi = \langle \phi | \psi \rangle := \gamma_s^{-1} \int Dz\, \overline{\phi(z)} \psi(z)\,. \tag{2.31}
$$

We introduce the basis vectors $\pi_k^{(s)} = z_1^k z_2^{2s-k}$ for $\mathbb{P}_s$, in terms of which the inner product reads

$$
\langle \pi_k^{(s)} | \pi_l^{(s)} \rangle = \binom{2s}{k}^{-1} \delta_{kl}\,.
$$

For $x \in \mathbb{C}^2$, we define the **coherent state** $|x, s\rangle \in \mathbb{P}_s$ to be the functions

$$
|x, s\rangle(z) := (x^* z)^{2s} = (\bar{x}_1 z_1 + \bar{x}_2 z_2)^{2s}\,. \tag{2.32}
$$

Then we can restate (2.28) as

$$
\langle x, s | y, s \rangle = (y^* x)^{2s} \quad \text{for} \quad x, y \in \mathbb{C}^2. \tag{2.33}
$$

In particular, the coherent state $|x, s\rangle$ is normalized to norm 1 if and only if x has norm 1. Directly from (2.32), we see that

$$|0, s\rangle = 0, \quad |\lambda x, s\rangle = \lambda^{2s}|x, s\rangle, \tag{2.34}$$

so that it suffices in principle to look at coherent states with x of norm 1. In particular, choosing the parametrization $x = \binom{1}{w}$ gives the traditional **spin coherent states** of Radcliffe [225]. For coherent states, (2.23) implies

$$U(g)|x, s\rangle = |g^{-1*}x, s\rangle \quad \text{for } g \in SL(2, \mathbb{C})\,, \tag{2.35}$$

Thus coherent states define a representation of $L(2, \mathbb{C})$, the **spinor representation** of $L(2, \mathbb{C})$. We verify that we correctly have $U(g)U(h)|x, s\rangle = |g^{-1*}h^{-1*}x, s\rangle = |(gh)^{-1*}x, s\rangle = U(gh)|x, s\rangle$. One sees easily that only the subgroup $SU(2)$ is represented unitarily and we have

$$U(g)|x, s\rangle = |gx, s\rangle \quad \text{for } g \in SU(2)\,.$$

Note that the Schrödinger equation (2.26) implies that $\psi(t) = U(t)\psi(0)$, where $U(t) = e^{-itH/\hbar}$. Since the Hamiltonian (2.25) is an element of $su(2)$, we have $U(t) \in SU(2)$, and equation (2.35) implies the **temporal stability** of coherent states. This means that if the initial state vector is a coherent state, then under the time evolution determined by H the state vector remains for all times a coherent state. Since the norm of the wave function is invariant under the dynamics, too, one can work with normalized coherent states throughout.

In general, let $\mathbb{H}$ be a Hilbert space of functions on some space Ω. If we can write function evaluation as inner product, i.e., if for every $x \in \Omega$ there is an element $g_x \in \mathbb{H}$ such that $f(x) = \langle g_x|f\rangle$ for some , then we say that $\mathbb{H}$ has the **reproducing kernel property**.

We show that the space $\mathbb{P}_s$ has the reproducing kernel property. Expanding $(x^*z)^{2s}$ using the binomial series we obtain

$$|x, s\rangle = \sum_{m=0}^{2s} \binom{2s}{m} \overline{\pi_m^{(s)}(x)}\, \pi_m^{(s)}\,,$$

from which it follows

$$\pi_m^{(s)} = \gamma_s^{-1} \int_D Dx\, \pi_m^{(2s)}(x)|x, s\rangle\,,$$

so that the coherent states span $\mathbb{P}_s$. From (2.33) we find

$$\langle x, s|y, s\rangle = |y, s\rangle(x) \tag{2.36}$$

for all coherent states $|y, s\rangle$ and since these span $\mathbb{P}_s$, we have for all $\psi \in \mathbb{P}_s$

$$\langle x, s|\psi\rangle = \psi(x)\,, \quad \text{for all } \psi \in \mathbb{P}_s\,,$$

which is the reproducing kernel property. This implies that we can reproduce elements as follows. For all $\phi \in \mathbb{P}_s$ we have

$$\langle \phi|\psi\rangle = \gamma_s^{-1} \int Dz\, \overline{\phi(z)}\psi(z) = \gamma_s^{-1} \int Dz\, \langle \phi|z, s\rangle\langle z, s|\psi\rangle\,, \tag{2.37}$$

from which it follows that we can reproduce ψ

$$\psi = \gamma_s^{-1} \int Dx \psi(x) |x, s\rangle \quad \text{for all } \psi \in \mathbb{P}_s \,. \tag{2.38}$$

Equation (2.38) implies the **completeness relation**

$$\gamma_s^{-1} \int Dz |z, s\rangle\langle z, s| = 1 \,. \tag{2.39}$$

These properties characterize coherent states in general. For an extension of the coherent state concept to semisimple Lie groups see Perelomov [217] and Zhang et al. [300]. Coherent states for Heisenberg groups are called **Glauber coherent states**, and are basic for modern quantum optics. See Section and the book by Mandel & Wolf [181].

2.12 Particles and detection probabilities

Entanglement

The Stern–Gerlach Experiment. The Stern–Gerlach experiment is one of the most prominent and best known experiments in the history of quantum mechanics. The experiment provided a first experimental verification of the discrete nature of quantum mechanics. At the time of the experiment, which took place in 1922, the phenomenon of spin was not well-understood and, from the point of view of our present knowledge, a wrong model was used. Fortunately, the outcome of the experiment was in concordance with this model and the discrete nature of quantum mechanics was accepted as a fact.

When later a better model was invented, the theory and the Stern–Gerlach experiment showed discrepancies. It was perhaps partially because of these discrepancies that Goudsmit and Uhlenbeck postulated that the electron had half-integer spin: with the half-integer spin of the electron the experiment of Stern and Gerlach was again in agreement with the theory [2].

The setup of the Stern–Gerlach experiment is quite easy. To understand the physics behind the experiment, one only has to know that the energy of a small object with magnetic moment μ in an magnetic field B is given by the equation

$$U = -\mu \cdot B \,.$$

The energy is measured relative to the energy far away towards infinity where there is no magnetic field. Note that the magnetic moment is a vector. Hence, classically it lives in a

[2] As more often in the history of physics, it was a coincidence that determined the acceptance of a theory. Another such example was the measurement of the deflection of rays of the stars that can be seen close to the sun during a solar eclipse done by Eddington in 1919, thereby verifying the general theory of relativity of Einstein. The actual deflections are too small to be measured and hence the deflections found by Eddington have to be ascribed to noise; luckily the noise gave a pattern in agreement with the theoretical results.

representation of $SO(3)$, the representations of which are labelled by integers $l = 0, 1, 2, ...$ The dimension of the lth representation is $2l + 1$. In the Stern–Gerlach experiment a beam of particles with some fixed absolute value of μ is sent through an inhomogeneous magnetic field pointing in, say, the z-direction. Behind the magnetic field a screen is placed that will light up whenever a particle hits the screen. The force F exerted on a particle with magnetic moment $\mu = (\mu_x, \mu_y, \mu_z)$ is given by

$$F = -\nabla U = \mu_z \frac{\partial B_z}{\partial z} \,.$$

Thus, classically, the beam will be smeared out; the particles with μ pointing in the $+z$-direction will be deflected upwards, those with μ pointing in the $-z$-direction will be deflected downwards. Classically all positions of μ are possible and distributed in a Gaussian way, so that the screen will show a bounded strip, most intense in the center and fading out towards the ends. However, the result of the Stern–Gerlach experiment showed very clearly two blobs, centered at the positions corresponding to μ pointing up and down. Both blobs had the same intensity.

Assume that we have a bunch of particles (for example electrons), then they all have the same value of l, but the z-component of the magnetic moment might be different. Since the z-value can take $2l + 1$ values, the beam will split in $2l + 1$ different parts.

In their experiment, Stern and Gerlach used silver atoms, of which we now know that there is one electron in the outmost orbit and it is this electron which gives rise to the magnetic moment. The spin of an electron is however not in an $SO(3)$-representation, but in an $SU(2)$-representation and this correspondsn to $l = 1/2$. This representation is two-dimensional and thus the general state ψ of an electron can be described as

$$\psi = a|+\rangle + b|-\rangle \,, \quad |a|^2 + |b|^2 = 1 \,,$$

where $|+\rangle$ is the state with μ pointing in the $+z$-direction and $|-\rangle$ is the state with μ pointing in the $-z$-direction. When one measures the z-component of the magnetic moment, one finds with probability $|a|^2$ the value $+1/2$ and with probability $|b|^2$ the value $-1/2$. In a sample of heated silver atoms, there is no preferred direction for μ and thus in the end, the possibility that the value of the magnetic moment of a single silver atom is $+1/2$ is more or less $1/2$. This explains why the two blobs in the Stern–Gerlach experiment are equally bright.

2.13 Photons on demand

In this section we consider a quantum model for photons on demand, and its realization through laser-induced emission by a single calcium ion in a cavity. The exposition is based on Keller et al. [149].

In their paper, Keller et al. discuss in detail a model based on the simplified level scheme given in Figure 2.13 which ignores the fine structure of the Ca^+ states.

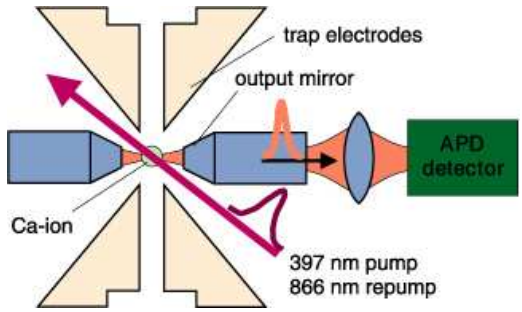


Figure 2.1: Experimental set-up for the generation of single-photon pulses with an ion-cavity system. The drawing shows a cross-section through the trap, perpendicular to the trap axis. (Figure 16 from [149])

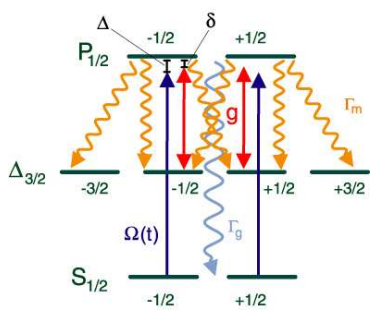
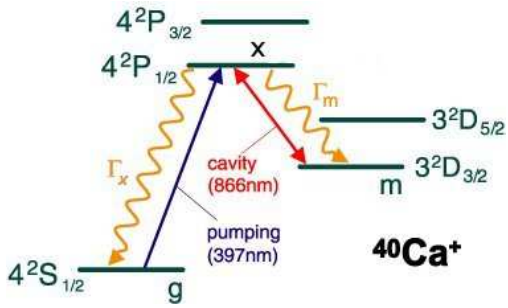
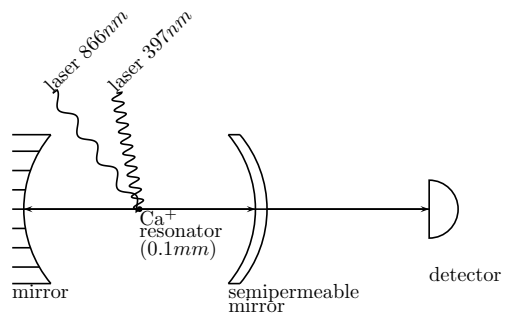


Figure 2.2: Scheme of the eight-level model on which we base our numerical calculations. Pump and cavity field are assumed to be linearly polarized in the direction of the quantization axis. For clarity, the four possible spontaneous decay transitions to the ground state are represented by a single arrow. (Figure 5 from [149])

- A **single** ion is localized in the cavity for many hours
- pulsating external fields (lasers) with a total cycle time 100kHz give a predictable rate of single photons
- pump laser at 397nm close to the excitation frequency $S \to P$
- Repeated excitation to P and decay to S until decay into the metastable D state; then inactive
- $\Rightarrow$ produces **exactly** one photon (not counting losses)
- reexcite ion into excited state with a reset laser at 866nm, until it falls back into the ground state
- ground state g, metastable state m, excited state x of Ca^+
- photons $\gamma_{\text{cavity}}, \gamma_{\text{pump}}, \gamma_{\text{reset}}$
- electron e bound in detector





Active processes

- a: $\gamma_{\text{cavity}} \rightleftharpoons \gamma_{\text{cavity}}$ (cavity detuning)
- b: $g + \gamma_{\text{pump}} \rightleftharpoons x$ (excitation)
- c: $x \rightleftharpoons m + \gamma_{\text{cavity}}$ (decay to metastable state)
- d: $\gamma_{\text{cavity}} + e \rightleftharpoons \emptyset$ (photodetection)
- e: $m + \gamma_{\text{reset}} \rightleftharpoons x$ (ion reset)

Only a, b, c are modelled explicitly by Keller et al..

But d, e can be modelled similarly.

Interaction picture model by Keller et al. (without reset and photodetection)

- $a =$ annihilator of cavity mode of photon
- $b = |g\rangle\langle x|$
- $c = |m\rangle\langle x|$
- Hamiltonian $H = \hbar(\delta a^* a + \Delta|g\rangle\langle g| + 2\,\mathrm{Re}(\Omega(t)b^* + \mu a c^*))$
- $\delta = \omega_{\text{cavity}} - \omega_{xm}$ cavity detuning

- $\Delta = \omega_{\text{pump}} - \omega_{gx}$ pump detuning
- $\Omega(t)$ classical pulse shape of pump laser
- μ (KELLER's g) ion–cavity coupling strength

- $\kappa = 0.02\,\Gamma_x$ cavity loss rate
- $\Gamma_x \approx 138$ MHz (KELLER's Γ_g) spontaneous decay rate into ground state
- $\Gamma_m \approx 11$ MHz spontaneous decay rate into metastable state

To account for losses, the dynamics of the density matrix is set up in the form of a

Lindblad master equation

$$\begin{aligned}\dot{\rho} \;\; = -\tfrac{i}{\hbar}[H,\rho] \;\; & +\kappa(2a\rho a^* - a^*a\rho - \rho a^*a) \\ & +\tfrac{\Gamma_x}{2}(2b\rho b^* - b^*b\rho - \rho b^*b) \\ & +\tfrac{\Gamma_m}{2}(2c\rho c^* - c^*c\rho - \rho c^*c)\end{aligned}$$

Note that the master equation is an equation for transition rates; probabilities are obtained by integration over time.

- time-dependent expectations $\langle f\rangle_t = \operatorname{tr} f\rho(t)$
- time dependent emission rate $p(t) = 2\kappa_{\text{tr}}\langle a^*a\rangle_t$ ($2\kappa_{\text{tr}}$ intensity transmission rate)
- probability of photon emerging from the cavity $\eta_{\text{photon}} = \int_0^\infty p(t)dt$
- single-photon efficiency $\eta_{\text{abs}} = (\kappa/\kappa_{\text{tr}} - 1)\eta_{\text{photon}}$

The Hilbert space on which the master equation is based is the tensor product of a single mode Fock space for the cavity photon and a 3-mode space for the Ca^+ ion.

An orthonormal basis of the space is given by the kets $|n,k\rangle$, where $n = 0,1,\ldots$ is the photon occupation number and $k \in \{g,x,m\}$ labels the ion level.

The structure of the Hamiltonian and the dissipation terms in the master equation is such that if the system is started in the ground state $|0,g\rangle$, it evolves to a mixed state in which the photon number is never larger than 1.

Thus multiphoton states do not contribute at all, and one can truncate the cavity photon Fock space to the two modes with occupation number $n = 0,1$, without changing the essence of the model.

Of interest for the photon production is the projection of the density matrix to the photon space, obtained by tracing over the ion degrees of freedom. This results in an effective time-dependent photon density matrix

$$\rho_{\text{photon}}(t) = \begin{pmatrix} \rho_{00}(t) & \rho_{01}(t) \\ \rho_{10}(t) & \rho_{11}(t) \end{pmatrix},$$

where $\rho_{11}(t) = p(t)$ is the probability density of finding a photon, $\rho_{00}(t)$ is the probability density of finding no photon, and $\rho_{01}(t) = \rho_{10}(t)^*$ measures the amount of entanglement between the 1-photon state and the vacuum state.

Semidefiniteness of the state requires $|\rho_{01}| \leq \sqrt{p(1-p)}$.

Assuming for simplicity that we have approximate equality, ρ_{photon} is essentially rank one, $\rho_{\text{photon}}(t) \approx \psi(t)\psi(t)^*, \quad \psi(t) = s(t)|0\rangle + c(t)|1\rangle$, where $s(t)$ and $c(t)$ are functions with $|s(t)|^2 + |c(t)|^2 = 1$, determined only up to a time-dependent phase factor. In particular, we may take $c(t)$ to be real and nonnegative.

Thus, in the approximation considered, the quantum electromagnetic field is in a superposition of the vacuum mode and the single-photon field mode, with a 1-photon amplitude $c(t) = \sqrt{p(t)}$ that varies with time and encodes the probability density $p(t)$ of detecting a photon particle.

In the actual experiments, $p(t)$ has a bell-shaped form, and the total photon detection probability, referred to as the **efficiency**, is significant, but smaller than 1.

Discarding the vacuum contribution corresponding to the dark, unexcited cavity, and giving up the interaction picture by inserting the field description $|1\rangle_t = e^{-i\omega t}\psi_0(\mathbf{x})$ of the photon mode, the (now time-dependent) 1-photon state takes the form $\mathbf{A}_{1\text{photon}}(\mathbf{x}, t) = \sqrt{p(t)}e^{-i\omega t}\psi_0(\mathbf{x})$.

(At this stage one notices a minor discrepancy with the field description, since the 1-photon state is no longer an exact solution of the Maxwell equations. To correct this deviation from Maxwell's equations, one has to work with quasi-monochromatic modes and the paraxial approximation.)

We now add the reset mechanism to get a continuous pulsed photon stream. Thus we consider a periodic sequence of excitation-reset cycles of the ion in the cavity. As before, we find that the electromagnetic field corresponding to the sequence of pulses is a single, periodically excited 1-photon mode of the electromagnetic field. Thus what appears at the photodetector as a **sequence** of photon particles arriving is from the perspective of quantum electrodynamics the manifestation of a **single** nonstationary, pulsed 1-photon state of the electromagnetic field!

2.14 Unitary representations of $SU(2)$

We call a set of linear operators L_0, L_1, L_2, L_3 on a Euclidean space $\mathbb{H}$ a **Pauli set** if L_0 is Hermitian positive definite and

$$[L_1, L_2] = 2iL_3, \quad [L_2, L_3] = 2iL_1, \quad [L_3, L_1] = 2iL_2, \tag{2.40}$$

$$(L_0 L_\mu)^* = L_0 L_\mu \quad \text{for } \mu = 1:3. \tag{2.41}$$

(In the infinite-dimensional case, we also require that L_0 and (2.41) are self-adjoint.) We say the Pauli set has **spin** j if

$$L_1^2 + L_2^2 + L_3^2 = 4j(j+1). \tag{2.42}$$

Definiteness of L_0 implies that the Hermitian inner product on $\mathbb{C}^s$ defined by

$$\overline{\phi}\psi := \phi^* L_0 \psi \quad \text{for } \phi, \psi \in \mathbb{C}^s \tag{2.43}$$

is positive definite, and

$$\overline{L_\mu \phi}\psi = \overline{\phi} L_\mu \psi \quad \text{for } \mu = 1, 2, 3. \tag{2.44}$$

We write

$$a \cdot L := a_1 L_1 + a_2 L_2 + a_3 L_3 \quad \text{for } a \in \mathbb{C}^3.$$

2.14.1 Proposition.
(i) Any Pauli set satisfies

$$[a \cdot L, b \cdot L] = 2i(a \times b) \cdot L \quad \text{for } a, b \in \mathbb{C}^3, \tag{2.45}$$

and hence defines a representation $\hat{X}$ of $so(3)$ by

$$\hat{X}(a) := a \cdot L/2i, \tag{2.46}$$

which is unitary in the inner product (2.43).

(ii) If $s \neq 1$ then $\mathbb{L} = \{a \cdot L \mid a \in \mathbb{C}^3\}$ is a Lie algebra isomorphic to $so(3)$.

(iii) $C := L_1^2 + L_2^2 + L_3^2$ is a Casimir operator of $\mathbb{L}$, i.e.,

$$[C, a \cdot L] = 0 \quad \text{for all } a \in \mathbb{R}^3. \tag{2.47}$$

(iv) For any Pauli set and an arbitrary rotation $Q = (e_1, e_2, e_3) \in SO(3)$, the $L'_k = e_k \cdot L$ form together with L_0 another Pauli set.

Proof. (i) (2.45) follows from

$$[a \cdot L, b \cdot L] = \sum_{\mu,\nu=1:3} a_\mu b_\nu [L_\mu, L_\nu] = \sum_{\mu<\nu} (a_\mu b_\nu - b_\mu a_\nu)[L_\mu, L_\nu] = 2i(a \times b) \cdot L,$$

and (iv) follows directly from (2.45).

(ii) (2.45) implies that $\mathbb{L}$ is closed under formation of commutators. Hence $\mathbb{L}$ is a Lie algebra. The isomorphism follows from Example (i) below.

(iii-iv) □

In contrast to (iv), the spin equation (2.42) is *not* preserved under general rotations.

2.14.2 Examples. The following examples all have $L_0 = 1$.

(i) On $\mathbb{C}^3$, a Pauli set of spin 1 is given by $a \cdot L = 2iX(a)$.

(ii) **(Angular momentum)** Let $J = q \times p$, where the components of position q and momentum p are the linear operators on $\mathbb{H} = C^\infty(\mathbb{R}^3)$ defined by

$$(p_\mu \psi)(x) = i\hbar \frac{\partial \psi(x)}{\partial x_\mu}, \quad (q_\mu \psi)(x) = x_\mu \psi(x) \quad \text{for } \mu = 1, 2, 3.$$

Then $L_\mu := 2J_\mu/\hbar$ for $\mu = 1, 2, 3$ defines a Pauli set on $\mathbb{H}$.

(iii) On any Euclidean space, a Pauli set of spin 0 is given by $L_1 = L_2 = L_3 = 0$.

(iv) A Pauli set of spin 1/2 on $\mathbb{C}^2$, exhibiting the isomorphism between the Lie algebras $u(3)$ and $so(3)$, is given by the **Pauli matrices**

$$s = 2, \quad L_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad L_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad L_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.48}$$

(iii) and (iv) from Example 2.14.2 are the first two cases of an infinite family of Pauli sets with arbitrary nonnegative half-integral spin:

2.14.3 Theorem. *The matrices $L_0, L_1, L_2, L_3 \in \mathbb{C}^{s \times s}$ defined by*

$$(L_1\psi)_k = (k-1)\psi_{k-1} + (s-k)\psi_{k+1},$$

$$(L_2\psi)_k = i(k-1)\psi_{k-1} - i(s-k)\psi_{k+1},$$

$$(L_3\psi)_k = (s+1-2k)\psi_k,$$

$$(L_0\psi)_k = \binom{s-1}{k-1}\psi_k$$

for $\psi \in \mathbb{C}^s$ form a Pauli set of spin $j = \frac{s-1}{2}$, called the **canonical Pauli set** *over $\mathbb{C}^s$. Written as matrices, the L_k and hence the $a \cdot L$ are tridiagonal, L_0 is diagonal, and the inner product* (2.43) *takes the form*

$$\overline{\phi}\psi = \sum_k \binom{s-1}{k-1} \phi_k^* \psi_k.$$

Proof. For $\mu = 1, 2$ we have

$$(L_\mu \psi)_k = \alpha_\mu(s-k)\psi_{k+1} + \beta_\mu(k-1)\psi_{k-1}, \tag{2.49}$$

where

$$\alpha_1 = \beta_1 = 1,\ \alpha_2 = -i,\ \beta_2 = i. \tag{2.50}$$

Therefore, for $\mu, \nu \in \{1, 2\}$,

$$\begin{aligned}(L_\mu L_\nu \psi)_k &= \alpha_\mu(s-k)(\alpha_\nu(s-k-1)\psi_{k+2} + \beta_\nu k\psi_k) \\ &\quad +\beta_\mu(k-1)(\alpha_\nu(s-k+1)\psi_k + \beta_\nu(k-2)\psi_{k-1}) \\ &= \alpha_\mu\alpha_\nu(s-k)(s-k-1)\psi_{k+2} + \beta_\mu\beta_\nu(k-1)(k-2)\psi_{k-2} \\ &\quad +(\alpha_\mu\beta_\nu k(s-k) + \alpha_\nu\beta_\mu(k-1)(s-k+1))\psi_k.\end{aligned} \tag{2.51}$$

Similarly,

$$(L_\mu L_3 \psi)_k = \alpha_\mu(s-k)(s-1-2k)\psi_{k+1} + \beta_\mu(k-1)(s+3-2k)\psi_{k-1}, \tag{2.52}$$

$$(L_3 L_\mu \psi)_k = (s+1-2k)\alpha_\mu(s-k)\psi_{k+1} + (s+1-2k)\beta_\mu(k-1)y_{k-1}, \tag{2.53}$$

Since $\alpha_1^2 + \alpha_2^2 = \beta_1^2 + \beta_2^2 = 0$, $\alpha_1\beta_1 + \alpha_2\beta_2 = 2$, (2.51) implies

$$((L_1^2 + L_2^2)\psi)_k = (2k(s-k) + 2(k-1)(s-k+1))\psi_k = (4k(s+1-k) - 2s - 2)\psi_k,$$

hence

$$((L_1^2 + L_2^2 + L_3^2)\psi)_k = (4k(s+1-k) - 2s - 2 + (s+1-2k)^2)\psi_k = (s^2-1)\psi_k,$$

giving (2.42). Taking differences in (2.51)–(2.53) gives

$$\begin{aligned}([L_1, L_2]\psi)_k &= (L_1L_2\psi)_k - (L_1L_2\psi)_k \\ &= (\alpha_1\beta_2 - \alpha_2\beta_1)(k(s-k) - (k-1)(s-k+1))\psi_k \\ &= 2i(s+1-2k)\psi_k = (2iL_3\psi)_k,\end{aligned}$$

$$([L_1, L_3]\psi)_k = -2\alpha_1(s-k)\psi_{k+1} + 2\beta_1(k-1)\psi_{k-1} = -(2iL_2\psi)_k,$$
$$([L_2, L_3]\psi)_k = -2\alpha_2(s-k)\psi_{k+1} + 2\beta_2(k-1)\psi_{k-1} = (2iL_1\psi)_k.$$

This gives the commutation relations (2.40). By writing the tridiagonal matrices out in full, using

$$(s-k)\binom{s-1}{k-1} = \frac{(s-1)!}{(k-1)!(s+1-k)!} = k\binom{s-1}{k},$$

(2.41) is easily verified. Since L_0 is positive definite, we have a Pauli set of spin j. □

Chapter 3

The symmetries of the universe

An understanding of the symmetries of the universe is necessary to be able to appreciate the modern concept of elementary particles.

The special orthogonal group $SO(3)$ of 3-dimensional rotations and the related special Euclidean group $ISO(3)$ of distance and orientation preserving affine mappings of 3-dimensional space are of exceptional importance in physics and mechanics. Indeed, the corresponding symmetries are inherent in many systems of interest and in the building blocks of most larger systems. The associated Lie algebra $so(3)$ of real, antisymmetric 3×3 matrices describes angular velocity and angular momentum, both in classical and in quantum mechanics; see Section 3.10. From a mathematical point of view, 3-dimensional rotations are also interesting due to the sporadic isomorphism between the Lie algebras $so(3)$ and $u(2)$ and the resulting isomorphism between $SO(3)$ and a quotient of $SU(2)$, see Section3.4.

3.1 Rotations and $SO(n)$

A matrix $U \in \mathbb{K}^{n\times n}$ is called **orthogonal** if $U^TU = 1$, equivalently, if U is invertible and $U^{-1} = U^T$. The set $O(n, \mathbb{K})$ of all orthogonal $n \times n$ matrices with entries in $\mathbb{K}$ is a matrix group, called a (full) **orthogonal group** over $\mathbb{K}$. Indeed, if $U, V \in O(n, \mathbb{K})$ then $(UV)^TUV = V^TU^TUV = V^TV = 1$ and $(U^{-1})^TU^{-1} = (U^T)^TU^{-1} = UU^{-1} = 1$, so that $UV, U^{-1} \in O(n, \mathbb{K})$. It is customary to write $O(n) := O(n, \mathbb{R})$. Note that $O(n)$ is a subgroup of $U(n)$. The orthogonal $n \times n$ matrices with determinant one form a matrix group $SO(n)$, called a **special orthogonal group**.

Every element $U \in O(n, \mathbb{K})$ satisfies $(\det U)^2 = detU^T \det U = \det(U^TU) = 1$, hence either $\det U = 1$ or $\det U = -1$. Therefore for odd n, we have $O(n, \mathbb{K}) = \{U, -U \mid U \in SO(n, \mathbb{K})$, and for any n, $O(n, \mathbb{K}) = \{U, MU \mid U \in SO(n, \mathbb{K})$, where M is the diagonal matrix with a $M_{nn} = -1$ and other diagonal entries one.

The elements of the special orthogonal group $SO(n)$ are called rotations. Thus, a **rotation**

is a real orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ with determinant one,

$$Q^TQ = QQ^T = 1, \quad \det Q = 1. \tag{3.1}$$

Since $|Qx|^2 = (Qx)^T(Qx) = x^TQ^TQx = x^Tx$ for $Q \in SO(n)$, rotations preserve the length $|x| = \sqrt{x^Tx}$ of a vector,

$$|Qx| = |x| \quad \text{for all } x \in \mathbb{R}^n.$$

Since $\det(QA) = \det Q \det A = \det A$ for $Q \in SO(n)$, rotations also preserve the orientation of volumes. Conversely, these condition together imply that $Q^TQ = 1$ and $\det Q = 1$, hence $Q \in SO(n)$. It can be shown that $SO(n)$ is a connected matrix group; hence every rotation is obtainable by a rotational motion. Since det is a continuous function of its entries and $\det 1 = 1$, $SO(n) = O(n)_0$ is the connected part of $O(n)$.

The natural metric for rotations is the **Frobenius distance**,

$$d(Q_1, Q_2) = \frac{1}{\sqrt{2n+2}}\|Q_1 - Q_2\|_F. \tag{3.2}$$

Here $\|A\|_F := \sqrt{A : A}$, where $A : B = \operatorname{tr} A^TB$ denotes the standard inner product between matrices, is the **Frobenius norm** of a matrix $A \in \mathbb{R}^{n\times n}$. (The reader is invited to check the triangle inequality $d(Q_1, Q_3) \le d(Q_1, Q_2) + d(Q_2, Q_3)$.)

3.1.1 Proposition. *The Frobenius distance has the invariance property*

$$d(Q_1, Q_2) = d(QQ_1, QQ_2) = d(Q_1Q, Q_2Q) \quad \text{if } Q \in SO(3), \tag{3.3}$$

and satisfies

$$d(Q_1, Q_2) = \frac{1}{2}\sqrt{n - Q_1 : Q_2} \in [0, 1]. \tag{3.4}$$

Proof. The inner product $A : B$ is orthogonal invariant,

$$QA : QB = \operatorname{tr}(QA)^TQB = \operatorname{tr} A^TQ^TQB = \operatorname{tr} A^TB = A : B,$$

$$AQ : BQ = \operatorname{tr}(AQ)^TBQ = \operatorname{tr} Q^TA^TBQ = \operatorname{tr} QQ^TA^TB = \operatorname{tr} A^TB = A : B.$$

Therefore $\|QA - QB\|_F^2 = Q(A - B) : Q(A - B) = (A - B) : (A - B) = \|A - B\|_F^2$ and $\|AQ - BQ\|_F^2 = (A - B)Q : (A - B)Q = (A - B) : (A - B) = \|A - B\|_F^2$, so that

$$\|QA - QB\|_F = \|A - B\|_F = \|AQ - BQ\|_F.$$

This implies (3.3). (3.4) follows from

$$\begin{aligned}
(2n+2)d(Q_1, Q_2)^2 &= \operatorname{tr}(Q_1 - Q_2)^T(Q_1 - Q_2) \\
&= \operatorname{tr} Q_1^TQ_1 - \operatorname{tr} Q_1^TQ_2 - \operatorname{tr} Q_2^TQ_1 + \operatorname{tr} Q_2^TQ_2 \\
&= 2\operatorname{tr} 1 - 2\operatorname{tr} Q_1^TQ_2 = 2n - 2Q_1 : Q_2 \\
&\le 2n + 2
\end{aligned}$$

by (3.24). □

A matrix $f \in \mathbb{K}^{n\times n}$ is called **antisymmetric** if $A^T = -A$. The set $o(n,\mathbb{K})o(n,\mathbb{K})$, orthogonal Lie algebra of all antisymmetric $n \times n$ matrices with entries in $\mathbb{K}$ is a matrix Lie algebra, called an **orthogonal Lie algebra** over $\mathbb{K}$. Indeed, if $f, g \in o(n,\mathbb{K})$ then $[f,g]^T = (fg-gf)^T = (g^T f^T - f^T g^T = (-g)(-f)-(-f)(-g) = -(fg-gf) = -[f,g]$, hence $[f,g] \in o(n,\mathbb{K})$. It is customary to write $o(n) := o(n,\mathbb{R})$. Note that $o(n)$ is a Lie subalgebra of $u(n)$. The antisymmetric $n \times n$ matrices with trace zero form a Lie algebra $so(n)$, called a **special orthogonal Lie algebra**. $so(n)$ is the Lie algebra of the matrix group $SO(n)$. Note that $so(n,\mathbb{K}) = o(n,\mathbb{K})$ since $f \in o(n,\mathbb{K})$ inplies $\operatorname{tr} f = \operatorname{tr} f^T = \operatorname{tr}(-f) = -\operatorname{tr} f$, hence the trace is automatically zero.

We briefly look at the smallest orthogonal groups and their Lie algebra. For $n = 1$, we have $O(1) = \{1, -1\}$, $SO(1) = \mathrm{Id}(1) = \{1\}$, and $o(1) = so(1) = \mathrm{id}(1) = \|0\}$.

For $n = 2$, the Lie algebra $o(2) = so(2)$ is 1-dimensional and consists of the antisymmetric 2×2 matrices

$$\begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix} = \alpha\mathbf{i},$$

where

$$\mathbf{i} := \begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix} \tag{3.5}$$

is the canonical generator. $SO(2)$ consists of the rotations

$$Q[\alpha] = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} = e^{\alpha\mathbf{i}} \tag{3.6}$$

the result of a uniform rotation $U(t) := e^{t\alpha\mathbf{i}}$ around zero by some angle α in counterclockwise direction. The product of rotations is a rotation by the sum of the angles,

$$Q[\alpha]Q[\beta] = Q[\alpha+\beta], \tag{3.7}$$

and the Frobenius distance of two rotations is a function of the difference of the angles,

$$d(Q[\alpha], Q[\beta]) = \sin(|\alpha-\beta|/2), \tag{3.8}$$

correctly taking account of the fact that angles differing by an integral multiple of 2π determine the same rotation. Note that $\mathbf{i}^2 = -1$, hence we may identify $\mathbf{i}$ with the imaginary unit i. This identification provides the isomorphisms $U(1) \cong SO(2)$ and $u(1) \cong so(2)$, reflecting the fact that the complex number plane is isomorphic to the 2-dimensional real plane.

The full orthogonal group $O(2)$ consists of the rotations and the matrices

$$R[\alpha] = \begin{pmatrix} \cos\alpha & \sin\alpha \\ \sin\alpha & -\cos\alpha \end{pmatrix} = R[0]e^{\alpha\mathbf{i}} \tag{3.9}$$

describing 2-dimensional **reflections** at the axis .

3.2 3-dimensional rotations and $SO(3)$

The general form of an antisymmetric 3×3 matrix is

$$X(\mathbf{a}) := \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix}, \quad a \in \mathbb{K}^3;$$

therefore

$$so(3, \mathbb{K}) = \{X(\mathbf{a}) \mid \mathbf{a} \in \mathbb{K}^3\}.$$

We note the rules

$$X(\mathbf{a})^T = -X(\mathbf{a}), \quad X(\mathbf{a})\mathbf{b} = \mathbf{a} \times \mathbf{b} = -X(\mathbf{b})\mathbf{a}, \quad X(\mathbf{a})\mathbf{a} = 0, \tag{3.10}$$

$$X(\mathbf{a} \times \mathbf{b}) = \mathbf{b}\mathbf{a}^T - \mathbf{a}\mathbf{b}^T, \tag{3.11}$$

$$X(\mathbf{a})X(\mathbf{b}) = \begin{pmatrix} -a_3b_3 - a_2b_2 & a_2b_1 & a_3b_1 \\ a_1b_2 & -a_3b_3 - a_1b_1 & a_3b_2 \\ a_1b_3 & a_2b_3 & -a_2b_2 - a_1b_1 \end{pmatrix} = \mathbf{b}\mathbf{a}^T - (\mathbf{a} \cdot \mathbf{b})1. \tag{3.12}$$

From (3.12) for $\mathbf{a} = \mathbf{b}$, we find by repeated multiplication with $X(\mathbf{a})$, using (3.10),

$$X(\mathbf{a})^2 = \mathbf{a}\mathbf{a}^T - \mathbf{a}^2 1, \quad X(\mathbf{a})^3 = -\mathbf{a}^2 X(\mathbf{a}), \quad X(\mathbf{a})^4 = -\mathbf{a}^2 X(\mathbf{a})^2; \tag{3.13}$$

and since $(1 - X(\mathbf{a}))((1 + \mathbf{a}^2)1 + X(\mathbf{a}) + X(\mathbf{a})^2) = (1 + \mathbf{a}^2)1$, we have

$$(1 - X(\mathbf{a}))^{-1} = 1 + (1 + \mathbf{a}^2)^{-1}(X(\mathbf{a}) + X(\mathbf{a})^2). \tag{3.14}$$

We use these relations for $\mathbb{K} = \mathbb{R}$ to prove the following explicit characterization of 3-dimensional rotations.

3.2.1 Theorem.
(i) For all $\mathbf{r} \in \mathbb{R}^3$ with $|\mathbf{r}| \leq 1$, the matrix

$$Q[\mathbf{r}] := 1 + 2\mathbf{r}_0 X(\mathbf{r}) + 2X(\mathbf{r})^2, \quad \text{where } \mathbf{r}_0 = \sqrt{1 - \mathbf{r}^2}, \tag{3.15}$$

is a rotation.

(ii) If $\mathbf{r} = 0$ then $Q[\mathbf{r}]$ is the identity; otherwise, $Q[\mathbf{r}]$ describes a rotation around the axis through the vector $\mathbf{r}$ by the angle

$$\alpha = 2 \arcsin |\mathbf{r}|, \tag{3.16}$$

and we have

$$Q\mathbf{r}\mathbf{r} = \mathbf{r}, \quad |\mathbf{r}| = \sin \frac{\alpha}{2}, \quad r_0 = \cos \frac{\alpha}{2} \geq 0. \tag{3.17}$$

(iii) Conversely, every rotation Q has the form $Q = Q[r]$ for some $\mathbf{r} \in \mathbb{R}^3$ with $\mathbf{r}^2 \leq 1$.

Proof. (i) Writing $X = X(\mathbf{r})$, $Q = Q[\mathbf{r}]$, we find from (3.13) that $X^4 = -\mathbf{r}^2 X^2 = (1-r_0^2)X^2$, hence

$$\begin{aligned} Q^T Q &= (1 - 2r_0 X + 2X^2)(1 + 2r_0 X + 2X^2) \\ &= 1 + (4 - 4r_0^2)X^2 + 4X^4 = 1. \end{aligned}$$

Thus $Q^{-1} = Q^T$, $QQ^T = QQ^{-1} = 1$. Since $(\det Q)^2 = \det Q \det Q^T = \det(QQ^T) = 1$, we have $\det Q[\mathbf{r}] = \pm 1$. Since the sign is positive for $\mathbf{r} = 0$, continuity of (3.15) implies that $\det Q[\mathbf{r}] = 1$ for all $\mathbf{r}$. Thus $Q[\mathbf{r}]$ is a rotation. Moreover,

$$X(Q + 1) = r_0(Q - 1), \tag{3.18}$$

since $(r_0 1 - X)Q = (r_0 1 - X)(1 + 2r_0 X + 2X^2) = r_0 1 + (2r_0^2 - 1)X^2 - 2X^3 = r_0 1 + X$.

(ii) The case $\mathbf{r} = 0$ is obvious; hence assume that $\mathbf{r} \neq 0$. Specializing the relation

$$\mathbf{a}^T Q[\mathbf{r}]\mathbf{b} = \mathbf{a} \cdot \mathbf{b} - 2(r_0(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{r} + (\mathbf{a} \times \mathbf{r}) \cdot (\mathbf{b} \times \mathbf{r})), \tag{3.19}$$

which follows using (3.10), to a unit vector $\mathbf{a}$ and $\mathbf{b} = \mathbf{a}$, we see that the angle α between a vector $\mathbf{a}$ and its rotated image $Q[\mathbf{r}]\mathbf{a}$ is $\cos\alpha = \mathbf{a}^T Q[\mathbf{r}]\mathbf{a} = 1 - 2|\mathbf{a} \times \mathbf{r}|^2$, hence

$$|\mathbf{a} \times \mathbf{r}| = \sqrt{(1 - \cos\alpha)/2} = \sin(\alpha/2). \tag{3.20}$$

In particular, a unit vector $\mathbf{a}$ orthogonal to $\mathbf{r}$ is rotated by the angle (3.16) since then $|\mathbf{a} \times \mathbf{r}| = |\mathbf{a}| \cdot |\mathbf{r}| = |\mathbf{r}|$. Since (3.10) implies $Q[\mathbf{r}]\mathbf{r} = \mathbf{r}$, the vector $\mathbf{r}$ is fixed by the rotation, and $Q[\mathbf{r}]$ describes a rotation around the vector $\mathbf{r}$ by the angle α given by (3.16).

(iii) Let Q be an arbitrary rotation.

Case 1. If $Q + 1$ is nonsingular, we define, motivated by (3.18),

$$\begin{aligned} \tilde{X} &:= (Q - 1)(Q + 1)^{-1} = (Q - Q^T Q)(Q + Q^T Q)^{-1} \\ &= (1 - Q^T)(1 + Q^T)^{-1} = -(1 - Q^T)^{-1}(Q^T - 1) = -\tilde{X}^T. \end{aligned}$$

Hence $\tilde{X}$ is antisymmetric, $\tilde{X} = X(\mathbf{a})$ for some $\mathbf{a}$. Now $\tilde{X}(Q + 1) = Q - 1$, hence we have $(1 - \tilde{X})Q = 1 + \tilde{X}$. Writing

$$r_0 := 1/\sqrt{1 + \mathbf{a}^2}, \quad \mathbf{r} := r_0 \mathbf{a},$$

we find from (3.14) and (3.13) that

$$\begin{aligned} Q &= (1 + r_0^2 \tilde{X} + r_0^2 \tilde{X})(1 + \tilde{X}) = 1 + (r_0^2 + 1 - r_0^2 \mathbf{a}^2)\tilde{X} + 2r_0^2 \tilde{X}^2 \\ &= 1 + 2r_0^2 X(\mathbf{a}) + 2r_0^2 X(\mathbf{a})^2 = 1 + 2r_0 X(\mathbf{r}) + 2X(\mathbf{r})^2. \end{aligned}$$

Since $1 - \mathbf{r}^2 = 1 - r_0^2 \mathbf{a}^2 = 1 - \mathbf{a}^2/(1 + \mathbf{a}^2) = 1/(1 + \mathbf{a}^2) = r_0^2 \geq 0$, we conclude that $Q = Q[\mathbf{r}]$.

Case 2. If $Q + 1$ is singular then -1 is an eigenvalue of Q. The other two eigenvalues must have product -1 since the determinant is the product of all eigenvalues, counted with their algebraic multiplicity. Since two complex conjugate eigenvalues have a positive product, this implies that the eigenvalues are all real. Any real eigenvalue λ has an associated real

eigenvector $\mathbf{x} \neq 0$ to with $Q\mathbf{x} = \lambda\mathbf{x}$, and $\mathbf{x}^2 = (Q\mathbf{x})^2 = \lambda^2\mathbf{x}^2$ implies $\lambda^2 = 1$, hence $\lambda = \pm 1$. Thus -1 is a double eigenvalue and $Q + 1$ has rank 1, $Q + 1 = \mathbf{r}\mathbf{s}^T$ with a unit vector $\mathbf{r}$. Now orthogonality implies $\mathbf{s} = 2\mathbf{r}$, giving $Q = -1 + 2\mathbf{r}\mathbf{r}^T = Q[\mathbf{r}]$, using (3.13). □

For angles $|\alpha| \leq \frac{\pi}{2}$ (corresponding to $\mathbf{r}^2 \leq \frac{1}{2} \leq r_0^2$), one may also use

$$\mathbf{q} = 2r_0\mathbf{r}, \qquad q_0 = \cos\alpha = 2r_0^2 - 1 = \sqrt{1 - \mathbf{q}^2}, \tag{3.21}$$

to rewrite $Q = Q[\mathbf{r}]$ as

$$Q = 1 + X(\mathbf{q}) + \frac{1}{1 + \mathbf{q}_0} X(q)^2 = (1 - \tfrac{1}{2}X(\mathbf{q}))^{-1}(1 + \tfrac{1}{2}X(\mathbf{q})), \tag{3.22}$$

which has nonlinearities only in the higher order term. Since 1 and $X(\mathbf{q})$ are symmetric, we see that

$$\mathbf{q} = \frac{1}{2}\begin{pmatrix} Q_{32} - Q_{23} \\ Q_{13} - Q_{31} \\ Q_{21} - Q_{12} \end{pmatrix} \tag{3.23}$$

is linear in the coefficients of Q. Therefore, (3.22) is referred to as the **linear parameterization**. From (3.31), one easily checks that $Q = Q[\mathbf{r}]$ satisfies

$$\operatorname{tr} Q = 4r_0^2 - 1 \geq -1. \tag{3.24}$$

Using also (3.23), we see that if $\operatorname{tr} Q > -1$ then $\mathbf{r}, r_0$ (and hence the rotation axis and angle) can be uniquely recovered from Q by

$$\mathbf{r} = \frac{\mathbf{q}}{\sqrt{1 + \operatorname{tr} Q}}, \qquad r_0 = \frac{1}{2}\sqrt{1 + \operatorname{tr} Q}. \tag{3.25}$$

And if $\operatorname{tr} Q = -1$ then $r_0 = 0$ (corresponding to a rotation by 180°) and $Q + 1$ has rank 1, hence $\mathbf{r}$ is one of the two unit vectors parallel to the columns of Q.

The exponential map. The Lie algebra $so(3)$ of all real, antisymmetric matrices consists of infinitesimal rotations, and the following result shows explicitly that every rotation can be written as a matrix exponential of an antisymmetric matrix. In particular, this implies that $SO(3)$ is connected.

3.2.2 Proposition. *If* $\mathbf{e}$ *is the unit vector in the direction of* $\mathbf{r}$ *(and an arbitrary unit vector if* $\mathbf{r} = 0$*) then, with* α *defined by* (3.16),

$$Q[\mathbf{r}] = e^{\alpha X(\mathbf{e})}. \tag{3.26}$$

Proof. Using the relations

$$\sin\alpha = 2\sin\frac{\alpha}{2}\cos\frac{\alpha}{2}, \qquad \cos\alpha = 1 - 2\sin^2\frac{\alpha}{2}, \qquad \mathbf{r} = \Big(\sin\frac{\alpha}{2}\Big)\mathbf{e},$$

we find

$$Q[\mathbf{r}] = 1 + (\sin\alpha)X(\mathbf{e}) + (1-\cos\alpha)X(\mathbf{e})^2 =: Q(\alpha). \tag{3.27}$$

Now $Q(0) = 1$ and

$$\frac{d}{d\alpha}Q(\alpha) = (\cos\alpha)X(\mathbf{e}) + (\sin\alpha)X(\mathbf{e})^2 = X(\mathbf{e})Q(\alpha),$$

using (3.13). Solving this differential equation gives (3.26). □

If we write (3.27) in terms of $\mathbf{a} = \alpha\mathbf{e}$, we conclude from (3.26) the **Rodrigues formula**

$$e^{X(\mathbf{a})} = 1 + \frac{\sin|\mathbf{a}|}{|\mathbf{a}|}X(\mathbf{a}) + \frac{1-\cos|\mathbf{a}|}{|\mathbf{a}|^2}X(\mathbf{a})^2 \quad \text{if } \mathbf{a} \neq 0 \tag{3.28}$$

for the exponential of a real, antisymmetric matrix. It describes a rotation along an axis parallel to $\mathbf{a}$ by an angle $\alpha = t|\mathbf{a}|$. The Rodrigues formula can also be obtained by writing the exponential as a power series and simplifying using (3.13). In particular, for small $\mathbf{a}$ we find $e^{X(\mathbf{a})} = 1 + X(\mathbf{a}) + O(|\mathbf{a}|^2)$ for small $\mathbf{a}$, showing explicitly that the $X(\mathbf{a}) \in so(3)$ are infinitesimal rotations.

As a useful application of the exponential form, we prove:

3.2.3 Proposition. *For any rotation Q,*

$$X(Q\mathbf{a}) = Q^T X(\mathbf{a})Q, \tag{3.29}$$

$$Q\mathbf{a} \times Q\mathbf{b} = Q(\mathbf{a}\times\mathbf{b}), \tag{3.30}$$

Proof. By differentiation, using (3.26). . □

3.3 Rotations and quaternions

In view of (3.15) and (3.13), we have

$$Q[\mathbf{r}] = 1 + 2\begin{pmatrix} -r_2^2 - r_3^2 & r_1r_2 - r_0r_3 & r_1r_3 + r_0r_2 \\ r_1r_2 + r_0r_3 & -r_1^2 - r_3^2 & r_2r_3 - r_0r_1 \\ r_1r_3 - r_0r_2 & r_2r_3 + r_0r_1 & -r_1^2 - r_2^2 \end{pmatrix}, \quad r_0 = \sqrt{1-|\mathbf{r}|^2}, \tag{3.31}$$

where 1 denotes the identity matrix and $\mathbf{r} \in \mathbb{R}^3$ satisfies $|\mathbf{r}| \leq 1$. Alternatively, we may write (3.31) in the homogeneous **quaternion parameterization**

$$Q[r_0, \mathbf{r}] = 1 + \frac{2}{r_0^2 + r_1^2 + r_2^2 + r_3^2}\begin{pmatrix} -r_2^2 - r_3^2 & r_1r_2 - r_0r_3 & r_1r_3 + r_0r_2 \\ r_1r_2 + r_0r_3 & -r_1^2 - r_3^2 & r_2r_3 - r_0r_1 \\ r_1r_3 - r_0r_2 & r_2r_3 + r_0r_1 & -r_1^2 - r_2^2 \end{pmatrix} \tag{3.32}$$

of rotations, with independent $r_0 \in \mathbb{R}$, $\mathbf{r} \in \mathbb{R}^3$, not both zero. $Q[r_0, \mathbf{r}]$ satisfies

$$Q[r_0, \mathbf{r}] = Q[\lambda r_0, \lambda \mathbf{r}] \quad \text{for all } \lambda \neq 0 \tag{3.33}$$

and reduces to $Q[\mathbf{r}]$ if the arbitrary scale is chosen such that $r_0^2 + r_1^2 + r_2^2 + r_3^2 = 1$ and $r_0 \geq 0$. Because of (3.33), parallel vectors $(r_0, \mathbf{r})$ in the quaternion parameterization give the same rotation. This shows that the 3-dimensional rotation group has the topology of a 3-dimensional projective space. (Note also that the linear parameterization (3.22) can be obtained from the homogeneous form (3.32) by choosing the arbitrary scale such that $r_0^2 + \mathbf{r}^2 = 2r_0$.)

In computational geometry, the quaternion parameterization of rotations is preferable to the frequently discussed (and more elementary) parameterization by Euler angles, since it does not need expensive trigonometric functions, its parameters have a geometric meaning independent of the coordinate system used, and it has significantly better interpolation properties (Shoemake [252], Ramamoorthi & Barr [226]). Note that the projective identification mentioned above has to be taken into account when constructing smooth motions joining two close rotations $Q[\mathbf{r}]$ with nearly opposite $\mathbf{r}$ of length close to 1.

Quaternions.

A **quaternion** is a 4×4 matrix of the form

$$U(r_0, \mathbf{r}) := \begin{pmatrix} r_0 & \mathbf{r}^T \\ -\mathbf{r} & r_0 1 + X(\mathbf{r}) \end{pmatrix}, \quad r_0 \in \mathbb{R},\ \mathbf{r} \in \mathbb{R}^3. \tag{3.34}$$

3.3.1 Theorem. *The set $\mathbb{Q}$ of quaternions is a* ***skew field****, i.e., an associative algebra in which every nonzero element has an inverse. We have*

$$U(r_0, \mathbf{r}) + U(s_0, \mathbf{s}) = U(r_0 + s_0, \mathbf{r} + \mathbf{s}), \tag{3.35}$$

$$\lambda U(r_0, \mathbf{r}) = U(\lambda r_0, \lambda \mathbf{r}), \tag{3.36}$$

$$U(r_0, \mathbf{r})^T = U(r_0, -\mathbf{r}), \tag{3.37}$$

$$U(r_0, \mathbf{r}) U(s_0, \mathbf{s}) = U(r_0 s_0 - r \cdot \mathbf{s},\ s_0 \mathbf{r} + r_0 \mathbf{s} + \mathbf{r} \times \mathbf{s}), \tag{3.38}$$

$$U(r_0, \mathbf{r})^{-1} = \frac{1}{r_0^2 + \mathbf{r}^2} U(r_0, -\mathbf{r}) \quad \text{if } r_0^2 + \mathbf{r}^2 \neq 0. \tag{3.39}$$

Proof. (3.35)–(3.37) are trivial, and (3.38) follows by direct computation, using (3.10), (3.12) and (3.11). Specializing (3.38) to $s_0 = r_0, \mathbf{s} = -\mathbf{r}$ gives

$$U(r_0, \mathbf{r}) U(r_0, -\mathbf{r}) = U(r_0^2 + \mathbf{r}^2, 0) = (r_0^2 + \mathbf{r}^2) 1, \tag{3.40}$$

which implies (3.39). Therefore $\mathbb{Q}$ is a vector space closed under multiplication, and every nonzero element in $\mathbb{Q}$ has an inverse. Since matrix multiplication is associative, $\mathbb{Q}$ is a skew field. □

In the standard treatment, quaternions are treated like complex numbers, as objects of the form

$$\mathbf{q}(r_0, \mathbf{r}) = r_0 1 + r_1 \mathbf{i} + r_2 \mathbf{j} + r_3 \mathbf{k}$$

with special unit quaternions $1, \mathbf{i}, \mathbf{j}, \mathbf{k}$. The correspondence is given by the identification

$$\mathbf{i} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{j} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \quad \mathbf{k} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \tag{3.41}$$

in terms of which $\mathbf{q}(r_0, \mathbf{r}) = U(r_0, \mathbf{r})$.

Identifying the imaginary unit i with the real 2×2 matrix (3.5), we expand to get the above real form:

$$\begin{aligned} r_0 + (r_1, r_2, -r_3)^T * \boldsymbol{\sigma} &= \begin{pmatrix} r_0 + ir_1 & r_2 + ir_3 \\ -r_2 + ir_3 & r_0 - ir_1 \end{pmatrix} \\ &= \begin{pmatrix} r_0 & r_1 & r_2 & r_3 \\ -r_1 & r_0 & -r_3 & r_2 \\ -r_2 & r_3 & r_0 & -r_1 \\ -r_3 & -r_2 & r_1 & r_0 \end{pmatrix} \\ &= r_0 + r_1 \mathbf{i} + r_2 \mathbf{j} + r_3 \mathbf{k}. \end{aligned}$$

3.4 Rotations and $SU(2)$

The isomorphism $su(2) \cong so(3)$. From (3.12) and (3.11), one finds immediately that

$$[X(\mathbf{a}), X(\mathbf{b})] = X(\mathbf{a} \times \mathbf{b}). \tag{3.42}$$

This implies that the spaces of real and complex antisymmetric matrices,

$$so(3) = \{X(\mathbf{a}) \mid \mathbf{a} \in \mathbb{R}^3\}, \quad so(3, \mathbb{C}) = \{X(\mathbf{a}) \mid \mathbf{a} \in \mathbb{C}^3\},$$

are closed under forming commutators, and hence form a Lie algebra. We shall see soon that the elements of $so(3)$ are infinitesimal rotations. Introducing

$$L_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad L_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad L_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

which form a basis of $so(3)$, we see that the correspondence $\frac{1}{2i}\sigma_k \mapsto L_k$ for $k = 1, 2, 3$ defines an isomorphism of Lie algebras.

Taking a closer look at $X(\mathbf{a})$ we see that there is a basis of $so(3)$ consisting of three elements J_i with $X(\mathbf{a}) = \sum_{i=1}^{3} \mathbf{a}_i J_i$, corresponding to infinitesimal rotations around the coordinate

axes. We assemble the three J's in a column vector and (ab-)use the notation $X(\mathbf{a}) = \mathbf{a}\cdot J$. Writing out $X(\mathbf{a})\angle X(\mathbf{a}') = X(\mathbf{a}\times\mathbf{a}')$ we get

$$J_k \angle J_l = \sum_m \epsilon_{klm} J_m \,, \tag{3.43}$$

with the Levi–Civitá symbol ϵ_{klm} defined in (2.20).

The group version. If g is an element of $SU(2)$ and $p \in su(2) \cong \mathbb{R}^3$ we see that

$$\mathrm{tr}(gpg^{-1}) = 0\,, \quad (gpg^{-1})^* = (g^{-1})^* p g^* = gpg^{-1}\,,$$

and we conclude that g induces a map $\mathbb{R}^3 \to \mathbb{R}^3$. Since

$$\mathrm{tr}(gpg^{-1}gqg^{-1}) = \mathrm{tr}(pq)\,,$$

the map induced by $g \in SU(2)$ defines an element of $O(3)$. But also $\mathbf{p}\times\mathbf{q}\cdot\mathbf{r}$ is invariant under the action of g and thus we found a map $R : SU(2) \to SO(3)$, whereby $g \in SU(2)$ gets mapped to the element $R(g)$ in $SO(3)$ corresponding to $p \mapsto gpg^{-1}$. The map $g \to R(g)$ is a group homomorphism; that is, $R(g_1 g_2) = R(g_1)R(g_2)$.

and hence the map $R : SU(2) \to SO(3)$ is surjective. Suppose now that $g(x, y)$ is mapped to the identity element in $SO(3)$. The kernel of $R : SU(2) \to SO(3)$ is easily checked to consist of $\{\pm 1\}$, which is the central $\mathbb{Z}_2$ subgroup of $SU(2)$. (Easy exercise: Prove that $\mathbb{Z}_2$ is the center of $SU(2)$.) As any kernel of group homomorphisms, the kernel is a normal subgroup. All in all we have shown

$$SO(3) \cong SU(2)/\mathbb{Z}_2\,.$$

3.5 Angular velocity

Quaternions are the most elegant way to derive a 3-dimensional analogue of the formulas (3.6) and (3.7) for 2-dimensional rotations in terms of rotation angles. The resulting product formula for 3-dimensional rotations, Theorem 3.5.1 in Section 3.5, allows us to derive the properties of angular velocity.

3.5.1 Theorem. ***(Product formula)***
Let $|\mathbf{r}|, |\mathbf{s}| \le 1$. *Then*

$$Q[\mathbf{r}]Q[\mathbf{s}] = Q[\mathbf{r}\oplus\mathbf{s}], \tag{3.44}$$

where with $r_0 = \sqrt{1-\mathbf{r}^2}$, $s_0 = \sqrt{1-\mathbf{s}^2}$, *and the sign chosen such that* $\pm(r_0 s_0 - \mathbf{r}\cdot\mathbf{s}) \ge 0$,

$$\mathbf{r}\oplus\mathbf{s} := \pm(s_0\mathbf{r} + r_0\mathbf{s} + \mathbf{r}\times\mathbf{s}). \tag{3.45}$$

Moreover,

$$Q[\mathbf{r}]^{-1} = Q[\mathbf{r}]^T = Q[-\mathbf{r}], \quad \mathbf{r}\oplus(-\mathbf{r}) = 0. \tag{3.46}$$

Note that $\oplus$ is not commutative!

Proof. Since $r_0^2 + \mathbf{r}^2 = s_0^2 + \mathbf{s}^2 = 1$, (3.39) implies that $U(r_0, \mathbf{r})$ and $U(s_0, \mathbf{s})$ are orthogonal 4×4 matrices. Writing

$$\mathbf{q} = \mathbf{r} \oplus \mathbf{s}, \;\; q_0 = |r_0 s_0 - \mathbf{r} \cdot \mathbf{s}|, \tag{3.47}$$

we may write (3.38) as

$$U(r_0, \mathbf{r}) U(s_0, \mathbf{s}) = U(q_0, \mathbf{q}), \tag{3.48}$$

hence $U(q_0, \mathbf{q})$ is also orthogonal, and (3.39) implies $q_0^2 + \mathbf{q}^2 = 1$, giving

$$(\mathbf{r} \oplus \mathbf{s})^2 \leq 1, \quad \sqrt{1 - (\mathbf{r} \oplus \mathbf{s})^2} = |r_0 s_0 - \mathbf{r} \cdot \mathbf{s}|. \tag{3.49}$$

Now

$$\begin{aligned} U(s_0, \mathbf{s}) U(0, \mathbf{x}) U(s_0, \mathbf{s})^T &= U(s_0, \mathbf{s}) U(0, \mathbf{x}) U_(s_0, -\mathbf{s}) = U(s_0, \mathbf{s}) U(\mathbf{s}^T \mathbf{x}, s_0 \mathbf{x} + X(\mathbf{s})\mathbf{x}) \\ &= U(0, s_0^2 \mathbf{x} + 2 s_0 X(\mathbf{s})\mathbf{x} + \mathbf{s}\mathbf{s}^T \mathbf{x} + X(\mathbf{s})^2 \mathbf{x}), \end{aligned}$$

hence

$$U(s_0, \mathbf{s}) U(0, \mathbf{x}) U(s_0, \mathbf{s})^T = U(0, Q[\mathbf{s}]\mathbf{x}). \tag{3.50}$$

Multiplication by $U(r_0, \mathbf{r})$ on the left and by $U(r_0, \mathbf{r})^T$ on the right gives, using (3.48),

$$U(q_0, \mathbf{q}) U(0, \mathbf{x}) U(q_0, \mathbf{q})^T = U(0, Q[\mathbf{r}] Q[\mathbf{s}]\mathbf{x}). \tag{3.51}$$

On the other hand

$$U(q_0, \mathbf{q}) U(0, \mathbf{x}) U(q_0, \mathbf{q})^T = U(q_0, \mathbf{q}) U(0, \mathbf{x}) U(q_0, \mathbf{q})^T = U(0, Q[\mathbf{q}]\mathbf{x}),$$

and comparing this with (3.51) implies (3.44). Finally, (3.46) is immediate. □

Computationally, (3.47) is numerically stable in finite precision arithmetic, while the direct formula $q_0 = \sqrt{1 - \mathbf{q}^2}$ suffers from loss of accuracy if q_0 is tiny, due to cancellation of leading digits.

Differentiation of the product formula gives a useful formula for the derivative of a rotation.

3.5.2 Theorem. ***(Differentiation formula)***
If $\mathbf{r}$ *is a function of* t *then*

$$\frac{d}{dt} Q[\mathbf{r}] = X(\boldsymbol{\omega}) Q[\mathbf{r}], \quad \boldsymbol{\omega} = 2(\mathbf{r} \times \dot{\mathbf{r}} + r_0 \dot{\mathbf{r}} - \dot{\mathbf{r}}_0 \mathbf{r}), \tag{3.52}$$

and we have

$$\dot{\mathbf{r}} = \frac{1}{2}(r_0 \boldsymbol{\omega} - \mathbf{r} \times \boldsymbol{\omega}), \quad \dot{r}_0 = \frac{1}{2} \mathbf{r} \cdot \boldsymbol{\omega}. \tag{3.53}$$

Proof. Writing

$$\mathbf{r} = \mathbf{r}(t), \quad \tilde{\mathbf{r}} = \mathbf{r}(t + h) = \mathbf{r} + h\dot{\mathbf{r}} + O(h^2),$$

we have

$$\begin{aligned} Q[\tilde{\mathbf{r}}]Q[-\mathbf{r}] &= Q[\tilde{\mathbf{r}} \oplus (-\mathbf{r})] = Q[-\tilde{r}_0\mathbf{r} + r_0\tilde{\mathbf{r}} - \tilde{\mathbf{r}} \times \mathbf{r}] \\ &= Q[-(r_0 + h\dot{r}_0)\mathbf{r} + r_0(\mathbf{r} + h\dot{\mathbf{r}}) - (\mathbf{r} + h\dot{\mathbf{r}}) \times \mathbf{r} + O(h^2)] \\ &= Q[h(\mathbf{r} \times \dot{\mathbf{r}} + r_0\dot{\mathbf{r}} - \dot{r}_0\mathbf{r})] + O(h^2) \\ &= 1 + hX(\boldsymbol{\omega}) + O(h^2). \end{aligned}$$

Multiplication by $Q[\mathbf{r}]$ gives

$$\begin{aligned} Q[\mathbf{r}(t+h)] &= Q[\tilde{\mathbf{r}}] = (1 + hX(\boldsymbol{\omega}) + O(h^2))Q[\mathbf{r}] \\ &= Q[\mathbf{r}] + hX(\boldsymbol{\omega})Q[\mathbf{r}] + O(h^2), \end{aligned}$$

and (3.52) follows. Now

$$2r_0\dot{r}_0 = (r_0^2)^\bullet = (1 - \mathbf{r}^2)^\bullet = -2\mathbf{r}^T\dot{\mathbf{r}}, \tag{3.54}$$

hence

$$\begin{aligned} \mathbf{r} \times \boldsymbol{\omega} &= 2(\mathbf{r} \times (\mathbf{r} \times \dot{\mathbf{r}}) + r_0\mathbf{r} \times \dot{\mathbf{r}}) \\ &= 2(\mathbf{r}\mathbf{r}^T\dot{\mathbf{r}} - \mathbf{r}^2\dot{\mathbf{r}} + r_0\mathbf{r} \times \dot{\mathbf{r}}) = r_0\boldsymbol{\omega} - 2\dot{\mathbf{r}}, \end{aligned}$$

giving $\dot{\mathbf{r}} = \frac{1}{2}(r_0\boldsymbol{\omega} - \mathbf{r} \times \boldsymbol{\omega})$. Multiplication by $\mathbf{r}^T$ gives $\mathbf{r}^T\dot{\mathbf{r}} = \frac{1}{2}r_0\boldsymbol{\omega}$, and the formula for $\dot{r}_0$ follows from (3.54) if $r_0 \neq 0$. For $r_0 = 0$, the formula follows by continuity. □

3.5.3 Proposition. *In the quaternion parameterization, we have*

$$d(Q[\mathbf{r}], Q[\mathbf{s}]) = |(-\mathbf{r}) \oplus \mathbf{s}| = \sqrt{1 - (r_0s_0 + \mathbf{r} \cdot \mathbf{s})^2}. \tag{3.55}$$

Proof. Since

$$\operatorname{tr} Q[\mathbf{r}]^T Q[\mathbf{s}] = \operatorname{tr} Q[-\mathbf{r}]Q[\mathbf{s}] = \operatorname{tr} Q[(-\mathbf{r}) \oplus \mathbf{s}] = 4((-\mathbf{r}) \oplus \mathbf{s})_0^2 - 1 = 3 - 4((-\mathbf{r}) \oplus \mathbf{s})^2$$

by (3.24), (3.55) follows from (3.4) and (3.47). □

3.6 Rigid motions and Euclidean groups

Translations $_(n) = T(\mathrm{Id}(1), \mathrm{id}(n))$ and $\exp \begin{pmatrix} 0 & 0 \\ ; x & 1_n \end{pmatrix}$

This motivates a more general triangular construction for Lie groups $T(\mathbb{G}_1, \ldots, \mathbb{G}_m)$ and Lie algebras $t(\mathbb{L}_1, \ldots, \mathbb{L}_m)$, which will later also produce the Galilean group and the Poincare group. $T(n) = T(\mathbb{R}, \ldots, \mathbb{R})$

$D(\mathbb{G}_1, \ldots, \mathbb{G}_m)$ diagonal, direct produt, $D(n)$. and corresponding Lie algebras.

$ISO(n)$ as subgroup of $L(n+1,\mathbb{R})$, and their Lie algebra

The **Euclidean group** or **inhomogeneous special orthogonal group** $ISO(n)$ consists of all distance preserving affine mappings

$$x \in \mathbb{R}^n \to x' = Qx + c \in \mathbb{R}^n,$$

with $Q \in SO(n)$ and $c \in \mathbb{R}^n$. In homogeneous coordinates,

$$\begin{pmatrix} x' \\ 1 \end{pmatrix} = \begin{pmatrix} Q & c \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ 1 \end{pmatrix},$$

hence we can write $ISO(n)$ as a matrix group,

$$ISO(n) = \left\{ \begin{pmatrix} Q & c \\ 0 & 1 \end{pmatrix} \middle| \, Q \in SO(n), \quad c \in \mathbb{R}^n \right\}.$$

In the special case special case $n = 3$, the corresponding Lie algebra of infinitesimal generators is the Lie algebra

$$iso(3) = \left\{ \begin{pmatrix} X(\omega) & v \\ 0 & 0 \end{pmatrix} \middle| \, \omega, v \in \mathbb{R}^3 \right\},$$

parameterizing one-parameter families of Euclidean motions defined by the differential equation

$$\dot{x}(t) = X(\omega(t))x(t) + v(t),$$

or short

$$\dot{x} = \omega \times x + v.$$

If we write

$$\hat{X}(a) = \begin{pmatrix} X(a) & 0 \\ 0 & 0 \end{pmatrix}, \quad b \cdot p = \begin{pmatrix} 0 & b \\ 0 & 0 \end{pmatrix}. \tag{3.56}$$

the commutator relations of $iso(3)$ can be compactly written as

$$[\hat{X}(a), \hat{X}(b)] = \hat{X}(a \times b) \quad \text{for } a, b \in \mathbb{R}^3, \tag{3.57}$$

$$[\hat{X}(a), b \cdot p] = (a \times b) \cdot p \quad \text{for } a, b \in \mathbb{R}^3, \tag{3.58}$$

$$[a \cdot p, b \cdot p] = 0 \quad \text{for } a, b \in \mathbb{R}^3. \tag{3.59}$$

Spinors, vectors, tensors in Lie algebras containing a distinguished $so(3)$.

Levi-Malcev theorem (Kirillov p.91, Barut & Raczka p.19)

A maximal chain of ideals

$$\mathbb{L} = \mathbb{L}_0 \supseteq \mathbb{L}_1 \supseteq \ldots \supseteq \mathbb{L}_s$$

with $\mathbb{L}_{k-1} \angle \mathbb{L}_k \subseteq \mathbb{L}_k$ should give the triangular structure; cf. Lie's theorem. Is this related to Ado's theorem?

3.7 Connected subgroups of $SL(2,\mathbb{R})$

$SL(2,\mathbb{R})$ is a matrix group of dimension 3. Up to conjugacy , proper connected subgroups of are:
For $d=1$: $ISO(1)$, $O(2)$, $O(1,1)$, $SD(2)=\left\{\begin{pmatrix} t & 0 \\ 0\&t^{-1} & \end{pmatrix}\right\}$,
for $d=2$ apparently only $ST(2)=\left\{\begin{pmatrix} t & 0 \\ s\&t^{-1} & \end{pmatrix}\right\}$,
Is this list complete, irredundant?

$SL(2,\mathbb{R})$ is an example of a connected matrix group in which not every element can be written as an exponential of an element of its Lie algebra. Indeed, any $f\in sl(2,\mathbb{R})$ has trace zero, hence its eigenvalues are $\pm\lambda$ for some $\lambda\in\mathbb{C}$. The eigenvalues of e^f are therefore $e^{\pm\lambda}$, and $\operatorname{tr} e^f = e^\lambda + e^{-\lambda}$. Since the product of the eigenvalues is the real determinant, λ is either real or purely imaginary. In the first case, $\operatorname{tr} e^f \geq 0$, while in the second case, $\lambda = i\omega$ and $\operatorname{tr} e^f = e^{i\omega}+e^{-i\omega} = 2\cos\omega \geq -2$. Since the element $\begin{pmatrix} -2 & 0 \\ 0 & -1/2 \end{pmatrix} \in sl(2,\mathbb{R})$ has trace < -2, it cannot be written as e^f with $f\in sl(2,\mathbb{R})$.

3.8 Connected subgroups of $SL(3,\mathbb{R})$

$SL(3,\mathbb{R})$ is a matrix group of dimension 6. Up to conjugacy, proper connected subgroups of dimension $0<d<6$ are $ISO(2)$, $O(3)$, $O(1,2)$, $H(1)$. Is this list complete?

3.9 Classical mechanics and Heisenberg groups

$H(n)$ and its Lie algebra; CCR script p.37f

Poisson representations script p.4-7

units p.29-30

restricted direct sum

The oscillator group $Os(n)$

The Schrödinger group?

3.10 Angular momentum, isospin, quarks

Angular momentum, commutation relations

$SU(n)$ for n flavors, and their Lie algebra

Isospin ($n = 2$), quarks ($uds\ldots$)

Structure hints from the mass spectrum of elementary particles

Standard model gauge group: $S(U(2) \times U(3))$

The local symmetry group of the universe: $ISO(1,3) \times S(U(2) \times U(3))$

3.11 Connected subgroups of $SL(4,\mathbb{R})$

$SL(4,\mathbb{R})$ is a matrix group of dimension 15. Up to conjugacy, the connected subgroups of dimension $d = 10$ are:

$ISO(3)$ (homogeneous Galilei transformations)

$O(4)$; $SO(4) \cong SO(3) \times SO(3)$ (hydrogen)

$O(1,3)$ (Lorentz group)

$O(2,2)$ (no physical relevance)

Find the symmetry group of a Lorentz cone (also needed for completely positive maps)

Other dimensions?

3.12 The Galilean group

script p.24-26,28-30,34f

Galilean spacetime. Until the beginning of the twentieth century, one thought that time for all observers was the same in the following sense: if two events take place at two different places in space, then the question whether the events took place at the same time has an observer independent answer. Space was thought of as a grid on which the motions of all objects took place and time was thought to be completely independent from space. The 'distance' between two events therefore consisted of two numbers: a difference in time and a spatial distance. For example, the distance between when I woke up and when I took the subway to work is characterized by saying that from the moment I woke up it took me half an hour to reach the subway station, which is 500 meter from my bed. We call the spacetime described in this manner the **Galilean spacetime**.

There are three important kinds of symmetries in the Galilean spacetime and the group

that these symmetries generate is called the **Galilean symmetry group**[1]. If we shift the clock an hour globally, which is possible in Galilean spacetime, the laws of nature cannot alter. Hence one symmetry generator is the time-shift: $t \mapsto t + a$ for some fixed number a. Likewise, the laws of nature should not change if we shift the origin of our coordinate system; hence a second symmetry is the shift symmetry $(x^1, x^2, x^3) \mapsto (x^1+b^1, x^2+b^2, x^3+b^3)$ for some fixed vector (b^1, b^2, b^3). The third kind of symmetries are rotations, that is, the group $SO(3)$, which we have seen before. There are some additional discrete symmetries, like space reflection, where a vector (x^1, x^2, x^3) is mapped to $(-x^1, -x^2, -x^3)$. We focus, however, on the connected part of the Galilean symmetry group. The subgroup of the Galilean symmetry group obtained by discarding the time translations is the group $ISO(3)$. Below, when we discuss the Poincaré group, we give more details on the group $ISO(3)$ as it is a subgroup of the Poincaré group.

3.13 The Lorentz groups $O(1,3)$, $SO(1,3)$, $SO(1,3)_0$

script p.30-33

When $\mathbb{K} = \mathbb{R}$, one has for symmetric bilinear forms another subdivision, since B can have a definite signature (p, q) where $p + q$ is the dimension of V. If B is of signature (p, q), this means that there exists a basis of V in which B can be represented as

$$B(v, w) = v^T A w\,, \quad \text{where} \quad A = \mathrm{diag}(\underbrace{-1, \ldots, -1}_{p \text{ times}}, \underbrace{1, \ldots, 1}_{q \text{ times}})\,.$$

The group of all linear transformations that leaves B invariant is denoted by $O(p, q)$. The subgroup of $O(p, q)$ of transformations with determinant one is the so-called **special orthogonal group** and is denoted by $SO(p, q)$. The associated real Lie algebra is denoted $so(p, q)$ and its elements are linear transformations $A : V \to V$ such that for all $v, w \in V$ we have $B(Av, w) + B(v, Aw) = 0$. The Lie product is given by the commutator of matrices.

More general, the standard representation of $so(p, q)$ is the one that defines $so(p, q)$ and is thus given by $(p + q) \times (p + q)$-matrices that leave a metric of signature (p, q) invariant; in Lie algebra theory the standard representation is called the **fundamental representation**. In the fundamental representation of $so(3, 1)$ (which is not unitary), the Minkowski inner product is invariant.

The group $SO(3)$ is a subgroup of $SO(3, 1)$ and consists of all those $SO(3, 1)$-rotations that act trivially on the time-component of four-vectors. The Galilean symmetry group is the subgroup of $ISO(3, 1)$ consisting of the $SO(3)$-rotations together with the time translations.

An element of $SO(3, 1)$ is called a Lorentz boost if the element acts nontrivially on the zeroth component of four-vectors. By multiplying with an appropriate element of the $SO(3)$

[1]The group is also called the **Galilei group** or the **Galileo group**. We follow the tradition that proceeds in analogy with the use of Euclidean space or Hermitian matrix.

subgroup we may assume that a Lorentz boost only mixes the zeroth and first component of four-vectors. Then a Lorentz boost L takes the following form (recall $c = 1$):

$$L(v)^0 = \frac{x^0 - vx^1}{\sqrt{1-v^2}}\,, \quad L(v)^1 = \frac{x^1 - vx^0}{\sqrt{1-v^2}}\,, \tag{3.60}$$

and $L(v)^2 = v^2$, $L(v)^3 = v^3$. Physically the Lorentz boost (3.60) describes how coordinates transform when one goes from one coordinate system to another coordinate system that moves with respect to the first system in the positive x^1-direction with velocity v. Since v has to be smaller than one, as is apparent from (3.60), one concludes that special relativity excludes superluminal velocities. The number

$$\gamma = \frac{1}{\sqrt{1-v^2}}\,, \tag{3.61}$$

is called the **γ-factor**. The γ-factor gives an indication whether we should treat a physical situation with special relativity or whether a nonrelativistic treatment would suffice. The **Lorentz contraction** factor is the inverse of γ and measures how distances shrink when measured in another coordinate system, moving at a velocity v with respect to the original coordinate system. For α-particles, moving with a typical speed of 15,000 kilometers per second, we have $v = 0.05$ and so $\gamma \sim 1.03$ and $\gamma^{-1} \sim 0.97$, which implies that if we take a rod of 100 meter and let an α-particle fly along the rod, it measures only $97m$ (assuming that α-particles can measure). The γ-factor thus tells us that if we want accuracy of more than 3%, we need to treat the α-particle relativistically.

The nonrelativistic limit. In order to discuss the nonrelativistic limit, we restore the presence of the velocity of light c in the formulas. For a particle at rest, the space momentum $\mathbf{p}$ vanishes. The formula $p^2 = -(mc)^2$ therefore implies that, at rest, $p_0 = mc$ and the **rest energy** is seen to be $E = mc^2$. This suggests to define the **kinetic energy** (which vanishes at rest) by the formula

$$H := p_0 c - mc^2.$$

Introducing **velocity** $\mathbf{v}$ and **speed** v by

$$\mathbf{v} = \mathbf{p}/m, \quad v = |\mathbf{v}| = \sqrt{\mathbf{v}^2},$$

we find from $\mathbf{p}^2 - p_0^2 = -(mc)^2$ that $p_0 = \sqrt{(mc)^2 + \mathbf{p}^2} = mc\sqrt{1 + (v/c)^2}$, so that

$$H = mc^2(\sqrt{1+(v/c)^2} - 1) = mc^2 \frac{1 + (v/c)^2 - 1}{\sqrt{1+(v/c)^2} + 1} = \frac{mv^2}{\sqrt{1+(v/c)^2} + 1}\,.$$

Similarly, the energy becomes

$$E = p_0 c = \frac{mc^2}{\sqrt{1-(v/c)^2}}\,.$$

Taking the limit $c \to \infty$ we find that H becomes the kinetic energy $\frac{1}{2}mv^2$ of a nonrelativistic particle of mass m, The **nonrelativistic approximation** $H \approx \frac{1}{2}mv^2$ for the kinetic energy

is valid for small velocities $v = |\mathbf{p}/m| \ll c$, where we may neglect the term $(v/c)^2$ in the square root of the denominator.

Lorentz group as $SL(2,\mathbb{C})$. We mention some further properties of spin coherent states. Because of the identity

$$|-x,s\rangle = (-1)^{2s}|x,s\rangle$$

fermionic representations ($s \notin \mathbb{Z}$) are called **chiral**. Since fermions are chiral, they are not invariant under the $\mathbb{Z}_2$-subgroup of $SL(2,\mathbb{C})$ and thus fermions do not constitute a representation of the restricted Lorentz group.

We use the notation introduced in Section 2.11 and identify four-vectors $p \in \mathbb{R}^{1,3}$ with the 2×2-matrices $p\cdot\sigma_+$. For any four-vector $p \in \mathbb{R}^{1,3}$ the Minkowski norm is given by

$$\det(p\cdot\sigma_+) = p\cdot p\,.$$

The group $SL(2,\mathbb{C})$ acts on $\mathbb{R}^{1,3}$ through

$$A(p\cdot\sigma_+)A^*\,, \quad \text{for} \quad A \in SL(2,\mathbb{C})\,.$$

Clearly this defines for each $A \in SL(2,\mathbb{C})$ an element of $SO(3,1)$, and hence we have a map $SL(2,\mathbb{C}) \to SO(3,1)$. The group $SL(2,\mathbb{C})$ is a real connected manifold of dimension 6. Indeed, any complex 2×2 matrix has 4 complex entries making 8 real numbers. The constraint $\det A = 1$ gives two equations, for the real and imaginary part, and hence removing two dimensions.

Let us show that $SL(2,\mathbb{C})$ is connected. For $A \in SL(2,\mathbb{C})$ we can apply the Gram–Schmidt proces to the column vectors of A. Looking at how the Gram–Schmidt procedure works, we see that any element of $A \in SL(2,\mathbb{C})$ can be written as a product of an upper triangular matrix N with positive entries on the diagonal and a unitary matrix $U \in U(2)$. We can write $U = e^{i\phi}U'$ with $U' \in SU(2)$ making clear that $U(2) \cong S^2 \times S^1$ so that $U(2)$ is connected and the matrix U can be smoothly connected to the identity. For N we may write

$$N = \begin{pmatrix} a & b \\ 0 & c \end{pmatrix}$$

with $ac = 1$ and $a > 0$ and $c > 0$. Then $t \mapsto tN + (1-t)1_{2\times 2}$ is a smooth path in $L(2,\mathbb{C})$ for $t \in [0,1]$ that connects the unit matrix to N. Dividing by the square root of the determinant gives the required path in $SL(2,\mathbb{C})$. Hence $SL(2,\mathbb{C})$ is connected.

The map $SL(2,\mathbb{C}) \to SO(3,1)$ is a smooth group homomorphism and thus any two points in the image can be joined by a smooth path. Hence the image is a connected subgroup of $SO(3,1)$. Since the dimensions of $SO(3,1)$ and $SL(2,\mathbb{C})$ are the same, the image contains an open connected neighborhood O of the identity (this is nothing more than the statement that the induced map $sl(2,\mathbb{C}) \to so(3,1)$ is an isomorphism). But the subgroup of $SO(3,1)$ generated by a small open neighborhood of the identity is the connected component containing the identity. Indeed, call G' the group generated by the open neighborhood O. We may assume $O^{-1} := \{g^{-1}, g \in O\} = O$, since if not we just replace O by $O \cap O^{-1}$. If $x \in G'$

then $xO \subset G'$ is an open neighborhood containing x so that G' is open. If $x \notin G'$, then $xO \cap G' = \emptyset$, since if $y \in xO \cap G'$, then there is $z \in O$ such that $xz = y$, but then $x = yz^{-1}$ lies in G'. Hence G' is an open and closed subgroup of the component that contains the identity, but then G' is the component that contains the identity.

Hence the map $SL(2,\mathbf{C}) \to SO(3,1)_0$ is surjective and we only have to check the kernel. An element A is in the kernel if and only if $Ap \cdot \sigma_+ A^* = p \cdot \sigma_+$ for all $p \in \mathbb{R}^{1,3}$. This is a linear equation in p so we may as well take $p \in \mathbb{C}^{1,3}$. Choosing $p \cdot \sigma_+ = \sigma_1 + i\sigma_2$ and writing

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

we find $a\bar{b} = 0$, $a\bar{d} = 1$ and $|c| = 0$. Hence $b = c = 0$ and $a\bar{d} = 1$. But since $\det A = 1$ we have $ad = 1$ so that $a^2 = 1$ giving $a = \pm 1$. The kernel is therefore the normal subgroup $\mathbb{Z}_2 = \{1, -1\}$.

3.14 The Poincare group $ISO(1,3)$

The group of all translations in V generates together with $SO(p,q)$ the group of **inhomogeneous special orthogonal transformations**, which is denoted $ISO(p,q)$. One can obtain $ISO(p,q)$ from $SO(p,q+1)$ by performing a contraction; that is, by rescaling some generators with some parameter ϵ and then choosing a singular limit $\epsilon \to 0$ or $\epsilon \to \infty$. The group $ISO(p,q)$ can also be seen as the group of $(p+q+1) \times (p+q+1)$-matrices of the form

$$\begin{pmatrix} Q & b \\ 0 & 1 \end{pmatrix} \quad \text{with} \quad Q \in SO(p,q)\,,\ b \in V\,.$$

The Lie algebra of $ISO(p,q)$ is denoted $iso(p,q)$ and can be described as the Lie algebra of $(p+q+1) \times (p+q+1)$-matrices of the form

$$\begin{pmatrix} A & b \\ 0 & 0 \end{pmatrix} \quad \text{with} \quad A \in so(p,q)\,,\ b \in V\,.$$

Again, the Lie product in $iso(p,q)$ is the commutator of matrices.

Minkowski spacetime. With the advent of special relativity, the classical spacetime view was altered in the sense that time and space made up one spacetime, called **Minkowski spacetime**. As a topological vector space Minkowski spacetime is nothing more than $\mathbb{R}^4$, but it is equipped with the **Minkowski metric**[2] (also see Section 5.6 and Example 11.4.5):

$$(x-y)^2 = -(x^0-y^0)^2 + (x^1-y^1)^2 + (x^2-y^2)^2 + (x^3-y^3)^2 = (\mathbf{x}-\mathbf{y})^2 - (x^0-y^0)^2.$$

The time component of the **four-vectors** is the zeroth component. We write a general four-vector as

$$v = \begin{pmatrix} v^0 \\ \mathbf{v} \end{pmatrix}, \quad \mathbf{v} = \begin{pmatrix} v^1 \\ v^2 \\ v^3 \end{pmatrix},$$

[2]We choose units such that $c = 1$, and work with the signature $(-,+,+,+)$.

where $\mathbf{v}$ is the space-like part of v and v^0 is the time-like component of v. With the notation introduced we see that the Minkowski metric can be written as $v^2 = -(v^0)^2 + \mathbf{v}^2$, where $\mathbf{v}^2$ is the usual Euclidean norm for three-vectors. The Minkowski inner product is derived from the Minkowski metric and given by

$$\begin{pmatrix} v^0 \\ \mathbf{v} \end{pmatrix} \begin{pmatrix} w^0 \\ \mathbf{w} \end{pmatrix} = -v^0 w^0 + \mathbf{v}\mathbf{w}\,.$$

Note that in a strict sense the Minkowski inner product, the Minkowski norm and the Minkowski metric are not an inner product, norm and metric respectively as the positivity condition is clearly not satisfied.

The **Poincaré group** is a subgroup of the group of all symmetries that leave the Minkowski metric invariant. The Poincaré group is often denoted as $ISO(3,1)$. On a four-vector v the Poincaré group acts as $v \mapsto Av + b$, where A is an element of $SO(3,1)$ and b is some four-vector. Hence the Poincaré group consists of rotations and translations. An explicit representation of $ISO(3,1)$ can be given in terms of the matrices

$$\begin{pmatrix} A & b \\ 0 & 1 \end{pmatrix},$$

where A is a 4×4-matrix in $SO(3,1)$ and b is a four-vector. Recall that A is in $SO(3,1)$ if A satisfies

$$A^T \eta A = \eta\,, \quad \eta = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The affine linear transformations contain the translations and $SO(3,1)$-rotations. The generators of the translations we call the momenta, and since they have four components, we sometimes refer to them as four-momenta.

The (real) Lie algebra of $ISO(3,1)$ is described by the matrices of the form

$$(A,b) := \begin{pmatrix} A & b \\ 0 & 0 \end{pmatrix},$$

with $A \in so(3,1)$ and $b \in \mathbb{R}^3$. The Lie product is given by the commutator of matrices, and takes the form

$$(A,b)\angle(A',b') = ([A,A'], Ab' - A'b)\,,$$

where Ab' is the usual matrix action of A on b'. In particular, we have

$$(0,b)\angle(0,b') = 0\,, \quad (A,0)\angle(0,b') = (0, Ab')\,,$$

from which we read off that the translations form a commutative subalgebra. The translations form an ideal such that the momenta form the standard representation of $so(3,1)$, that is, the defining representation.

General spacetime. The generalization of Minkowski spacetime is a manifold with a **pseudo-Riemannian metric** g; the latter turns the tangent space at each point of the

manifold into a Minkowski space. Thus around every point there is a chart and a coordinate system such that g takes the form of a Minkowski metric. It is clear that a proper description of general relativity requires differential geometry and the development of tensor calculus.

In general relativity but also already in special relativity physicists use some conventions that are worth explaining. Spacetime indices indicating components of four-vectors are indicated by Greek letters $\mu, \nu, \ldots$. To denote a four-vector $x = (x^\mu)$ one writes simply x^μ. If an index appears ones upstairs and once downstairs, it is to be summed over; this is called the **Einstein convention**. Derivatives are objects with indices downstairs; $\partial_\mu = \partial/\partial x^\mu$. The **Kronecker delta** δ^μ_ν is an invariant tensor and we have $\partial_\mu x^\nu = \delta^\mu_\nu$ and $\partial_\mu x^\mu = 4$. The Minkowski metric is usually denoted by the Greek letter η and again one usually just writes $\eta_{\mu\nu}$ to denote the metric and not just the $\mu\nu$-component; as a matrix the Minkowski metric is given by:

$$\eta = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} .$$

The Minkowski inner product is now written as $v \cdot w = v^\mu w^\nu \eta_{\mu\nu}$. If v and w are two elements of the tangent space at a point x their inner product in general relativity is given by $v^\mu w^\nu g_{\mu\nu}(x)$, from which it is clear that general relativity is the curved generalization of special relativity. To denote the metric g physicists often describe a line element, which is to mean the distance of an infinitesimal displacement $ds = (dx^\mu)$;

$$ds^2 = g_{\mu\nu}(x) dx^\mu dx^\nu .$$

The metric $g_{\mu\nu}$ and its pointwise inverse $g^{\mu\nu}$ are used to lower and to raise indices; indeed, the metric gives an isomorphism between the tangent space and the cotangent space. Hence ∂^μ is defined as $g^{\mu\nu}\partial_\nu$, and a check of consisteny gives $g^{\mu\nu} = g^{\mu\lambda} g^{\nu\rho} g_{\rho\lambda}$. As a further exercise in the conventions the reader might verify $g^{\mu\lambda} g_{\lambda\nu} = \delta^\mu_\nu$, $g^{\mu\nu} g_{\mu\nu} = 4$. The described conventions are used a lot in physics literature and more on its nature and why it works can be found in many text books on relativity, e.g., in the nice introductory textbook by D'Inverno [72]).

The symmetry group of a manifold M with a pseudo-Riemannian metric g is huge; it consists of all diffeomorphisms of the manifold, as any diffeomorphism preserves a metric. The vector fields on M describe the infinitesimal generators of the group of diffeomorphisms.

3.15 A Lorentz invariant measure

The reason that one uses the integration measure

$$\frac{d^3\mathbf{k}}{(2\pi)^3 2\omega(k)}, \quad \omega(k) = \sqrt{c^2\mathbf{k}^2 + \frac{m^2c^4}{\hbar^2}}. \tag{3.62}$$

is due to Lorentz covariance. The integration measure is clearly rotation invariant. Hence to study the behavior under a general Lorentz transformation L we may assume that L

only mixes the x-direction and the time-direction. In that case we have, using the γ-factor (3.61)

$$\begin{aligned} L(k_x) &= \frac{k_x - vk_t}{\sqrt{1-\frac{v^2}{c^2}}} = \gamma(k_x - vk_t)\,, \\ L(k_y) &= k_y\,, \quad L(k_z) = k_z\,, \\ L(k_t) &= \frac{k_t - \frac{v}{c^2}k_x}{\sqrt{1-\frac{v^2}{c^2}}} = \gamma(k_t - \frac{v}{c^2}k_x)\,. \end{aligned}$$

One easily checks that $L(k)^2 = k^2$. Since $\omega(k)$ is the zeroth component of the wave vector k, we see that the factors $\sqrt{1-\frac{v^2}{c^2}}$ cancel out. Another way to see the covariance is to note the equality

$$\frac{d^3\mathbf{k}}{(2\pi)^3 2\omega(k)} = \frac{d^4k}{(2\pi)^3}\delta\Big(k^2 + \frac{m^2c^2}{\hbar^2}\Big)\theta(k_0)\,, \tag{3.63}$$

where θ is the **Heaviside function** defined by $\theta(x) = 1$ if $x \geq 0$ and $\theta(x) = 0$ if $x < 0$. The Heaviside function selects the positive sign of the square root in (3.62). The equality of the two integration measures in (3.63) is proven by integration of both sides. It is clear that the expression (3.63) is invariant under Lorentz transformations.

3.16 Kepler's laws, the hydrogen atom, and $SO(4)$

3.17 The periodic systemand the conformal group $SO(2,4)$

$SO(2,4) \cong SU(4)$? containing $SO(1,3)$

conformal transformations and Poisson representation

$H(3)$ as subgroup and the hydrogen atom

The periodic system

3.18 The interacting boson model and $U(6)$

3.19 Casimirs

faithful representations

sum and product of reps

universal envelope (classical and quantum),

Casimirs,

splitting representations through common eigenspaces of Casimirs

$so(3)$, $sl(2)$, spin

3.20 Unitary representations of the Poincaré group

This section is neither in a good form nor complete in contents.

Knowing the simple and semisimple Lie algebras is of course interesting, but in physics there are also important non-semisimple Lie algebras that play an important role. In this section we treat one of the most important Lie algebras in physics, the Poincaré Lie algebra. The Poincaré Lie algebra is not semisimple since it contains an abelian (and thus solvable) ideal.

In physics, the irreducible unitary representations of the Poincaré algebra correspond to **elementary particles**, more precisely to particles considered at distances so large that their internal structure can be safely ignored. Using the Casimir operators in the universal enveloping algebra, one can label the different representations, since a Casimir must take a constant value in any irreducible representation.

There are two independent Casimirs. One is the number p^2, which is an invariant since the Minkowski inner product is invariant. With our choice of signature $(-+++)$, one has $p^2 = \mathbf{p}^2 - p_0^2 = -(mc)^2$ for a constant m called the **mass** of the representation (or the associated particles); for the signature $(+---)$, we have instead $p^2 = p_0^2 - \mathbf{p}^2 = (mc)^2$. In physically relevant representations, $m \geq 0$ and $p_0 > 0$.

A second Casimir accounts for the **spin** s of the representation; for unitary representations, it is quantized, and takes nonnegative, half integral values. The particles are called **bosons** if the spin of this representation is integral, and **fermions** otherwise, i.e., if the spin is half an odd integer. For example, electrons have spin $s = 1/2$ and are fermions, while photons have spin $s = 1$ and are bosons. The name "spin" derives from relations to the representation theory of the rotation group; see Section 21.1, where also the dichotomic nature of integral and nonintegral spin is explained, which justifies using different names for bosons and fermions.

Clearly, representations which differ in mass or spin are nonequivalent. Less trivial is the fact that, among the **physical representations** (i.e., those with $m \geq 0$ and $p_0 > 0$), there is an up to equivalence unique irreducible representation for each combination $m > 0$ and $s \in \frac{1}{2}\mathbb{Z}_+$. In the massless case $m = 0$, there are precisely two for each $s \in \frac{1}{2}\mathbb{Z}_+$, a right-handed and a left-handed one.

Given an irreducible unitary representation, we can choose a basis such that the components of p act diagonally, since they are Hermitian and commute. Thus we can assign to a vector in the representation the four momentum components. The momentum components will also

be denoted p_ν. The number $E = p_0 c$ is called the **energy**, and depends on the basis chosen, since the $so(3,1)$ rotations mix the momenta. Having fixed a basis of the translations, there is only a $SO(3)$ subgroup that leaves the energy invariant. Intuitively this is clear, rotating a reference frame does not change the energies. In general, for a given basis, the subgroup of $so(3,1)$ that leaves the vector $(1,0,0,0)$ invariant is $SO(3)$ and the elements of the $SO(3)$ subgroup are rotations. There are three independent $SO(3,1)$ elements that do not leave $(1,0,0,0)$ invariant, these transformations and their linear combinations are called **Lorentz boosts** in the physics literature. The Lorentz boosts mix time and space coordinates. A basis of Poincaré Lie algebra thus consists of the generators of three rotations, three Lorentz boosts and four translations.

3.21 Some representations of the Poincare group

mass and spin

The Foldy construction

relation to the invariant measure form; Foldy-Wouthuisen transform?

Galilei version and classical limit

3.22 Elementary particles

Elementary particle = irreducible unitary representation of the Poincare group with quantized spin, $p^2 \geq 0$, and $p_0 > 0$.

massless particles and gauge freedom

3.22.1 Proposition. *For real $a \in \mathbb{R}^3$ and any Pauli set of spin j,*

$$|\overline{\psi}(a \cdot \sigma)\psi| \leq 2j|a|\overline{\psi}\psi \quad \textit{for all } \psi \in \mathbb{C}^s. \tag{3.64}$$

Equality holds iff ψ satisfies the **Weyl equation**

$$(a \cdot \sigma)\psi = \pm 2j|a|\psi.$$

Proof. We need to show that the symmetric matrix $\sigma_0(2j|a| - a \cdot \sigma)$ is positive semidefinite. The matrix $A = \sigma_0((s-1)|a| - a \cdot \sigma)$ is tridiagonal with nontrivial entries

$$A_{kk} = \binom{s-1}{k-1}((s-1)|a| - (s+1-2k)a_3),$$

$$A_{kk-1} = -\binom{s-1}{k-1}(k-1)(a_1 + ia_2),$$

$$A_{kk+1} = -\binom{s-1}{k-1}(s-k)(a_1 - ia_2) = A^*_{k+1k}.$$

If $a_3 \neq |a|$ then $a_3 < |a|$, and we may define the lower triangular tridiagonal matrix L and the diagonal matrix D with nontrivial entries

$$L_{kk} = 1, \quad L_{k+1k} = -\frac{a_1 + ia_2}{|a| - a_3}, \quad D_{kk} = (|a| - a_3)k\binom{s-1}{k} \geq 0.$$

Now $A = LDL^*$; therefore, A is Hermitian positive semidefinite.

If $a_3 = |a|$ then $a_1 = a_2 = 0$ and A is diagonal with nonnegative diagonal entries $A_{kk} = \binom{s-1}{k-1}2(k-1)|a|$, and again positive semidefinite. Now

$$0 \leq \psi^* A\psi = (s-1)|a|\overline{\psi}\psi - \overline{\psi}(a \cdot \sigma)\psi,$$

and replacing a by $-a$ gives the desired inequality. Equality holds iff $A\psi = 0$, which is the Weyl equation. □

Note that the Weyl equation is solved for $a_3 < |a|$ by ψ iff $L^*\psi$ is zero except in the last component (since $A = LDL^*$ and the other diagonal entries of D are positive).

More precisely, $a \cdot \sigma$ has the simple eigenvalues $(s + 1 - 2l)|a|$ $(l = 1 : s)$.

3.23 The position operator

Chapter 4

From the theoretical physics FAQ

4.1 To be done

The present chapter will be merged into the preceding chapters. Some of the sections in later chapters, whose content is already in Part I will be eliminated.

The section on "Heisenberg groups and Poisson representations" is at the start of Chapter 3 since to define the Lie algebra of angular momentum already requires the CCR and Poisson brackets.

Perhaps the two chapters could be integrated better via a sequence like:

- Reflections, Rotations and classical angular momentum (which could contain a lot of math on SO(3) including some Lie stuff).

- Galilei group, which builds on rotations.

- Symplectic/Hamiltonian stuff (classical non-relativistic dynamical groups)

- Classical relativistic stuff (Poincare) Maybe also classical electromagnetism in here somewhere, since it stands astride both the classical and quantum worlds. It's also the natural place to introduce the concept of (classical) gauge invariance.

- Non-relativistic QM (Heisenberg, Oscillator, Schrodinger, etc).

- Re-visit SO(3) in the quantum context and show how the requirement of being a symmetry of a positive-definite inner product is enough to imply stunningly unexpected facts about the spectrum of angular momentum experiments. This then becomes the archetype for how representations, Casimirs, etc, are at the heart of modern physics. This is also a good place to emphasize how Schrödinger wave functions, etc, are not the last word and about how a more general algebraic framework is cleaner and powerful (having shown that this is sufficient to make impressive predictions).

- Continue on to Isospin and gauge symmetries.

- Quantum dynamical groups (conformal, H-atom, etc).

Thus, each step in the mathematical sequence of ideas is presented and developed in a suitable physics context.

4.2 Postulates for the formal core of quantum mechanics

Quantum mechanics consists of a formal core that is universally agreed upon (basically being a piece of mathematics with a few meager pointers on how to match it with experimental reality) and an interpretational halo that remains highly disputed even after 85 years of modern quantum mechanics. The latter is the subject of the foundations of quantum mechanics; it is addressed elsewhere in this FAQ.

Here I focus on the formal side. The relativistic case is outside the scope of the present axioms, though presumably very little needs to be changed.

As in any axiomatic setting (necessary for a formal discipline), there are a number of different but equivalent sets of axioms or postulates that can be used to define formal quantum mechanics. Since they are equivalent, their choice is a matter of convenience.

My choice presented here is the formulation which gives most direct access to statistical mechanics but is free from allusions to measurement. The reason for the first is that statistical mechanics is the main tool for applications of quantum mechanics to the macroscopic systems we are familiar with. The reason for the second is that real measurements consitute a complex process involving macroscopic detectors, hence should be explained by quantum statistical mechanics rather than be part of the axiomatic foundations themselves. (This is in marked contrast to other foundations, and distinguishes the present axiom system.)

Thus the following describes nonrelativistic quantum statistical mechanics in the Schroedinger picture. (As explained later, the traditional starting point is instead the special case of this setting where all states are assumed to be pure.)

For brevity, I assume the knowledge of some basic terms from functional analysis, which are precisely defined in many mathematics books. [For a discussion of the difference between a Hermitian and a

self-adjoint operator, see e.g., Definition 3 in
http://arxiv.org/pdf/quant-ph/9907069 . The importance of this
difference is that Hermitian operators have a real spectrum if and
only if they are self-adjoint. Moreover, the Hille-Yosida theorem says
that e^{iX) exists (and is unitary) for a Hermitian operator X if and
only iff X is self-adjoint. A detailed discussion and the HY theorem
itself are discussed in Vol.3 of the math physics treatise by Thirring.]
The statements of my axioms contain in parentheses some additional
explanations that, strictly speaking, are not part of the axioms but
make them more easily intelligible; the list of examples given only
has illustrative character and is far from being exhaustive.

Quantum mechanics is governed by the following six axioms:

A1. A generic system (e.g., a 'hydrogen molecule') is defined by
specifying a Hilbert space K and a (densely defined, self-adjoint)
Hermitian linear operator H called the _Hamiltonian_ or the _energy_.

A2. A particular system (e.g., 'the ion in the ion trap on this
particular desk') is characterized by its _state_ rho(t)
at every time t in R (the set of real numbers).
Here rho(t) is a Hermitian, positive semidefinite, linear trace class
operator on K satisfying at all times the conditions
   trace rho(t) = 1.   (normalization)

A3. A system is called _closed_ in a time interval [t1,t2]
if it satisfies the evolution equation
   d/dt rho(t) = i/hbar [rho(t),H] for t in [t1,t2],
and _open_ otherwise. (hbar is Planck's constant, and is often set
to 1.)
If nothing else is apparent from the context, a system is assumed to
be closed.

A4. Besides the energy H, certain other (densely defined, self-adjoint)
Hermitian operators (or vectors of such operators) are distinguished
as _observables_.
(E.g., the observables for a system of N distinguishable particles
conventionally include for each particle several 3-dimensional vectors:
the _position_ x^a, _momentum_ p^a, _orbital_angular_momentum_ L^a
and the _spin_vector_ (or Bloch vector) sigma^a of the particle with
label a. If u is a 3-vector of unit length then u dot p^a, u dot L^a
and u dot sigma^a define the momentum, orbital angular momentum,
and spin of particle a in direction u.)

A5. For any particular system, and for every vector X of observables

with commuting components, one associates a time-dependent monotone linear functional <.>_t defining the _expectation_

<f(X)>_t:=trace rho(t) f(X)

of bounded continuous functions f(X) at time t.
(This is equivalent to a multivariate probability measure dmu_t(X) on a suitable sigma algebra over the spectrum spec(X) of X) defined by

integral dmu_t(X) f(X) := trace rho(t) f(X) =<f(X)>_t.

The signma algebra is uniquely determined.)

A6. Quantum mechanical predictions consist of predicting properties (typically expectations or conditional probabilities) of the measures defined in Axiom A5, given reasonable assumptions about the states (e.g., ground state, equilibrium state, etc.)

Axiom A6 specifies that the formal content of quantum mechanics is covered exactly by what can be deduced from Axioms A1-A5 without anything else added (except for restrictions defining the specific nature of the states and observables), and hence says that Axioms A1-A5 are complete.

The description of a particular closed system is therefore given by the specification of a particular Hilbert space in A1, the specification of the observable quantities in A4, and the specification of conditions singling out a particular class of states (in A6). Given this, everything else is determined by the theory, and hence is (in principle) predicted by the theory.

The description of an open system involves, in addition, the specification of the details of the dynamical law. (For the basics, see the entry 'Open quantum systems' in this FAQ.)

In addition to these formal axioms one needs a rudimentary interpretation relating the formal part to experiments.
The following _minimal_interpretation_ seems to be universally accepted.

MI. Upon measuring at times t_l (l=1,...,n) a vector X of observables with commuting components, for a large collection of independent identical (particular) systems closed for times t<t_l, all in the same state

rho_0 = lim_{t to t_l from below} rho(t)

(one calls such systems _identically_prepared_), the measurement results are statistically consistent with independent realizations of a random vector X with measure as defined in axiom A5.

Note that MI is no longer a formal statement since it neither defines what 'measuring' is, nor what 'measurement results' are and what 'statistically consistent' or 'independent identical system' means. Thus MI has no mathematical meaning - it is not an axiom, but already part of the interpretation of formal quantum mechanics.

MI relates the axioms not to a hypothetical classical realm but to a nonphysical entity: the social conventions of the community of physicists. The terms 'measuring', 'measurement results', 'statistically consistent', and 'independent' already have informal meaning in the reality as perceived by a physicist. Everything stated in Axiom MI is understandable by every trained physicist.
Thus statement MI is not an axiom for formal logical reasoning but a bridge to informal reasoning in the traditional cultural setting that defines what a trained physicist understands by reality.

The lack of precision in statement MI is on purpose, since it allows the statement to be agreeable to everyone in its vagueness; different philosophical schools can easily fill it with their own understanding of the terms in a way consistent with the remainder.

Interpretational axioms necessarily have this form, since they must assume some unexplained common cultural background for perceiving reality. (This is even true in pure mathematics, since the language stating the axioms must be assumed to be common cultural background.)

MI is what _every_ interpretation I know of assumes (and has to assume) at least implicitly in order to make contact with experiments. Indeed, all interpretations I know of assume much more, but they differ a lot in what they assume beyond MI.

Everything beyond MI seems to be controversial. In particular, already what constitutes a measurement of X is controversial. (E.g., reading a pointer, different readers may get marginally different results. What is the true pointer reading?)

On the other hand there is an informal consensus on how to perform measurements in practice. Good foundations including a good measurement theory should be able to properly justify this informal consensus by defining additional formal concepts that behave within the theory just as their informal relatives with the same name behave in reality.

In complete foundations, there would be formal objects in the mathematical theory corresponding to all informal objects discussed by physicists, such that talking about the formal objects and talking about the real objects is essentially isomorphic. We are currently far from such complete foundations.

A state rho is called _pure_ at time t if rho(t) maps the Hilbert space K to a 1-dimensional subspace, and _mixed_ otherwise.

Although much of traditional quantum mechanics is phrased in terms of pure states, this is a very special case; in most actual experiments the systems are open and the states are mixed states. Pure states are relevant only if they come from the ground state of a Hamiltonian in which the first excited state has a large energy gap. Indeed, assume for simplicity that H has discrete spectrum. In an orthonormal basis of eigenstates psi_k,

```
   f(H) = sum_k f(E_k) psi_k psi_k^*
```

for every function f defined on the spectrum. Setting the Boltzmann constant to 1 to simplify the formulas, the equilibrium density is the canonical ensemble,

```
   rho(T) = 1/Z(T) exp(-H/T) = sum_k exp(-E_k/T)/Z(T) psi_k psi_k^*.
```

(Of course, equating this ensemble with equilibrium in a closed system is an additional step beyond our axiom system, which would require justification.) Taking the trace (which must be 1) gives

```
   Z(T) = sum_k exp(-E_k/T),
```

and in the limit T -> 0, all terms exp(-E_k/T)/Z(T) become 0 or 1, with 1 only for the k corresponding to the states with least energy Thus, if the ground state psi_1 is unique,

```
   lim_{T->0} rho(T) = psi_1 psi_1^*.
```

This implies that for low enough temperatures, the equilibrium state is approximately pure. The larger the gap to the second smallest energy level, the better is the approximation at a given nonzero temperature. In particular (reinstalling the Boltzmann constant kbar), the approximation is good if the energy gap exceeds a small multiple of E^* := kbar T.

States of simple enough systems with a few levels only can often be prepared in nearly pure states, by realizing a source governed by a Hamiltonian in which the first excited state has a much larger energy than the ground state. Dissipation then brings the system into equilibrium, and as seen above, the resulting equilibrium state is nearly pure.

To see how the more traditional setting in terms of the

Schroedinger equation arises, we consider the case of a closed system in a pure state rho(t) at some time t.

If psi(t) is a unit vector in the range of the pure state rho(t) then psi(t), called the _state_vector_ of the system at time t, is determined up to a phase, and one easily verifies that

rho(t) = psi(t)psi(t)^*.

Remarkably, under the dynamics for a closed system specified in the above axioms, this property persists with time (only) if the system is closed, and the state vector satisfies the Schroedinger equation

i hbar psi(t) = H psi(t)

Thus the state remains pure at all times. Conversely, for every pure state, the phases of psi(t) at all times t can be chosen such that the Schroedinger equation holds.

Moreover, if X is a vector of observables with commuting components and the spectrum of X is discrete, then the measure from Axiom A5 is discrete,

integral dmu(X) f(X) = sum_k p_k f(X_k)

with nonnegative numbers p_k summing to 1, commonly called _probabilities_. Associated with the p_k are eigenspaces K_k such that

X psi = X_k psi for psi in K_k,

and K is the direct sum of the K_k. Therefore, every state vector psi can be uniquely decomposed into a sum

psi = sum_k psi_k with psi_k in K_k.

psi_k is called the _projection_ of psi to the eigenspace K_k.

A short calculation using Axiom A5 now reveals that for a pure state rho(t)=psi(t)psi(t)^*, the probabilities p_k are given by the so-called _Born_rule_

p_k = |psi_k(t)|^2, (B)

where psi_k(t) is the projection of psi(t) to the eigenspace K_k.

Deriving the Born rule (B) from Axioms A1-A5 makes it completely natural, while the traditional approach starting with (B) makes it an irreducible rule full of mystery and only justifiable by its miraculous agreement with experiment.

Note that Born's 1926 paper (reprinted in English translation in pp.52-55 of the reprint volume ''Quantum Theory and Measurement'' by Wheeler and Zurek) - which introduced the probabilistic interpretation that earned him a Nobel prize - didn't relate his interpretation to measurement. Born's formulation doesn't depend on anything being measured (let alone to be assigned a precise numerical measurement value): ''gives the probability for the electron, arriving from the z-direction, to be thrown out into the direction designated by the

angles alpha, beta, gamma, with the phase change delta''.

Nevertheless, it is often (see, e.g.,
    http://en.wikipedia.org/wiki/Born_rule)
claimed as part of Born's rule that the results of the measurement should equal exactly the eigenvalues. But unless the lambda_i are (as for polarization, spin or angular momentum in a particular direction - the common subjects of experiments involving Alice and Bob) system-independent, discrete, and known a priori - in which case one can label each measurement record with these numbers -, this form of the rule is highly unrealistic.

I didn't mention indistinguishable particles in my examples illustrating the axioms, for two reasons:
 1. One cannot easily specify the set of relevant observables without introducing lots of additional notation or terminology - whereas the explanations of the axioms should be very short.
 2. I think that the concept of indistinguishable particles is completely superseded by the concept of a quantum field.
The latter gives much better intuition about the meaning of the formalism, and the former (which is difficult to justify and even more difficult to interpret intuitively) is then completely dispensable.

4.3 Lie groups and Lie algebras

Lie groups can be illustrated by continuous rigid motion of a ball with painted patterns on it in 3-dimensional space. The Lie group ISO(3) consists of all rigid transformations.

A rigid transfromation is essentially the act of picking the ball and placing it somewhere else, ignoring the detailed motion in between and the location one started.
Special transformations are for example a translation in northern direction by 1 meter, or a rotation by one quarter around the vertical axis at some particular point (think of a ball with a string attached).
'Rigid' means that the distances between marked points on the ball remains the same; the mathematician talks about 'preserving distances', and the distances are therefore labeled 'invariants'.

One can repeat the same transformation several times, or two different transformations and get another one - This is called the product of

these transformations. For example, the product of a translations by 1 meter and another one by 2 meters in the same direction gives one of 1+2=3 meters in the same direction. In this case, the distances add, but if one combines rotations about different axes the result is no longer intuitive. To make this more tractable for calculations, one needs to take some kind of logarithms of transformations - these behave again additively and make up the corresponding Lie algebra iso(3) [same letters but in lower case]. The elements of the Lie algebra can be visualized as very small, or 'infinitesimal', motions.

General Lie groups and Lie algebras extend these notions to to more general manifolds. A manifold is just a higher-dimensional version of space, and transformations are generalized motions preserving invariants that are important in the manifold. The transformations preserving these invariants are also called 'symmetries', and the Lie group consisting of all symmetries is called a 'symmetry group'. The elements of the corresponding Lie algebra are 'infinitesimal symmetries'.

For example, physical laws are invariant under rotations and translations, and hence unter all rigid motions. But not only these: If one includes time explicitly, the resulting 4-dimensional space has more invariant motions or ''symmetries''.
The Lie group of all these symmetry transformations is called the Poincar'e group, and plays a basic role in the theory of relativity. The transformations are now about space-time frames in uniform motion. Apart from translations and rotations there are symmetries called 'boosts' that accelerate a frame in a certain direction, and combinations obtained by taking products. All infinitesimal symmetries together make up a Lie algebra, called the Poincar'e algebra.

Much more on Lie groups and Lie algebras from the perspective of classical and quantum physics can be found in:

Arnold Neumaier and Dennis Westra,
Classical and Quantum Mechanics via Lie algebras,
Cambridge University Press, to appear (2009?).
http://www.mat.univie.ac.at/~neum/papers/physpapers.html#QML
arXiv:0810.1019

4.4 The Galilei group as contraction of the Poincare group

The group of symmetries of special relativity is the Poincare group.

However, before Einstein invented the theory of relativity, physics was believed to follow Newton's laws, and these have a different group of symmetries - the Galilei group, and its infinitesimal symmetries form the Galilei algebra.

Now Newton's physics is just a special case of the theory of relativity in which all motions are very slow compared to the speed of light. Physicists speak of the 'nonrelativisitic limit'.
Thus one would expect that the Galilei group is a kind of nonrelativistic limit of the Poincar'e group.

This notion has been made precise by Inonu. He looked at the Poincar'e algebra and 'contracted' it in an ingenious way to the Galilei algebra. The construction could then be lifted to the corresponding groups. Not only that, it turned out to be a general machinery applicable to all Lie algebras and Lie groups, and therefore has found many applications far beyond that for which it was originally developed.

4.5 Representations of the Poincare group

Whatever deserves the name ''particle'' must move like a single, indivisible object. The Poincare group must act on the description of this single object; so the state space of the object carries a unitary representation of the Poincare group. This splits into a direct sum or direct integral of irreducible reps. But splitting means divisibility; so in the indivisible case, we have an irreducible representation.

On the other hand, not all irreducible unitary reps of the Poincare group qualify. Associated with the rep must be a consistent and causal free field theory. As explained in Volume 1 of Weinberg's book on quantum field theory, this restricts the rep further to those with positive mass, or massless reps with quantized helicity.

Weinberg's book on QFT argues for gauge invariance from causality + masslessness. He discusses massless fields in

Chapter 5, and observes (probably there, or in the beginning of Chapter 8 on quantum electrodynamics) roughly the following:

Since massless spin 1 fields have only two degrees of freedom, the 4-vector one can make from them does not transform correctly but only up to a gauge transformation making up for the missing longitudinal degree of freedom. Since sufficiently long range elementary fields (less than exponential decay) are necessarily massless, they must either have spin <=1/2 or have gauge behavior.

To couple such gauge fields to matter currents, the latter must be conserved, which means (given the known conservation laws) that the gauge fields either have spin 1 (coupling to a conserved vector current), or spin 2 (coupling to the energy-momentum tensor). [Actually, he does not discuss this for Fermion fields, so spin 3/2 (gravitinos) is perhaps another special case.]

Spin 1 leads to standard gauge theories, while spin 2 leads to general covariance (and gravitons) which, in this context, is best viewed also as a kind of gauge invariance.

There are some assumptions in the derivation, which one can find out by reading Weinberg's papers

Phys.Rev. 133 (1964), B1318-B1322	any spin (massive)
Phys.Rev. 134 (1964), B882-B896	any spin II (massless)
Phys.Rev. 135 (1964), B1049-B1056	grav. mass = inertial mass
Phys.Rev. 138 (1965), B988-B1002	derivation of Einstein
Phys.Rev. 140 (1965), B516-B524	infrared gravitons
Phys.Rev. 181 (1969), 1893-1899	any spin III (general reps.)

on 'Feynman rules for any spin' and some related questions, which contain a lot of important information about applying the irreducible representations of the Poincare group for higher spin to field theories, and their relation to gauge theories and general relativity. A perhaps more understandable version of part of the material is in

D.N. Williams,
The Dirac Algebra for Any Spin,
Unpublished Manuscript (2003)
http://www-personal.umich.edu/~williams/papers/diracalgebra.pdf

Note that there are plenty of interactions that can be constructed using the representation theory of the Lorentz group (and Weinberg's constructions), and there are plenty of (compound) particles with spin >2. See the tables of the particle data group, e.g., Delta(2950) (randomly chosen from http://pdg.lbl.gov/2003/bxxxpdf.html).

R.L. Ingraham,
Prog. Theor. Phys. 51 91974), 249-261,

http://ptp.ipap.jp/link?PTP/51/249/
constructs covariant propagators and complete vertices for spin J bosons with conserved currents for all J. See also
H Shi-Zhong et al.,
Eur. Phys. J. C 42 (2005), 375-389
http://www.springerlink.com/content/ww61351722118853/

4.6 Forms of relativistic dynamics

Relativistic multiparticle mechanics is an intricate subject, and there are no-go theorems that imply that the most plausible possibilities cannot be realized. However, these no-go theorems depend on assumptions that, when questioned, allow meaningful solutions. The no-go theorems thus show that one needs to be careful not to introduce plausible but inappropriate intuition into the formal framework.

To pose the problem, one needs to distinguish between kinematical and dynamical quantities in the theory. Kinematics answers the question "What are the general form and properties of objects that are subject to the dynamics?" Thus it tells one about conceivable solutions, mapping out the properties of the considered representation of the phase space (or what remains of it in the quantum case). Thus kinematics is geometric in nature. But kinematics does not know of equations of motions, and hence can only tell general (kinematical) features of solutions.

In contrast, dynamics is based on an equation of motion (or an associated variational principle) and answers the question 'What characterizes the actual solution?', given appropriate initial or boundary conditions. Although the actual solution may not be available in closed form, one can discuss their detailed properties and devise numerical approximation schemes.

The difference between kinematical and dynamical is one of convention, and has nothing to do with the physics. By choosing the representation, i.e., the geometric setting, one chooses what is kinematical; everything else is dynamical.

Since something which is up to the choice of the person describing an experiment can never be distinguished experimentally, the physics is unaffected. However, the formulas look very different in different descriptions, and - just as in choosing coordinate systems - choosing

a form adapted to a problem may make a huge difference for actual computations.

Dirac distinguishes in his seminal paper
Rev. Mod. Phys. 21 (1949), 392-399
three natural forms of relativistic dynamics, the instant form, the point form, and the fromt form. They are distinguished by what they consider to be kinematical quantities and what are the dynamical quantities.

The familiar form of dynamics is the instant form, which treats space (hence spatial translations and rotations) as kinematical and time (and hence time translation and Lorentz boosts) as dynamical. This is the dynamics from the point of view of a hypothetical observer (let us call it an 'instant observer') who has knowledge about all information at some time t (the present), and asks how this information changes as time proceeds.

Because of causality (the finite bound of c on the speed of material motion and communication), the resulting differential equations should be symmetric hyperbolic differential equations for which the initial-value problem is well-posed.
Because of Lorentz invariance, the time axis can be any axis along a timelike 4-vector, and (in special relativity) space is the 3-space orthogonal to it. For a real observer, the natural timelike vector is the momentum 4-vector of the material system defining its reference frame (e.g., the solar system).

While very close to the Newtonian view of reality, it involves an element of fiction in that no real observer can get all the information needed as intial data. Indeed, causality implies that it is impossible for a physical observer to know the present anywhere except at its own position.

A second, natural form of relativistic dynamics is, according to Dirac, the point form. This is the form of dynamics in which a particular space-time point x=0 (the here and now) in Minkowski space is distinguished, and the kinematical object replacing space is, for fixed L, a hyperboloid x^2=L^2 (and x_0<0) in the past of the here and now.
The Lorentz transformations, as symmetries of the hyperboloid, are now kinematical and take the role that space translations and rotations had in the instant form. On the other hand, _all_ space and

time translations are now dynamical, since they affect the position of the here-and-now.

This is the form of dynamics which is manifestly Lorentz invariant, and in which space and time appear on equal footing. An observer in the here and now (let us call it a 'point observer') can - in principle, classically - have arbitrarily accurate information about the particles and/or fields on the past hyperboloid; thus causality is naturally accounted for. Information given on the past hyperboloid of a point can be propagated to information on any other past hyperboloid using the dynamical equations that are defined via the momentum 4-vector P, which is a 4-dimensional analogue of the nonrelativistic Hamiltonian. The Hamiltonian corresponding to motion in a fixed timelike direction u is given by H=u dot P. The commutativity of the components of P is the condition for the uniqueness of the resulting state at a different point x independent of the path x is reached from 0.

In principle, there are many other forms of relativistic dynamics: As Dirac mentions on p. 396 of his paper, any 3-dimensional surface in Minkowski space works as kinematical space if it meets every world line with time like tangents exactly once. In general, those transformations are kinematical which are also symmetries of the surface one treats as kinematical reference surface. By choosing a surface without symmetries _all_ transformations become dynamical. For reasons of economy, one wants however, a large kinematical symmetry group. The full Poincare group is possible only for free dynamics.

This leaves as interesting large subgroups two with 6 linearly independent generators, the Euclidean group ISO(3), leading to the instant form, and the Lorentz group SO(1,3), leading to the point form, and one with 7 linearly independent generators, the stabilizer of a front (or infinite momentum plane), a 3-space with lightlike normal, leading to the front form. This third natural form of relativistic dynamics according to Dirac, has many uses in quantum field theory, but here I won't discuss it further.

All forms are equivalent, related classically by canonical transformations preserving algebraic operations and the Poisson bracket, and quantum mechanically by unitary transformations preserving algebraic operations and hence the commutator. This means that any statement about a system in one of the forms can be translated into an equivalent statement of an equivalent system in any of the other

forms.

Preferences are therefore given to one form over the other depending solely on the relative simplicity of the computations one wants to do. This is completely analogous to the choice of coordinate systems (cartesian, polar, cylindric, etc.) in classical mechanics.

For a multiparticle theory, however, the different forms and the need to pick a particular one seem to give different pictures of reality. This invites paradoxes if one is not careful.

This can be seen by considering trajectories of classical relativistic many-particle systems. There is a famous theorem by

Currie, Jordan and Sudarshan
Rev. Mod. Phys. 35 (1963), 350-375

which asserts that interacting two-particle systems cannot have Lorentz invariant trajectories in Minkowski space. Traditionally, this was taken by mainstream physics as an indication that the multiparticle view of relativistic mechanics is inadequate, and a field theoretical formulation is essential.
However, as time proceeded, several approaches to valid relativistic multi-particle (quantum) dynamics were found (see the FAQ entry on 'Is there a multiparticle relativistic quantum mechanics?'), and the theorem had the same fate as von Neumann's proof that hidden-variable theories are impossible. Both results are now simply taken as an indication that the assumptions under which they were made are too strong.

In particular, once the assumption by Currie, Jordan and Sudarshan that all observers see the same trajectories of a system of interacting particles is rejected, their no-go theorem no longer applies.
The question then is how to find a consistent and covariant description without this at first sight very intuitive property. But once it is admitted that different observers see the same world but represented in different personal spaces, the formerly intuitive property becomes meaningless. For objectivity, it is enough that one can consistently translate the views of any observer into that of any other observer. Precisely this is the role of the dynamical Poincare transformations.

Thus nothing forbids an instant observer to observe particle trajectories in its present space, or a point observer to observe particle trajectories in its past hyperboloid. However, the present space (or the past hyperboloid) of two different observers is related not by kinematical transforms but dynamically, with the result that trajectories seen by different observers on

their different kinematical 3-surface look different.
Classically, this looks strange on first sight, although
the Poincare group provides well-defined recipes for translating
the trajectories seen by one observer into those seen by another
observer.

Quantum mechanically, trajectories are fuzzy anyway, due to the
uncertainty principle, and as various successful multiparticle
theories show, there is no mathematical obstacle for such a description.

The mathematical reason of this superficially paradoxical situation
lies in the fact that there is no observer-independent definition
of the center of mass of relativistic particles, and the related fact
that there is no observer-independent definition of space-time
coordinates for a multiparticle system.
The best one can do is to define either a covariant position operator
whose components do not commute (thus definig a noncommutative
space-time), or a spatial position operator, the so-called
Newton-Wigner position operator, which has three commuting coordinates
but is observer-dependent.
(See the FAQ entry on 'Localization and position operators'.)

4.7 Is there a multiparticle relativistic quantum mechanics?

In his QFT book, Weinberg says no, arguing that there is no way to
implement the cluster separation property. But in fact there is:

There is a big survey by Keister and Polyzou on the subject
    B.D. Keister and W.N. Polyzou,
    Relativistic Hamiltonian Dynamics in Nuclear and Particle Physics,
    in: Advances in Nuclear Physics, Volume 20,
    (J. W. Negele and E.W. Vogt, eds.)
    Plenum Press 1991.
    www.physics.uiowa.edu/~wpolyzou/papers/rev.pdf
that covered everything known at that time. This survey was quoted
at least 116 times, see
    http://www.slac.stanford.edu/spires/find/hep?c=ANUPB,20,225
looking these up will bring you close to the state of the art
on this.

They survey the construction of effective few-particle models.
There are no singular interactions, hence there is no need for

renormalization.

The models are _not_ field theories, only Poincare-invariant few-body dynamics with cluster decomposition and phenomenological terms which can be matched to approximate form factors from experiment or some field theory. (Actually many-body dynamics also works, but the many particle case is extremely messy.)
They are useful phenomenological models, but somewhat limited; for example, it is not clear how to incorporate external fields.

The papers by Klink at
http://www.physics.uiowa.edu/~wklink/
and work by Polyzou at
http://www.physics.uiowa.edu/~wpolyzou/
contain lots of multiparticle relativistic quantum mechanics, applied to real particles. See also the Ph.D. thesis by Krassnigg at
http://physik.uni-graz.at/~ank/dissertation-f.html

Other work in this direction includes Dirac's many-time quantum theory, with a separate time coordinate for each particle; see, e.g.,
Marian Guenther, Phys Rev 94, 1347-1357 (1954)
and references there. Related multi-time work was done under the name of 'proper time quantum mechanics' or 'manifestly covariant quantum mechanics', see, e.g.,
L.P. Horwitz and C. Piron, Helv. Phys. Acta 48 (1973) 316,
but it apparently never reached a stage useful to phenomenology.

4.8 What is a photon?

According to quantum electrodynamics, the most accurately verified theory in physics, a photon is a single-particle excitation of the free quantum electromagnetic field. More formally, it is a state of the free electromagnetic field which is an eigenstate of the photon number operator with eigenvalue 1.

The pure states of the free quantum electromagnetic field are elements of a Fock space constructed from 1-photon states.
A general n-photon state vector is an arbitrary linear combinations of tensor products of n 1-photon state vectors; and a general pure state of the free quantum electromagnetic field is a sum of n-photon state vectors, one for each n. If only the 0-photon term contributes, we have the dark state, usually called the vacuum; if only the 1-photon term contributes, we have a single photon.

A single photon has the same degrees of freedom as a classical vacuum radiation field. Its shape is characterized by an arbitrary nonzero real 4-potential A(x) satisfying the free Maxwell equations, which in the Lorentz gauge take the form

```
   nabla dot nabla A(x) = 0,
   nabla dot A(x) = 0,
```

expressing the zero mass and the transversality of photons. Thus for every such A there is a corresponding pure photon state |A>.
Here A(x) is _not_ a field operator but a photon amplitude; photons whose amplitude differ by an x-independent phase factor are the same. For a photon in the normalized state |A>, the observable electromagnetic field expectations are given by the usual formulas relating the 4-potential and the fields,

```
   <\E(x)> = <A|\E(x)|A>
           = - partial \A(x)/partial x_0 - c nabla_\x A_0(x),
```

and

```
   <\B(x)> = <A|\B(x)|A> = nabla_\x x \A(x)
```

[hmmm. check if this really is the case...]
Here \x (fat x) and x_0 are the space part and the time part of a relativistic 4-vector, \E(x), \B(x) are the electromagnetic field operators (related to the operator 4-potential by analogous formulas), and c is the speed of light. Amplitudes A(x) producing the same \E(x) and \B(x) are equivalent and related by a gauge transformation, and describe the same photon.

In momentum space (frequently but not always the appropriate choice), single photon states have the form

```
   |A> = integral d\p^3/p_0 A(\p)|\p>,
```

where |\p> is a single particle state with definite 3-momentum \p (fat p), p_0=|\p| is the corresponding photon energy divided by c, and the photon amplitide A(\p) is a polarization 4-vector.
Thus a general photon is a superposition of monochromatic waves with arbitrary polarizations, frequencies and directions.
(The Fourier transform of A(\p) is the so-called analytic signal A^(+)(x), and by adding its complex conjugate one gets the real 4-potential A(x) in the Lorentz gauge.)

The photon amplitude A(\p) can be regarded as the photon's wave function in momentum space. Since photons are not localizable (though they are localizable approximately), there is no meaningful photon wave function in coordinate space; see the next entry in this FAQ. One could regard the 4-potential A(x) as coordinate space wave function, but because of its gauge dependence, this is not really useful.

```
[
This is second quantized notation, as appropriate for quantum fields.
This is how things always look in second quantization, even for a
harmonic oscillator. The wave function psi(x) or psi(p) in standard
(first quantized) quantum mechanics becomes the state vector
   psi = integral dx psi(x) |x>   or   integral dp psi(p) |p>
in Fock space; the wave function at x or p turns into the coefficient
of |x> or |p>. In quantum field theory, x, A (the photon amplitude), and
E(x) (the electric field operator) correspond to  k (a component of the
momentum), x, and p_k. Thus the coordinate index k is inflated to the
spacetime position x, the argument of the wave function is inflated to
a solution of the free Maxwell equations, the momentum operator is
inflated to a field operator, and the integral over x becomes a
functional integral over photon amplitudes,
   psi = integral dA psi(A) |A>.
Here psi(A) is the most general state vector in Fock space; for a
single photon, psi depends linearly on A,
   psi(A) = integral d\p^3/p_0 A(\p)|\p> = |A>.
Observable electromagnetic fields are obtained as expectation values
of the field operators \E(x) and \B(x) constructed by differentiation of
the textbook field operator A(x). As the observed components of
the mean momentum, say, in ordinary quantum mechanics are
   <p_k> = integral dx psi(x)^* p_k psi(x),
so the observed values of the electromagnetic field are
   <\E(x)> = <psi|\E(x)|psi> = integral dA psi(A)^* \E(x) psi(A).
   <\B(x)> = <psi|\B(x)|psi> = integral dA psi(A)^* \B(x) psi(A).
]
In a frequently used interpretation (valid only approximately),
the term A(\p)|\p> represents the one-photon part of a monochromatic
beam with frequency nu=cp_0/h, direction \n(\p)=\p/p_0, and
polarization determined by A(\p). Here h = 2 pi hbar, where hbar is
Planck's number; omega=cp_0/hbar is the angular frequency.

The polarization 4-vector A(\p) is orthogonal to the 4-momentum p
composed of p_0 and \p, obtained by a Fourier transform of the
4-potential A(x) in the Lorentz gauge. (The wave equation translates
into the condition p_0^2=\p^2, causality requires p_0>0, hence
p_0=|\p|, and orthogonality p dot A(\p) = 0 expresses the Lorentz
gauge condition. For massless particles, there remains the additional
gauge freedom to shift A(\p) by a multiple of the 4-momentum p, which
can be used to fix A_0=0.)

A(\p) is usually written (in the gauge with vanishing time component) as
a linear combination of two specific polarization vectors eps^+(p) and
eps^-(p) for circularly polarized light (corresponding to helicities +1
and -1), forming together with the direction vector \n(\p) an
```

```
orthonormal basis of complex 3-space. In particular,
   eps^+(p) eps^+(p)^* + eps^-(p)eps^-(p)^* + \n(\p)\n(\p)^* = 1
is the 3x3 identity matrix. (This is used in sums over helicities for
Feynman rules.) Specifically, eps^+(p) and eps^-(p) can be obtained by
finding normalized eigenvectors for the eigenvalue problem
[check. The original eigenvalue problem is p dot J eps = lambda eps.]
   p x eps = lambda eps
with lambda = +-i|p|. For example, if p is in z-direction then
   eps^+(p) = (1, -i, 0)/sqrt(2),
   eps^-(p) = (i, -1, 0)/sqrt(2),
and the general case can be obtained by a suitable rotation.
An explicit calculation gives almost everywhere
    eps^+(p) = u(p)/p_0
where p_0=|p| and
    u_1(p) = p_3 - i p_2 p'/p'',
    u_2(p) = -i p_3 - i p_1 p'/p''
    u_3(p) = p'
with
   p' = p_1+ip_2,
   p''= p_3+p_0.
[what is eps^-(p)?]
These formulas become singular along the negative p_3-axis,
so several charts are needed to cover
```

For experiments one usually uses nearly monochromatic light bundled into narrow beams. If one also ignores the directions (which are usually fixed by the experimental setting, hence carry no extra information), then only the helicity degrees of freedom remain, and the 1-photon part of the beam behaves like a 2-level quantum system ('a single spin').

A general monochromatic beam with fixed direction in a pure state is given by a second-quantized state vector, which is a superposition of arbitrary multiphoton states in the Bosonic Fock space generated by the two helicity degrees of freedom. This is the basis for most quantum optics experiments probing the foundations of quantum mechanics.

```
The simplest state of light (generated for example by
lasers) is a coherent state, with state vector proportional to
    e(A) = |vac> + |A> + 1/sqrt(2!) |A> tensor |A>
                 + 1/sqrt(3!) |A> tensor |A> tensor |A> + ...
where |A> is a one-photon state. Thus coherent states also have the
same degrees of freedom as classical electromagnetic radiation.
Indeed, light in coherent states behaves classically in most respects.
```

At low intensity, the higher order terms in the expansion are negligible, and since the vacuum part is not directly observable, a low intensity coherent states resembles a single photon state.

On the other hand, true single photon states are very hard to produce to good accuracy, and were created experimentally only recently:
B.T.H. Varcoe, S. Brattke, M. Weidinger and H. Walther,
Preparing pure photon number states of the radiation field,
Nature 403, 743--746 (2000).
see also
http://www.qis.ucalgary.ca/quantech/fock.html
Ordinary light is essentially never, and high-tech light almost never, describable by single photons.

A good informal discussion of what a photon is from a more practical perspective was given by Paul Kinsler in
http://www.lns.cornell.edu/spr/2000-02/msg0022377.html
But this does not tell the whole story. An interesting collection of articles explaining different current views is in
The Nature of Light: What Is a Photon?
Optics and Photonics News, October 2003
http://www.osa-opn.org/Content/ViewFile.aspx?Id=3185

The standard reference for quantum optics is
L. Mandel and E. Wolf,
Optical Coherence and Quantum Optics,
Cambridge University Press, 1995.
Mandel and Wolf write (in the context of localizing photons), about the temptation to associate with the clicks of a photodetector a concept of photon particles. [If there is interest, I can try to recover the details.] The wording suggests that one should resist the temptation, although this advice is usually not heeded. However, the advice is sound since a photodetector clicks even when it detects only classical light! This follows from the standard analysis of a photodetector, which treats the light classically and only quantizes the detector. Thus the clicks are an artifact of photodetection caused by the quantum nature of matter, rather than a proof of photons arriving!!!

A coherent light source (laser) produces a coherent state of light, which is a superposition of the vacuum state, a 1-photon state, a 2-photon state, etc, with squared amplitudes given by a Poisson

distribution. At low intensity, this is misinterpreted in practice as random single photons arriving at the end of the beam in a random Poisson process, because the photodetector produces clicks according to this distribution.

Incoherent light sources usually consist of thermal mixtures and produce other distributions, but otherwise the description (and misinterpretation) is the same.
Nevertheless, one must understand this misinterpretation in order to follow much of the literature on quantum optics.

Thus the talk about photons is usually done inconsistently; almost everything said in the literature about photons should be taken with a grain of salt.
There are even people like the Nobel prize winner Willis E. Lamb (the discoverer of the Lamb shift) who maintain that photons don't exist. See towards the end of

http://web.archive.org/web/20040203032630/www.aro.army.mil/phys/proceed.htm

The reference mentioned there at the end appeared as

W.E Lamb, Jr.,
Anti-Photon,
Applied Physics B 60 (1995), 77--84

This, together with the other reference mentioned by Lamb, is reprinted in

W.E Lamb, Jr.,
The interpretation of quantum mechanics,
Rinton Press, Princeton 2001.

I think the most apt interpretation of an 'observed' photon as used in practice (in contrast to the photon formally defined as above) is as a low intensity coherent state, cut arbitrarily into time slices carrying an energy of h*nu = hbar*omega, the energy of a photon at frequency nu and angular frequency omega.
Such a state consists mostly of the vacuum (which is not directly observable hence can usually be neglected), and the contributions of the multiphoton states are negligible compared to the single photon contribution.
With such a notion of photon, most of the actual experiments done make sense, though it does not explain the quantum randomness of the detection process (which comes from the quantized electrons in the detector).

A nonclassical description of the electromagnetic field where states of light other than coherent states are required is necessary mainly for special experiments involving recombining split beams, squeezed

state amplification, parametric down-conversion, and similar
arrangements where entangled photons make their appearance.
There is a nice booklet on this kind of optics:
U. Leonhardt,
Measuring the Quantum State of Light,
Cambridge, 1997.

Nonclassical electromagnetic fields are also relevant in the
scattering of light, where there are quantum corrections
due to multiphoton scattering. These give rise to important effects
such as the Lamb shift, which very accurately confirm the quantum
nature of the electromagnetic field. They involve no observable
photon states, but only virtual photon states, hence they are unrelated
to experiments involving photons. Indeed, there is no way to observe
virtual particles, and their name was chosen to reflect this.
(Observed particles are always onshell, hence massless for photons,
whereas it is an easy exercise that the virtual photon mediating
electromagnetic interaction of two electrons in the tree approximation
is never onshell.)

4.9 Particle positions and the position operator

The standard probability interpretation for quantum particles
is based on the Schr"odinger wave function psi(x), a square integrable
single- or multicomponent function of position x in R^3.
Indeed, with ^* denoting the conjugate transpose,
rho(x) := psi(x)^*psi(x)
is generally interpreted as the probability density to find (upon
measurement) the particle at position x. Consequently,
Pr(Z) := integral_Z dx |psi(x)|^2
is interpreted as the probability of the particle being in the open
subset Z of position space. Particles in highly localized states
are then given by wave packets which have no appreciable size
|psi(x)| outside some tiny region Z.

If the position representation in the Schr"odinger picture exists,
there is also a vector-valued position operator x, whose components
act on psi(x) by multiplication with x_j (j=1,2,3). In particular,
the components of x commute, satisfy canonical commutation relations
with the conjugate momentum
p = -i hbar partial_x,
and transform under rotations like a 3-vector, so that the commutation
relations with the angular momentum J take the form
[J_j,x_k] = i eps_{jkl} x_l.

Moreover, in terms of the (unnormalizable) eigenstates |x,m> of the position operator correponding to the spectral value x (and a label m to distinguish multiple eigenstates) we can recover the position representation from an arbitrary representation by defining psi(x) to be the vector with components

psi_m(x) := <x,m|psi>.

Therefore, if we have a quantum system defined in an arbitrary Hilbert space in which a momentum operator is defined, the necessary and sufficient condition for the existence of a spatial probability interpretation of the system is the existence of a position operator with commuting components which satisfy standard commutation relations with the components of the momentum operator and the angular momentum operator.

Thus we have reduced the existence of a probability interpretation for particles in a bounded region of space to the question of the existence of a position operator with the right properties.
We now investigate this existence problem for elementary particles, i.e., objects represented by an irreducible representation of the full Poincare group. We consider first the case of particles of mass m>0, since the massless case needs additional considerations.

A. Massive case, m>0:

Let M := R^3 be the manifold of 3-momenta p. On the Hilbert space H_m^d obtained by completion of the space of all C^infty functions with compact support from M to the space C^d of d-component vectors with complex entries, with inner product defined by

<phi|psi> := integral d\p/sqrt(p^2+m^2) phi(p)^*psi(p),

we define the position operator

q := i hbar partial_p,

which satisfies the standard commutation relations, the momentum in time direction,

p_0 := sqrt(m^2+|p|^2),

where m>0 is a fixed mass, and the operators

J := q x p + S,

K := (p_0 q + q p_0)/2 + p x S/(m+p_0),

where S is the spin vector in a unitary representation of so(3) on the vector space C^d of complex vectors of length d, with the same commutation relations as J.

This is a unitary representation of the Poincare algebra; verification of the standard commutation relations (given, e.g., in Weinberg's Volume 1, p.61) is straightforward.
It is not difficult to show that this representation is irreducible

and extends to a representation of the full Poincare group.
Obviously, this representation carries a position operator.

Since the physical irreducible representations of the Poincare group are uniquely determined by mass and spin, we see that in the massive case, a position operator must always exist. An explicit formula in terms of the Poincare generators is obtained through division by m in the formula

mq = K - ((K dot p) p/p_0 + J x p)/(m+p_0),

which is straightforward, though a bit tedious to verify from the above. That there is no other possibility follows from

T.F. Jordan
Simple derivation of the Newton-Wigner position operator
J. Math. Phys. 21 (1980), 2028-2032.

Note that the position operator is always observer-dependent, in the sense that one must choose a timelike unit vector to distinguish space and time coordinates in the momentum operator. This is due to the fact that the above construction is not invariant under Lorentz boosts (which give rise to equivalent but different representations).

Note also that in case of the Dirac equation, the position operator is _not_ the operator multiplying a solution psi(x) of the Dirac equation by the spacelike part of x (which would mix electron and positron states), but a related operator obtained by first applying a so-called Foldy-Wouthuysen transformation.

L.L. Foldy and S.A. Wouthuysen,
On the Dirac Theory of Spin 1/2 Particles and Its Non-Relativistic Limit,
Phys. Rev. 78 (1950), 29-36.

B. Massless case, m=0:

Let M_0 := R^3\{0} be the manifold of nonzero 3-momenta p, and let

p_0 := |p|, n := p/p_0.

The Hilbert space H_0^d (defined as before but now with m=0 and with M_0 in place of M)
obtained by completion of the space of all C^infty functions with compact support from M to the space C^d of d-component vectors with complex entries, with inner product defined by

<phi|psi> := integral d\p/sqrt(p^2+m^2) phi(p)^*psi(p),

carries a natural massless representation of the Poincare algebra, defined by

J := q x p + S,
K := (p_0 q + q p_0)/2 + n x S,

where q = i hbar partial_p is the position operator, and S is the spin vector in a unitary representation of so(3) on C^d, with the same commutation relations as J.
Again, verification of the standard commutation relations is straightforward. (Indeed, this representation is the limit of the above massive representation for m --> 0.)

It is easily seen that the helicity
   lambda := n dot S
is central in the (suitably completed) universal envelope of the Lie algebra, and that the possible eigenvalues
of the helicity are s,s-1,...,-s, where s=(d-1)/2. Therefore, the eigenspaces of the helicity operator carry by restriction unitary representations of the Poincare algebra, which are easily seen to be irreducible. They extend to a representation of the connected Poincare group. Moreover, the invariant subspace H_s formed by the direct sum of the eigenspaces for helicity s and -s form a massless irreducible spin s representation of the full Poincare group.

(It is easy to see that changing K to K-t(p_0)p for an arbitrary differentiable function t of p_0 preserves all commutation relations, hence gives another representation of the Poincare algebra.
Since the massless irreducible representations of the Poincare group are uniquely determined by their spin, the resulting representations are equivalent. This corresponds to the freedom below in choosing a position operator.)

Now suppose that a Poincare invariant subspace H of L^2(M_0)^d has a position operator x satisfying the canonical commutation relations with p and the above commutator relations with J. Then F=q-x commutes with p, hence its components must be a (possibly matrix-valued) function F(p) of p. Commutation with p implies that partial_p x F = 0, and, since M_0 is simply connected, that F is the gradient of a scalar function f. Rotation invariance then implies that this function depends only on p_0=|p|. Thus
    F = partial_p f(p_0) = f'(p_0) n.
Thus the position operator takes the form
   x = q - f'(p_0) n.
In particular,
   x x p = q x p.
Now the algebra of linear operators on the dense subspace of C^infty functions in H contains the components of p, J, K and x, hence those of
   J - x x p = J - q x p = S.
Thus the (p-independent) operators from the spin so(3) act on H.
But this implies that either H=0 (no helicity) or H = L^2(M_0)^d (all helicities between s and -s).

Since the physical irreducible representations of the Poincare group are uniquely determined by mass and spin, and for s>1/2, the spin s Hilbert space H_s is a proper, nontrivial subspace of L^2(M_0)^d, we proved the following theorem:

Theorem.
An irreducible representations of the full Poincare group with mass m>=0 and finite spin has a position operator transforming like a 3-vector and satisfying the canonical commutation relations if and only if either m>0 or m=0 and s<=1/2 (but s=0 if only the connected poincare group is considered).

This theorem was announced without giving details in
T.D. Newton and E.P. Wigner,
Localized states for elementary systems,
Rev. Mod. Phys. 21 (1949), 400-406.
A mathematically rigorous proof was given in
A. S. Wightman,
On the Localizability of Quantum Mechanical Systems,
Rev. Mod. Phys. 34 (1962), 845-872.
See also
T.F. Jordan
Simple proof of no position operator for quanta with zero mass and nonzero helicity
J. Math. Phys. 19 (1980), 1382-1385.
who also considers the massless representations of continuous spin, and
D Rosewarne and S Sarkar,
Rigorous theory of photon localizability,
Quantum Opt. 4 (1992), 405-413.

For spin 1, the case relevant for photons, we have d=3, and the subspace of interest is the space H obtained by completion of the space of all vector-valued C^infty functions A(p) of a nonzero 3-momentum p with compact support satisfying the transversality condition p dot A(p)=0,
with inner product defined by
<A|A'> := integral dp/|p| A(p)^* A'(p).
It is not difficult to see that one can identify the wave functions A(p) with the Fourier transform of the vector potential in the radiation gauge where its 0-component vanishes. This relates the present discussion to that given in the FAQ entry ''What is a photon?''.

As a consequence of our discussion, photons (m=0, s=1) and gravitons (m=0, s=2) cannot be given natural probabilities for being in any given bounded region of space. Chiral spin 1/2 particles also do not have a position operator and hence have no such probabilities, by the same argument, applied to the connected Poincare group.

(Note that measured are only frequencies, intensities and S-matrix elements; these don't need a well-defined position concept but only a well-defined momentum concept, from which frequencies can be found via omega=p_0/hbar - since c=1 in the present setting, and directions via n = p/p_0.)

However, assuming there are scalar massless Higgs particles (s=0), one could combine such a higgs, a photon, and a graviton into a single reducible representation on L^2(M_0)^5, using the above construction. By our derivation, one can find position eigenstates which are superpositions of Higgs, photon, and graviton. Thus to be able to regard photons and gravitons as particles with a proper probability interpretation, one must consider Higgs, photons, and gravitons as aspects of the same localizable particle, which we might call a graphoton. (Without gravity, a phiggs particle would also do.)

Related papers:

M.H.L. Pryce,
Commuting Co-ordinates in the new field theory,
Proc. Roy. Soc. London Ser. A 150 (1935), 166-172.
(first construction of position operators in the massive case)

B. Bakamjian and L.H. Thomas,
Relativistic Particle Dynamics. II,
Phys. Rev. 92 (1953), 1300-1310.
(first construction of massive representations along the above lines)

L.L. Foldy,
Synthesis of Covariant Particle Equations,
Physical Review 102 (1956), 568-581.
(nice and readable version of the Bakamjian-Thomas construction for massive representations of the Poincare group)

R. Acharya and E. C. G. Sudarshan,
''Front'' Description in Relativistic Quantum Mechanics,

J. Math. Phys. 1 (1960), 532-536.
(a ''most local'' description of the photon by wave fronts)

I. Bialynicki-Birula,
Photon wave function,
http://arxiv.org/abs/quant-ph/0508202
(A 53 page recent review article, covering various possibilities to define photon wave functions without a position operator acting on them. The best is (3.5), with a nonstandard inner product (5.8). What is left of the probability interpretation is (5.28) and its subsequent discussion.)

See also the entry ''Localization and position operators'' in this FAQ.

There are a few papers by M. Hawton, e.g.
http://arxiv.org/abs/quant-ph/0101011
http://arxiv.org/abs/0711.0112v1
on a nonstandard position operator which does not transform like a 3-vector. This is unphysical since it does not give orientation independent probabilities for observing a photon in a given region of space. Claims to the contrary in
http://lanl.arxiv.org/pdf/0804.3773v2,
supposedly constructing a Lorentz invariant photon number density, are erroneous; see
http://groups.google.at/group/sci.physics.research/browse_thread/thread/815435df4b

Other nonstandard position operators violating the conditions necessary for a probability interpretation were discussed earlier, starting with
M.H.L. Pryce,
The Mass-Centre in the Restricted Theory of Relativity and Its Connexion with the Quantum Theory of Elementary Particles,
Proc. Roy. Soc. London, Ser. A, 195 (1948), 62-81.

4.10 Localization and position operators

Position operators are part of the toolkit of relativistic quantum mechanics.

In a relativistic setting, one always has a representation of the Poincare algebra. From the generators of the Poincare algebra (namely the 4-momentum p, the angular momentum \J, and the boost generators \K) one can make up (in massive representations)

a nonlinear expression for a 3-dimensional \x (the position operator) that together with the space part \p of the 4-momentum has canonical commutation rules and hence gives a Heisenberg algebra.
(The backslash is a convenient ascii notation to indicate bold face letters, corresponding to 3-vectors.)

The position operator so constructed is unique, once the time coordinate is fixed, and is usually called the Newton-Wigner position operator, although it appears already in earlier work of Pryce. Relevant applications are related to the names Foldy and Wuythousen (for their transform of the Dirac equation, widely used in relativistic quantum chemistry) and Bakamjian and Thomas (for their relativistic multi-particle theories); both groups rediscovered the Newton-Wigner results independently, not being aware of their work.

That the time coordinate has to be fixed means that the position operator is observer-dependent. Each observer splits space-time into its personal time (in direction of its total 4-momentum) and personal 3-space (orthogonal to it), and the position operator relates to this 3-space. By a Lorentz transformation, one can transform the 4-momentum to the vector (E_obs 0 0 0), which makes time the 0-component. Most papers on the subject work in the latter setting.

For massless representations of spin >1/2, the construction breaks down. This is related to the fact that massless particles with spin >1/2 don't have modes of all helicities allowed by the spin (e.g., photons have spin 1 but no longitudinal modes), which makes them being always spread out, and hence not completely localizable. For details, see the FAQ entry
    ''Particle positions and the position operator''

Here are a few references:

J.P. Costella and B.H.J. McKellar,
The Foldy-Wouthuysen transformation,
arXiv:hep-ph/9503416
* This paper discusses the physical relevance of the Newton-Wigner representation, and its relation to the Foldy-Wouthuysen transformation

T. D. Newton, E. P. Wigner,
Localized States for Elementary Systems,
Rev. Mod. Phys. 21 (1949) 400-406
* The original paper on localization

L. L. Foldy and S. A. Wouthuysen,

On the Dirac Theory of Spin 1/2 Particles and Its Non-Relativistic
Limit,
Phys. Rev. 78 (1950), 29-36.
* On the transform of the Dirac equation now carrying the author's name

B. Bakamjian and L. H. Thomas
Relativistic Particle Dynamics. II
Phys. Rev. 92 (1953), 1300-1310.
and related papers in
Phys. Rev. 85 (1952), 868-872.
Phys. Rev. 121 (1961), 1849-1851.
* First constructive papers on relativistic multiparticle dynamics,
based on a 3D position operator

L. L. Foldy,
Synthesis of Covariant Particle Equations,
Phys. Rev. 102 (1956), 568-581
* A lucid exposition of Poincare representations which start with
a 3D position operator, and a discussion of electron localization
Before eq. (189), he notes that an observer-independent localization
of a Dirac electron (which generally is considered to be a pointlike
particle since it can be exactly localized in a given frame)
necessarily leaves a fuzziness of the order of the Compton wavelength
of the particle. (This is also related to the so-called Zitterbewegung,
see, e.g., the discussion in Chapter 7 of Paul Strange's
"Relativistic Quantum Mechanics".)

A. S. Wightman,
On the Localizability of Quantum Mechanical Systems,
Rev. Mod. Phys. 34 (1962) 845-872
* A group theoretic view in terms of systems of imprimitiviy

T. O. Philips,
Lorentz invariant localized states,
Phys. Rev. 136 (1964), B893-B896.
* A covariant coherent state alternative which does not require
to single out a time coordinate

V. S. Varadarajan,
Geometry of Quantum Theory
(second edition), Springer, 1985
* A book discussing some of this stuff

L. Mandel and E. Wolf,
Optical Coherence and Quantum Optics,
Cambridge University Press, 1995.

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* The bible on quantum optics, a thick but very useful book.
Relevant here since it contains a good discussion of the
localizability of photons (which can be done only approximately,
in view of the above) from a reasonably practical point of view.

G.N. Fleming,
Reeh-Schlieder meets Newton-Wigner
http://philsci-archive.pitt.edu/archive/00000649/
* This paper gives some relations to quantum field theory
```

4.11 $SO(3) = SU(2)/\mathbb{Z}_2$

In this appendix we wish to show that $SO(3)SU(2)/\mathbb{Z}_2$. First we collect some basics on $SO(3)$ and $SU(2)$.

A real 3×3 matrix R is called special orthogonal if

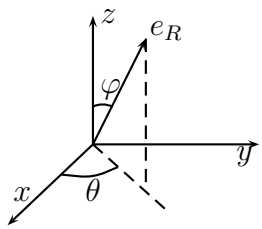
$$R^T R = 1\,, \quad \det R = 1\,.$$

Note that 1 here denotes the 3×3 identity matrix in the first equation. It is easy to check that the special orthogonal matrices form a group; we denote this group by $SO(3)$ and call it the special orthogonal group, or the rotation group. An element of $SO(3)$ is also called a rotation.

If λ is an eigenvalue of $R \in SO(3)$ we see that $\lambda = \pm 1$. We want to show that there is always an eigenvector with eigenvalue 1. The characteristic polynomial of R has three roots λ_1, λ_2 and λ_3. The modulus of the roots has to be 1 and if there is a imaginary eigenvalue μ, then so is its conjugate $\bar{\mu}$ an eigenvalue. If all the three eigenvalues are real, then the only possibilities are that all three are 1 or that two are -1 and the third is 1. Let now λ_1 be imaginary and take $\lambda_2 = \bar{\lambda}_1$. Then $\lambda_3 = \frac{1}{\lambda_1 \lambda_1}$ is real and positive and since it has to be of unit modulus $\lambda_3 = 1$. We see that there is always an eigenvalue 1. If R is a rotation and not the identity there is just one eigenvector with eigenvalue one; we denote this eigenvector by e_R. We thus have $Re_R = e_R$ and if $R \neq 1$ then e_R is unique. The vector e_R determines a one-dimensional subspace of $\mathbb{R}$ that is left invariant under the action of R. We call this one-dimensional invariant subspace the axis of rotation.

Consider an arbitrary $SO(3)$ element R with axis of rotation determined by e_R over an angle ψ and denote the rotation by $R(e_R, \psi)$. Call the angle between the plane in which e_R and the z-axis lie and the plane in xz-plane θ. Call the angle between e_R and the z-axis φ. See figure 4.1. The rotation can now be broken down into three rotations. First we use two rotations two go to a coordinate system with coordinates x', y' and z' in which the e_R points in the z'-direction, and then we rotate around the z'-axis over an angle ψ. The two rotation to go to the new coordinate system are: (a) a rotation around the z-axis around an angle θ to align the x-axis with the projection of e_R onto the xy-plane, (b) a rotation

Figure 4.1: Rotation around e_R. Any axis is characterized by two angles φ and θ.



over an angle φ around the image of the y-axis under the first rotation. Hence we can write $R(e_R, \psi)$ as a product

$$R(e_R, \psi) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\varphi & 0 & \sin\varphi \\ 0 & 1 & 0 \\ -\sin\varphi & 0 & \cos\varphi \end{pmatrix} \begin{pmatrix} \cos\psi & -\sin\psi & 0 \\ \sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{pmatrix} .$$

In this way we obtain a system of coordinates on the manifold $SO(3)$. The three angles are then called the Euler angles.

We note in particular the following: The group $SO(3)$ is generated by all elementary rotations $R_x(\alpha)$, $R_y(\beta)$ and $R_z(\gamma)$ given by

$$\begin{aligned} R_x(\alpha) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix} , \quad R_y(\beta) = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} , \\ R_z(\gamma) &= \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} . \end{aligned}$$

A 2×2 complex matrix U is called special unitary if it satisfies

$$U^\dagger U = 1 , \quad \det U = 1 .$$

It is easily checked that the special unitary matrices form a group, which is called the special unitary group and is denoted $SU(2)$.

We now wish to show that $SU(2)$ is a real manifold that is isomorphic to the three sphere S^3. We do this by finding an explicit parametrization of $SU(3)$ in terms of two complex numbers x and y satisfying $|x|^2 + |y|^2 = 1$. If one splits up x and y in a real and imaginary parts, one sees that x and y define a point on S^3.

We write an element $U \in SU(2)$ as

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix} .$$

Writing out the equation $U^\dagger U = 1$ and $\det U = 1$ one finds the following equations:

$$\begin{aligned} &|a|^2 + |c|^2 = 1 , \qquad |b|^2 + |d|^2 = 1 , \\ &\bar{a}b + \bar{c}d = 0 , \qquad ad - bc = 1 . \end{aligned}$$

We first assume $b = 0$ and find then that $ad = 1$ and $\bar{c}d = 0$, implying that $c = 0$ and U is diagonal with $a = \bar{d}$. Next we suppose $b \neq 0$ and use $a = -\frac{c\bar{d}}{b}$ to deduce that $|b| = |c|$ and $|a| = |d|$; we thus have $b \neq 0 \Leftrightarrow c \neq 0$. We also see that we can use the ansatz

$$\begin{aligned} a &= e^{i\alpha}\cos\theta\,, \qquad b = e^{i\beta}\sin\theta\,, \\ c &= -e^{i\gamma}\sin\theta\,, \quad d = e^{i\delta}\cos\theta\,. \end{aligned}$$

Using again $a = -\frac{c\bar{d}}{b}$ we see $\alpha + \delta = \beta + \gamma$ and writing out $ad - bc = 1$ we find $\alpha = -\delta$ and $\beta = -\gamma$. We thus see $a = \bar{d}$ and $b = -\bar{c}$. Hence the most general element of $SU(2)$ can be written as

$$U(x, y) = \begin{pmatrix} x & y \\ -\bar{y} & \bar{x} \end{pmatrix}, \quad \text{with } |x|^2 + |y|^2 = 1\,.$$

The map $S^3 \to SU(2)$ given by $(x, y) \mapsto U(x, y)$ is clearly injective, and from the above analysis bijective. Furthermore the map is smooth. Hence we conclude that $SU(2) \cong S^3$ as a real manifold.

We introduce the Pauli matrices[1]

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that the Pauli-matrices are precisely all the traceless Hermitian 2×2 complex matrices and make up a three-dimensional vector space. Therefore they provide a realization of the Lie algebra $su(2)$. It is easy to check that the Pauli-matrices satisfy the relations

$$\sigma^i\sigma^j = \delta^{ij} + i\epsilon^{ijk}\sigma^k\,,$$

where we also used the Levi–Civitá symbol ϵ^{ijk}; if (ijk) is not a permutation of (123) ϵ^{ijk} is zero and if (ijk) is a permutation of (123) then ϵ^{ijk} is the sign of the permutation. In particular we note the commutator relations

$$[\sigma^i, \sigma^j] = \sigma^i\sigma^j - \sigma^j\sigma^i = 2i\epsilon^{ijk}\sigma^k\,,$$

which resembles the vector product in $\mathbb{R}^3$. We also note the identities

$$\mathrm{tr}(\sigma^i) = 0\,, \quad \mathrm{tr}(\sigma^i\sigma^j) = 2\delta^{ij}\,, \quad \mathrm{tr}([\sigma^i, \sigma^j]\sigma^k) = 4i\epsilon^{ijk}\,.$$

For every vector $\vec{x} \in \mathbb{R}$ we identify an element x of $su(2)$ as follows

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \leftrightarrow x = \sum_{i=1}^{3} x_i\sigma^i\,.$$

From now on we simply identify the elements with each other and thus write equality signs instead of arrows. We see that $\vec{x} \times \vec{y}$ corresponds to the element $\frac{1}{2i}[x, y]$;

$$\vec{x} \times \vec{y} = \frac{1}{2i}[x, y]\,.$$

[1] Actually they are rescaled versions of the Pauli-matrices

And similarly we find

$$\vec{x}\cdot\vec{y} = \frac{1}{2}\,\mathrm{tr}(xy)\,, \quad \vec{x}\times\vec{y}\cdot\vec{z} = \frac{1}{4i}\,\mathrm{tr}([x,y]z)\,.$$

If U is an element of $SU(2)$ and $x \in su(2) \cong \mathbb{R}^3$ we see that

$$\mathrm{tr}(UxU^{-1}) = 0\,, \quad (UxU^{-1})^\dagger = (U^{-1})^\dagger x U^\dagger = UxU^{-1}\,,$$

and we conclude that U induces a map $\mathbb{R}^3 \to \mathbb{R}^3$. In fact, U defines a special orthogonal transformation since

$$\vec{x}\cdot\vec{y} \mapsto \mathrm{tr}(UxU^{-1}UyU^{-1}) = \vec{x}\cdot\vec{y}$$

is invariant, so that U preserves the inner product on $\mathbb{R}^3$ and similarly $\vec{x}\times\vec{y}\cdot\vec{z}$ is invariant so that the action of U preserves the orientation. We thus found a map $R : SU(2) \to SO(3)$, whereby $U \in SU(2)$ gets mapped to the element $R(U)$ in $SO(3)$ corresponding to $x \mapsto UxU^{-1}$. Since $U_1(U_2xU_2^{-1})U_1^{-1} = (U_1U_2)x(U_1U_2)^{-1}$ the map $SU(2) \to SO(3)$ is a group homomorphism; $R(U_1U_2) = R(U_1)R(U_2)$.

Explicitly we find

$$\begin{aligned}
U(x,y)\sigma^1U(x,y)^{-1} &= \mathrm{Re}(x^2-y^2)\sigma^1 - \mathrm{Im}(x^2-y^2)\sigma^2 + 2\mathrm{Re}(x\bar{y})\sigma^3\,,\\
U(x,y)\sigma^2U(x,y)^{-1} &= \mathrm{Im}(x^2+y^2)\sigma^1 + \mathrm{Re}(x^2+y^2)\sigma^2 + 2\mathrm{Im}(x\bar{y})\sigma^3\,,\\
U(x,y)\sigma^3U(x,y)^{-1} &= -2\mathrm{Re}(xy)\sigma^1 + 2\mathrm{Im}(xy)\sigma^2 + (|x|^2-|y|^2)\sigma^3\,.
\end{aligned}$$

Therefore

$$R(U(x,y)) = \begin{pmatrix} \mathrm{Re}(x^2-y^2) & \mathrm{Im}(x^2+y^2) & -2\mathrm{Re}(xy) \\ -\mathrm{Im}(x^2-y^2) & \mathrm{Re}(x^2+y^2) & 2\mathrm{Im}(xy) \\ 2\mathrm{Re}(x\bar{y}) & 2\mathrm{Im}(x\bar{y}) & |x|^2-|y|^2 \end{pmatrix}\,.$$

We find

$$\begin{aligned}
R(U(\cos\alpha/2, -i\sin\alpha/2)) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix} = R_x(\alpha)\,,\\
R(U(\cos\beta/2, -\sin\beta/2)) &= \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix} = R_y(\beta)\,,\\
R(U(e^{-i\gamma/2}, 0)) &= \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} = R_z(\gamma)\,,
\end{aligned}$$

and hence the map $R : SU(2) \to SO(3)$ is surjective. Suppose now that $U(x,y)$ is mapped to the identity element in $SO(3)$. We see then that $x\bar{y} = 0$, so that either $x = 0$ or $y = 0$. Since also $|x|^2 - |y|^2 = 1$, we cannot have $x = 0$ and hence $y = 0$. Furthermore from $\mathrm{Re}x^2 = |x|^2 = 1$ we see $x = \pm 1$: indeed we see that $R(U(x,y)) = R(U(-x,-y))$. The kernel of $R : SU(2) \to SO(3)$ is thus given by ± 1 times the identity matrix, which is the $\mathbb{Z}_2$-subgroup of $SU(2)$[2]. As any kernel of group homomorphisms, the kernel is a normal subgroup. All in all we have shown

$$SU(2) \cong SO(3)/\mathbb{Z}_2\,.$$

[2]Easy exercize: Prove that there is only one $\mathbb{Z}_2$-subgroup in $SU(2)$.

Chapter 5

Classical oscillating systems

In this chapter, we discuss in detail an important family of classical physical systems: harmonic or anharmonic oscillators, and their multivariate generalization, which describe systems of coupled oscillators such as macromolecules or planetary systems.

Understanding classical oscillators is of great importance in understanding many other physical systems. The reason is that an arbitrary classical system behaves close to equilibrium like a system of coupled linear oscillators. The equations we deduce are therefore approximately valid in many other systems. For example, a nearly rigid mechanical structure such as a high-rise building always remains close enough to equilibrium so that it can be approximately treated as a linear oscillating system for the elements into which it is decomposed for computational purposes via the finite element method.

We shall see that the equations of motion of coupled oscillators can be cast in a form that suggest a Lie algebra structure behind the formalism. This will provide the connection to Part III of the book, where Lie algebras are in the center of our attention.

Besides the (an-)harmonic oscillators we discuss some basic linear partial differential equations of physics: the Maxwell equations describing (among others) light and gamma rays, the Schrödinger equation and the Klein–Gordon equation (describing alpha rays), and the Dirac equation (describing beta rays). The solutions of these equations can be represented in terms of infinitely many harmonic oscillators, whose quantization (not treated in this book) leads to quantum field theory.

5.1 Systems of damped oscillators

For any quantity x depending on time t, differentiation with respect to time is denoted by $\dot{x}$:

$$\dot{x} = \frac{d}{dt}x\,.$$

Analogously, n dots over a quantity represents differentiating this quantity n times with respect to time.

The **configuration space** is the space of possible positions that a physical system may attain, including external constraints. For the moment, we think of it as a subset in $\mathbb{R}^n$. A point in configuration space is generally denoted q. For example, for a system of N point masses, q is an N-tuple of vectors $\mathbf{q}_k \in \mathbb{R}^3$ arranged below each other; each $\mathbf{q}_k$ denotes the spatial coordinates of the kth moving point (planet, atom, node in a triangulation of the body of a car or building, etc.), so that $n = 3N$.

A **system of damped oscillators** is defined by the differential equation

$$M\ddot{q} + C\dot{q} + \nabla V(q) = 0\,. \tag{5.1}$$

The reader wishing to see simple examples should turn to Section 5.2; here we explain the contents of equation (5.1) in general terms. As before, q is the configuration space point $q \in \mathbb{R}^n$. The M and C are real $n \times n$-matrices, called the **mass matrix** and the **friction matrix**, respectively. The mass matrix is always symmetric and positive definite (and often diagonal, the diagonal entries being the masses of the components). The friction matrix need not be symmetric but is always positive semidefinite. The **potential** V is a smooth function from $\mathbb{R}^n$ to $\mathbb{R}$, i.e., $V \in C^\infty(\mathbb{R}^n, \mathbb{R})$, and ∇V is the gradient of V,

$$\nabla V = \left(\frac{\partial V}{\partial q_1}, \ldots, \frac{\partial V}{\partial q_n}\right)^T .$$

Here the **gradient operator** ∇ is considered as a vector whose components are the differential operators $\partial/\partial q_k$. In finite-element applications in structural mechanics, the mass matrix is created by the discretization procedure for a corresponding partial differential equation. In general, the mass may here be distributed by the discretization over all adjacent degrees of freedom. However, in many applications the mass matrix is diagonal;

$$M_{ij} = m_i \delta_{ij}\,,$$

where m_i is the mass corresponding to the coordinate q_i, and δ_{ij} is the **Kronecker symbol** (or Kronecker delta), which is 1 if $i = j$ and zero otherwise. In the example where $\mathbf{q}_k$ is a three-vector denoting the position of an object, then i is a multi-index $i = (k, j)$ where k denotes an object index and $j = 1, 2, 3$ is the index of the coordinate of the kth object which sits in position i of the vector q. Then m_i is the mass of the kth object.

The quantity F defined by

$$F(q) := -\nabla V(q)\,,$$

is the **force** on the system at the point q due to the potential $V(q)$. We define the **velocity** v of the oscillating system by

$$v := \dot{q}\,.$$

The **Hamiltonian energy** H is then defined by

$$H := \frac{1}{2} v^T M v + V(q)\,. \tag{5.2}$$

The first term on the right-hand side is called the **kinetic energy** since it depends solely on the velocity of the system. The second term on the right-hand side is called the **potential energy** and it depends on the position of the system. For more complex systems the potential energy can also depend on the velocities. Calculating the time-derivative of the Hamiltonian energy H we get

$$\dot{H} = v^T M\dot{v} + \nabla V(q) \cdot \dot{q} = \dot{q}^T(M\ddot{q} + \nabla V(q)) = -\dot{q}^T C\dot{q} \leq 0\,, \tag{5.3}$$

where the last equality follows from the differential equation (5.1) and the final inequality follows since C is assumed to be positive semidefinite. If $C = 0$ (the idealized case of no friction) then the Hamiltonian energy is constant, $\dot{H} = 0$, and in this case we speak of **conservative dynamics** (the Hamiltonian H is conserved). If C is positive definite we have $\dot{H} < 0$ unless $\dot{q} = 0$ and there is energy loss. This is called **dissipative dynamics**. In the dissipative case, the sum of the kinetic and potential energy has to decrease.

If the potential V is unbounded from below, it might happen that the system starts falling in a direction in which the potential is unbounded from below and the system becomes unphysical; the velocity could increase without limits. Thus, in a realistic and manageable physical system, the potential is always bounded from below, and we shall make this assumption throughout. It follows that the Hamiltonian is bounded from below.

Since in the dissipative case the Hamiltonian energy is decreasing and is bounded below, it will approach a limit as $t \to \infty$. Therefore, $\dot{H} \to 0$, and by (5.3), $\dot{q}^T C\dot{q} \to 0$. Since C is positive definite for a dissipative system, this forces $\dot{q} \to 0$. Thus, the velocities will get smaller and smaller, and asymptotically the system will approach the configuration of being in a state with $\dot{q} = 0$, at the level of the accuracy of the model. Typically this implies that q tends to some constant value q_0. Note that it does not follow rigorously that q tends to a constant value; it is possible that $q \to \infty$. Nevertheless we assume that q does not walk away to infinity and then it follows from $\dot{q} = 0$ that $\ddot{q} = 0$, so that (5.1) implies $\nabla V(q_0) = 0$, and we conclude that q tends to a stationary point q_0 of the potential. If this is a saddle point, small perturbations can (and will) cause the system to move towards another stationary point. Because of such stability reasons, the system ultimately moves towards a local minimum.

In practice, the perturbations come from imperfections in the model. Remember that the deterministic equation (5.1) is a mathematical idealization of the real world situation. A more appropriate model (but still an approximation) is the equation

$$M\ddot{q} + C\dot{q} + \nabla V(q) = \varepsilon\,,$$

where ε is a stochastic force, describing the imperfections of the model. Typically, these are already sufficient to guarantee with probability 1 that the system will not end up in a saddle point. Usually, imperfections are small, irregular jumps due to friction, see, e.g., Bowden & Leben [49], or Brownian motion due to kicks by molecules of a solvent. See, e.g., Brown [52], Einstein & Brown [79], Garcia & Palacios [98], Hanggi & Marchesoni [121], for an overview on Brownian motion with lots of historical references and citations Duplantier [75], and for a discussion in the context of protein folding Neumaier [202, Section 4].

In many cases, the potential $V(q)$ has several local minima. Our argument so far says that the state of the system will usually move towards one of these local minima. Around the local minimum it can oscillate for a while, and in the absence of stochastic forces it will ultimately get into one of the local minima. If we assume that there are stochastic imperfections, we can say even more!

Suppose that the local minimum towards which the system tends is not a global minimum. Then occasional stochastic perturbations may suffice to push (or kick) the system over a barrier separating the local minimum from a valley leading to a different minimum. Such a barrier is characterized by a **saddle point**, a stationary point where the Hessian of the potential has exactly one negative eigenvalue. The energy needed to pass the barrier, called the **activation energy**, is simply the difference between the potential energy of the separating saddle point and the potential energy of the minimum. In a simple, frequently used approximation, the negative logarithm of the probability of exceeding the activation energy in a given time span is proportional to the activation energy. This implies that small barriers are easy to cross, while high barriers are difficult to cross. In particular, if a system can cross a barrier between a high-lying minimum to a much lower lying minimum, it is much more likely to cross it in the direction of the lower minimum than in the other direction. This means that (averaged over a population of many similar systems) most systems will spend most of their time near low minima, and if the energy barriers between the different minima are not too high, most systems will be most of the time close to the global minimum. Thus a global minimum characterizes an **absolutely stable** equilibrium, while other local minima are only **metastable** equilibrium positions, which can become unstable under sufficiently large stochastic perturbations.

There are famous relations called **fluctuation-dissipation theorems** that assert (in a quantitative way) that friction is related to stochastic (i.e., not directly modeled high frequency) interactions with the environment. In particular, if a system is sufficiently well isolated, both friction and stochastic forces become negligible, and the system can be described as a conservative system. Of course, from a fundamental point of view, the only truly isolated system is the universe as a whole, since at least electromagnetic radiation escapes from all systems not enclosed in an opaque container, and systems confined to a container interact quite strongly with the walls of the container (or else the wall would not be able to confine the system).

Thus on a fundamental level, a conservative system describes the whole universe from the tiniest microscopic details to the largest cosmological facts. Such a system would have to be described by a quantum field theory that combines the successful standard model of particle physics with general relativity. At present, no such theory is available.

On the other hand, conservative systems form a good first approximation to many small and practically relevant systems, which justifies that most of the book looks at the conservative case only. However, in Part IV, the dissipative case is in the center of the discussion.

The phase space formulation. So far, our discussion was framed in terms of position and velocity. As we shall see, the Hamiltonian description is most powerful in phase space coordinates. Here everything is expressed in terms of the phase space observables q and p,

where

$$p := Mv\,,$$

is called the **momentum** p of the oscillating system. The **phase space** for a system of oscillators is the space of points $(q,p) \in \mathbb{R}^n \times \mathbb{R}^n$. A **state** (in the classical sense) is a point (p,q) in phase space. The **Hamiltonian function** (or simply the **Hamiltonian**) is the function defining the Hamiltonian energy in terms of the phase space observables p and q. In our case, since a positive definite matrix is always invertible, we can express v in terms of p as $v = M^{-1}p$, and find that

$$H(p,q) = \frac{1}{2}p^T M^{-1} p + V(q)\,. \tag{5.4}$$

Note that H does not depend explictly on time. (In this book, we only treat such cases; but in problems with time-dependent external fields, an explicit time dependence would be unavoidable.)

5.2 The classical anharmonic oscillator

To keep things simple, we concentrate on the case of a single degree of freedom. Everything said has a corresponding generalization to systems of coupled oscillators, but the essentials are easier to see in the simplest case.

The **simple anharmonic oscillator** is obtained by taking $n = 1$. The differential equation (5.1) reduces to a scalar equation

$$m\ddot{q} + c\dot{q} + V'(q) = 0\,, \tag{5.5}$$

where the prime denotes differentiation with respect to q. This describes for example the behavior of an object attached to a spring; then q is the length of the spring, $m = M$ is the mass of the object, $c = C$ is the friction constant (collective of the air, some friction in the spring itself, or of a surface if the object is lying on a surface) and $V(q)$ describes the potential energy (see below) the spring has when extended or contracted to length q. Note that a constant shift in the potential does not alter the equations of motion of an anharmonic oscillator; hence the potential is determined only up to a constant shift.

The **harmonic oscillator** is the special case of the anharmonic oscillator defined by a potential of the form

$$V(q) = \frac{k}{2}(q - q_0)^2\,, \quad k > 0\,,$$

where q_0 is the equilibrium position of the spring. (Strictly speaking, only oscillators that are not harmonic should be called anharmonic, but we follow the mathematical practice where limiting cases are taken to be special cases of the generic concept: A linear function is also nonlinear, and a real number is also complex.) In this case, the force becomes

$$F(q) = -\nabla V(q) = -k(q - q_0) \tag{5.6}$$

The equation (5.6) is sometimes called **Hooke's law**, which asserts that the force needed to pull a spring from equilibrium is linear in the deviation $q - q_0$ from equilibrium, a valid approximation when $q - q_0$ is small. Since the force is minus the gradient of the potential, the potential has to be quadratic to reproduce Hookes' law. It is customary to shift the potential such that it vanishes in global equilibrium; then one gets the above form, and stability of the equilibrium position dictates the sign of k. Note that the shift does not change the force, hence has no physical effect.

The **mathematical pendulum** is described by the equation

$$V(q) = -k(1 - \cos q)\,, \quad k > 0\,, \tag{5.7}$$

where q is now the angle of deviation from the equilibrium, measured in radians. Looking at small q we can approximate as follows:

$$V(q) = \frac{k}{2}q^2 + O(q^4)\,,$$

and after dropping the error term, we end up with a harmonic oscillator. The same argument allows one to approximate an arbitrary anharmonic oscillator by a harmonic oscillator as long as the oscillations around a stable equilibrium position are small enough.

For q not small the mathematical pendulum is far from being harmonic. Physically this is clear; stretching a (good) spring further and further is harder and harder, but pushing the one-dimensional pendulum 'far' from its equilibrium position is really different. After rotating it over π radians the pendulum is upside down and pushing it further no longer costs energy.

Dynamics in phase space. We now restrict to conservative systems and analyze the conservative anharmonic oscillator ($\dot{H} = 0$) a bit more. Since $c = 0$, the differential equation (5.5) simplifies to

$$m\ddot{q} + V'(q) = 0\,. \tag{5.8}$$

The Hamiltonian energy is given by

$$H = \frac{1}{2}mv^2 + V(q).$$

Note the form of the kinetic energy familiar from school. Expressed in terms of the phase space observables p and q (which are now scalar variables, not vectors), we have

$$H = \frac{p^2}{2m} + V(q),$$

$$\dot{q} = v = \frac{p}{m}\,, \quad \dot{p} = m\dot{v} = m\ddot{q} = -V'(q)\,. \tag{5.9}$$

An observable is something you can calculate from the state; simple examples are the velocity and the kinetic, potential, or Hamiltonian energy. Thus arbitrary observables

can be written as smooth functions $f(p,q)$ of the phase space observables. In precise terms, an **observable** is (for an anharmonic oscillator) a function $f \in C^\infty(\mathbb{R}\times\mathbb{R})$. The required amount of smoothness can be reduced in practical applications; on the fundamental theoretical level, it pays to require infinite differentiability to get rid of troubling exceptions.

Introducing the shorthand notation

$$f_p := \frac{\partial f}{\partial p}\,, \quad f_q := \frac{\partial f}{\partial q}\,,$$

for partial derivatives, we can write the equations (5.9) in the form

$$\dot q = H_p\,, \quad \dot p = -H_q\,. \tag{5.10}$$

The equations (5.10) are called the **Hamilton equations** in **state form**. Although derived here only for the anharmonic oscillator, the Hamilton equations are of great generality; the equations of motions of many (unconstrained) conservative physical systems can be cast in this form, with more complicated objects in place of p and q, and more complex Hamiltonians $H(p,q)$. A dynamical system governed by the Hamilton equations is called an **isolated Hamiltonian system**. If there are external forces, the system is not truly isolated, but the Hamilton equations are still valid in many cases, provided one allows the Hamiltonian to depend explicitly on time, $H = H(p,q,t)$; in this case, there would appear additional partial derivatives with respect to time in various of our formulas.

Calculating the time-dependence of an arbitrary observable f we get

$$\dot f = \frac{\partial f}{\partial p}\dot p + \frac{\partial f}{\partial q}\dot q = f_p\dot p + f_q\dot q\,,$$

hence

$$\dot f = H_p f_q - H_q f_p\,. \tag{5.11}$$

In particular for $f = q$ or $f = p$ we recover (5.10). Thus this formulation is equivalent to the Hamilton equations. We call (5.11) the Hamilton equations in **general form**. Let us apply (5.11) to $f = H$ and calculate the change of the Hamiltonian:

$$\dot H = H_p H_q - H_q H_p = 0\,,$$

which is consistent since we knew from the start that energy is conserved, $\dot H = 0$. But now this relation has been derived for arbitrary isolated Hamiltonian systems!

When external forces are present, we have to consider time-dependent observables $f(p,q,t)$. In this case, we have in place of (5.11)

$$\dot f = f_p\dot p + f_q\dot q + f_t\dot t = H_p f_q - H_q f_p + f_t\,, \tag{5.12}$$

and in particular for the Hamiltonian,

$$\dot H = H_t = \partial H/\partial t.$$

However, we restrict the subsequent discussion to the isolated case.

The Hamiltonian equations can be cast in a form that turns out to be even more general and very useful. It brings us directly to the heart of the subject of the present book. We define a binary operation $\angle$ on $C^\infty(\mathbb{R}\times\mathbb{R})$ as follows:

$$f\angle g := f_p g_q - g_p f_q\,.$$

Physicists write $\{g, f\}$ for $f\angle g$ and call it the **Poisson bracket**. Our alternative notation will turn out to be very useful, and generalizes in many unexpected ways. The equation (5.11) can then be written in form of a **classical Heisenberg equation**

$$\dot{f} = H\angle f. \tag{5.13}$$

It turns out that this equation, appropriately interpreted, is extremely general. It covers virtually *all* conservative systems of classical and quantum mechanics.

A basic and most remarkable fact, which we shall make precise in the following chapter, is that the vector space $C^\infty(\mathbb{R}\times\mathbb{R})$ equipped with the binary operation $\angle$ is a Lie algebra. We shall take this up systematically in Section 12.1.

5.3 Harmonic oscillators and linear field equations

Historically, radiating substances which produce rays of α-, β- or γ-particles were fundamental for gaining an understanding of the structure of matter. Even today, many experiments in physics are performed by rays (or beams, which is essentially the same) generated by some source and then manipulated in the experiments.

The oldest, most familiar rays are light rays, α-rays, β-rays, and γ-rays. (Nowadays, we also have neutron rays, etc., and cosmic rays contain all sorts of particles.)

All kinds of rays are described by certain quantum fields, obtained by quantizing corresponding classical field equations, linear partial differential equations whose time-periodic solutions provide the possible **single-particle modes** of the quantum fields. In the following sections we look at these field equations in some detail; here we just make some introductory comments.

α-rays are modes (realizations) of the field of doubly ionized helium, He^{++}, which is modeled on the classical level by a Schrödinger wave equation or a Klein–Gordon wave equation. β-rays are modes of a charged field of electrons or positrons, modeled on the classical level by a Dirac wave equation. For radiation of only positrons one uses the notation β^+, and for rays with only electrons one uses β^-. Both light rays and γ-rays are modes of the electromagnetic field which are modeled on the classical level by the Maxwell wave equations. Their quantization (which we do not treat in this book) produces the corresponding quantum fields.

In the present context, the Schrödinger, Klein–Gordon, Dirac, and Maxwell equations are all regarded as classical field equations for waves in $3+1$ dimensions, though they can also be regarded as the equations for a single quantum particle (a nonrelativistic or relativistic

scalar particle, an electron, or a photon, respectively). This dual use is responsible for calling **second quantization** the quantum field theory, the quantum version of the classical theory of these equations. It also accounts for the **particle-wave duality**, the puzzling property that rays sometimes (e.g., in photodetection or a Geiger counter) behave like a beam of particles, sometimes (in diffraction experiments, of which the double slit experiments are the most famous ones) like a wave – in the case of light a century-old conflict dating back to the times of Newton and Huygens.

In the quantum field setting, quantum particles arise as eigenstates of an operator N called the **number operator**. This operator has a discrete spectrum with nonnegative integer eigenvalues, counting the number of particles in an eigenstate. The ground state, with zero eigenvalue, is essentially unique, and defines the **vacuum**; a quantum particle has an eigenstate corresponding to the eigenvalue 1 of N, and eigenstates with eigenvalue n correspond to systems of n particles. If a quantum system contains particles of different types, each particle type has its own number operator.

The states that are easy to prepare correspond to beams. The fact that beams have a fairly well-defined direction translates into the formal fact that beams are approximate eigenstates of the momentum operator. Indeed, often beams are well approximated by exact eigenstates of the momentum operator, which describe so-called **monochromatic beams**. (Real beams are at best quasi-monochromatic, a term we shall not explain.) Since the states of beams are not eigenstates of the number operator N, they contain an indefinite number of particles.

All equations mentioned are linear partial differential equations, and behave just like a set of infinitely many coupled harmonic oscillators, one at each space position. They describe non-interacting fields in a homogeneous medium. The definition of interacting fields leaves the linear regime and leads into the heart of nonlinear field theory, both in a classical and a quantum version. This is outside the scope of the present book. However, when position space (or momentum space) is discretized so that only a finite number of degrees of freedon remain to describe a field, one is back to nonlinear oscillators, which can be understood completely on the basis of the treatment given here, and indeed, number operator will play a prominent role in Part V of this book.

Fortunately, for understanding beam experiments, it usually suffices to quantize a few modes of the classical field, and these are harmonic oscillators. Indeed, by separation of variables, the linear field equations can be decoupled in time, leading to a system of uncoupled harmonic oscillators forming the Fourier modes. Beams correspond to solutions which have a significant intensity only in a small neighborhood of a line in 3-space. Frequently, beams correspond to solutions that have an (almost) constant frequency. Interactions with such (quasi-)monochromatic beams can be modelled in many situations simply as interactions with a harmonic oscillator.

On the other hand, when a beam containing all frequencies interacts with a system which oscillates only with certain frequencies, the beam will resonate with these frequencies. This allows the detection of a system's eigenfrequencies by observing its interaction with light or other radiation. This is the basis of spectroscopy, and will be discussed in more detail

in Chapter 6 and Chapter 23.

Note that, just as the free Maxwell equations describe both classical electromagnetic waves (in particular light and γ-rays) or single photons (particles of the corresponding quantum field), so the Schrödinger equation, the Klein–Gordon equation, and the Dirac equation describe both classical fields for α- and β-rays, or single α-particles or electrons and positrons (particles of the corresponding quantum field), respectively.

In the following, we consider four kinds of classical fields and their associated quantum particles, differing in spin and hence in the way rotations and Lorentz transformations affect the fields.

- Slow bosons of spin zero, such as slow α-particles. The equation describing them is the Schrödinger equation.
- Fast bosons of spin zero, such as fast α-particles. The equation describing them is the Klein–Gordon equation.
- Fermionic particles of spin 1/2, like electrons, positrons and neutrinos. The dynamical equation in this case is the Dirac equation.
- Light and γ-rays; electromagnetic radiation. The corresponding particles are photons, which have spin 1. The field describing these particles is the electromagnetic field. The equations governing their dynamics are the Maxwell equations.

Because of the differing spin, there is a significant difference between β-rays and the others: α-particles and photons have integral spin and are therefore so-called **bosons**, while electrons and positrons have non-integral spin and are therefore so-called **fermions**. Only fermions are subject to the so-called **Pauli exclusion principle** which is responsible for the extensivity of matter. This difference is reflected by the fundamental requirement that the fields of bosons, in particular of α-particles and photons, are quantized by imposing **canonical commutation relations** (discussed in Section 20.2), while fermions, and hence positrons and electrons, are quantized by imposing **canonical anticommutation relations** (discussed in Section 21.1).

5.4 Alpha rays

We first consider rays consisting of **α-particles**, helium atoms stripped of their two electrons, and consist of two protons and two neutrons. α-particles are released by other heavier nuclei during certain processes in the nucleus. For example, some elements are α-radioactive, which means that a nucleus of type A will want to go to a lower energy level, which can then be done by emitting two of its protons and two of its neutrons. The result is thus two nuclei, a Helium nucleus and a nucleus of type $A' \neq A$; schematically $A \to A' + \alpha$. But also during nuclear splitting α-particles are released. Yet even more, the

sun is emitting α-particles all the time; the sun produces heat by means of a chain of nuclear fusion reactions, during which some α-particles are produced. If the atmosphere would not be there, life on earth would be impossible due to the bombardment of α-particles. That α-particles are not healthy has been in the news lately (in 2007), since the former Russian spy Litvinenko is said to have been killed by a small amount of polonium, which is an α-emitter.

An α-particle emitted from a radioactive nucleus typically has a speed of 15,000 kilometers per second. Although this might look very fast, it is only 5% of the speed of light, which means that for a lot of calculations α-particles can be considered **nonrelativistically**, that is, without using special relativity. For some more accurate calculations though, special relativity is required.

For the nonrelativistic α-particle we have to use the Schrödinger equation. For a particle of mass m moving in a potential $V(x)$ the Schrödinger equation is given by

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\nabla^2\psi(x,t) + V(x)\psi(x,t)$$

where ψ is the wave function of the particle, and $\nabla^2 = \nabla\cdot\nabla$ is the **Laplace operator**. The wave function contains the information about the particle. The quantity $|\psi(x,t)|^2$ is the probability density for finding the particle at time t in a given position (x). For beam considerations, we take $V(x) = 0$. Since we shoot the α-particles just in one direction, we assume $\psi(x,t) = \phi(t)\chi(x)$. We obtain

$$\frac{i\dot{\phi}(t)}{\phi(t)} = -\frac{\hbar}{2m}\frac{\chi''(x)}{\chi(x)}\,, \tag{5.14}$$

where the dot denotes the derivative with respect to time t and the prime ' the derivative with respect to the coordinate x. The left-hand side of (5.14) only depends on time t and the right-hand side only on x, which implies that both sides are a constant (with the dimensions of time^{-1}) independent of t and x. We denote this constant by ω and obtain two linear ordinary differential equations for ϕ and χ with the solutions

$$\phi(t) = e^{-i\omega t}\,, \quad \chi(x) = ae^{ikx} + b^*e^{-ikx}\,, \quad k = \sqrt{\frac{2m\omega}{\hbar}}\,,$$

where a and b are some constants; we have normalized the constant in front of ϕ to 1 since we are only interested in the product of ϕ and χ. Note that we wrote the solution suggestively as if $\omega \geq 0$ and in fact, on physical grounds it is; the solutions with $\omega < 0$ are not integrable and hence cannot determine a probability distribution.

We can express E in terms of k, which plays the role of the inverse wavelength, getting $\omega(k) = \frac{\hbar k^2}{2m}$. Reintroducing an arbitrary direction unit vector $\mathbf{n}$ and the wave vector $\mathbf{k} = k\mathbf{n}$, we obtain the **dispersion relation** of the Schrödinger equation,

$$\omega_{\mathbf{k}} = \frac{\hbar\mathbf{k}^2}{2m}\,.$$

Therefore the general solution can be expanded as

$$\psi(x,t) = \int d\mathbf{k} \left(a(\mathbf{k}) e^{-i\omega_{\mathbf{k}} t - i\mathbf{k}\dot{\mathbf{x}}} + b(\mathbf{k})^* e^{-i\omega_k t + i\mathbf{k}\dot{\mathbf{x}}} \right).$$

If we have an experiment with a great number of non-interacting particles, all of which have the same wave function ψ, the quantity $|\psi(x,t)|^2$ is proportional to the particle density. However, α-particles interact and thus the Hamiltonian is different. If we assume the particle density is not too high we can still assume that the α-particles move as if there were no other α-particles. Under this assumption we may again take $|\psi(x,t)|^2$ as the particle density. The energy density is then proportional to $|\psi(x,t)|^2$. Putting as before the whole experiment in a box of finite volume V one can again arrive at a Hamiltonian corresponding to a collection of independent harmonic oscillators.

Now we look at relativistic α-particles, and remind the reader of the notation introduced in Section 3.13. The dynamics of relativistic α-particles of mass m is described by a real-valued function $\psi(x^\mu)$ whose evolution is governed by the **Klein–Gordon equation**, which is given by

$$\left(\Box - \frac{m^2 c^2}{\hbar^2} \right) \psi = 0 \tag{5.15}$$

with the second order differential operator

$$\Box := -\frac{\partial^2}{c^2 \partial t^2} + \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2},$$

called the **d'Alembertian**. Here c is the speed of light. We look for wave like solutions $\psi \sim e^{ik\cdot x}$ for some vector $\mathbf{k}^\mu$. Note that $\partial_\mu e^{ik\cdot x} = ik_\mu e^{ik\cdot x}$ and hence $\Box e^{ik\cdot x} = \mp k^2 e^{ik\cdot x}$, where $k^2 = k \cdot k$. Hence we obtain the condition on k

$$\pm k^2 + \frac{m^2 c^2}{\hbar^2} = 0. \tag{5.16}$$

Writing $k^0 = \omega$ and denoting the spatial parts of k with bold $\mathbf{k}$ we thus get the dispersion relation

$$\omega = \pm \sqrt{c^2 \mathbf{k}^2 + \frac{m^2 c^4}{\hbar^2}}. \tag{5.17}$$

We see that $\hbar|\omega| = E = mc^2$, combining Einstein's famous formula $E = mc^2$ and Planck's law $E = \hbar\omega$. The solution for a given choice of sign of ω is expanded in Fourier terms and most often written as

$$\psi(x,t) = \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega(k)} \left(a(\mathbf{k}) e^{i\omega(k)t - i\mathbf{k}\cdot\mathbf{x}} + a(\mathbf{k})^* e^{-i\omega(k)t + i\mathbf{k}\cdot\mathbf{x}} \right),$$

where we used the Lorentz-invariant measure (3.62) involving $\omega(k) = \sqrt{c^2\mathbf{k}^2 + \frac{m^2c^4}{\hbar^2}}$.

5.5 Beta rays

We now discuss beams composed of spin $\frac{1}{2}$ particles, the β-rays. β-radiation is emitted by radioactive material. Unstable nuclei can lose some of their energy and go to a more stable

nucleus under the emission of β-rays. There are two kinds of β-rays – those with positive charge and those with negative charge. The negatively charged version consists of nothing more than **electrons**. The positively charged counterpart consists of the antiparticles of the electrons, the so-called **positrons**.

Other examples of fermions are neutrinos. The sun emits a stream of neutrinos; in each second, there are approximately 10^{13} neutrinos flying through your body (it depends on which latitude you are, how big you are and whether you are standing or lying down, making a difference of a factor of 100 perhaps). Neutrinos fly very fast; the solar neutrinos travel at the speed of light (or very close). The reason they travel that fast is that neutrinos have a zero or very tiny mass, and massless particles (such as photons) always travel at the speed of light. For a long time, neutrinos were believed to be massless; only recently it became an established fact that at least one of the three generations of neutrinos must have a tiny positive mass. We do not feel anything of the many neutrinos coming from the sun and steadily passing through our body, because – unlike protons and electrons – they hardly interact with matter; for example, to absorb half of the solar neutrinos, one would need a solid lead wall of around 10^{16} meters thick! The reason is that they do not have charge: they are electrically neutral.

To discuss the case that the particles shot by the beam are fermions, we have to use the Dirac equation. It is convenient to use the same conventions for dealing with relativistic particles. In addition to the previously introduced symbols, we now introduce the so-called γ-matrices. In four dimensions there are four of them, called $\gamma^0, \ldots, \gamma^3$, and they satisfy

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu} \,. \tag{5.18}$$

The associative algebra generated by the γ-matrices subject to the above relation is a **Clifford algebra**. There are several possibilities to find a representation for the γ-matrices in terms of 4×4-matrices; a frequently made choice is

$$\gamma^0 = i\sigma_1 \otimes 1 \,, \quad \gamma^1 = \sigma_2 \otimes 1$$

$$\gamma^2 = \sigma^3 \otimes \sigma^1 \,, \quad \gamma^3 = \sigma^3 \otimes \sigma^2 \,,$$

where the σ_k are the Pauli matrices (2.7). however, we only need the defining relation (5.18). We assemble the γ-matrices in a vector $(\gamma^0, \gamma^1, \gamma^2, \gamma^3)$ and inner products with vectors p^μ are given by $\gamma \cdot p = \gamma^\mu p_\mu = \gamma^\mu p^\nu \eta_{\mu\nu}$.

A fermion is described by a vector-like object ψ, which takes values in the spinor representation of the Lie algebra $so(3,1)$. Hence we can think of ψ as a vector with four-components. In this case, the γ-matrices are 4×4-matrices; that such a representation exists is shown by the explicit construction above. We need a property of the γ-matrices, namely that they are traceless (in any representation). To prove this, take any γ^μ and choose another γ-matrix γ^ν, $\mu \neq \nu$. Then we have

$$\operatorname{tr} \gamma^\mu = \operatorname{tr}\Big(\gamma^\mu \gamma^\nu (\gamma^\nu)^{-1}\Big) = -\operatorname{tr}\Big(\gamma^\nu \gamma^\mu (\gamma^\nu)^{-1}\Big) = -\operatorname{tr} \gamma^\mu \,.$$

Hence $\operatorname{tr} \gamma^\mu = 0$.

With these preliminaries the Dirac equation is given by

$$\left(\gamma \cdot \partial + \frac{mc}{\hbar}\right) \psi = 0 \,.$$

Acting on the Dirac equation with $(\gamma \cdot \partial - \frac{mc}{\hbar})$ and using $\gamma \cdot p \gamma \cdot p = p^2$ for any four-vector p^μ, we see that each component of the spinor obeys the Klein–Gordon equation (5.15).

We look for solutions of the form $\psi = u e^{ik\cdot x}$. Putting this ansatz in the Dirac equation we obtain

$$\left(i\gamma \cdot k - \frac{mc}{\hbar}\right) u = 0 \,, \tag{5.19}$$

and the additional constraint $k^2 + \frac{m^2c^2}{\hbar^2} = 0$ follows from the Klein–Gordon equation. Equation (5.19) can be written as

$$\left(1 - i\frac{\hbar}{mc}\gamma \cdot k\right) u = 0 \,,$$

and it is easy to see that

$$P = \frac{1}{2}\left(1 - i\frac{\hbar}{mc}\gamma \cdot k\right)$$

satisfies $P^2 = P$. Hence P is a projection operator and $\mathbb{C}^4$ splits as $V \oplus V'$ with $V = P\mathbb{C}^4$ and $V' = (1-P)\mathbb{C}^4$. The Dirac equation thus tells us that u has to be in V'. Denote $p^\mu = \frac{mc}{\hbar} k^\mu$, then $p^2 = -1$. We now choose a frame moving along with the particle, so that in that frame the particle is not moving, hence we may choose $p^\mu = (1,0,0,0)$ in the chosen frame. It follows that $2P = 1 + i\gamma^0$. The eigenvalues of $i\gamma^0$ are ± 1 since $(i\gamma^0)^2 = 1$. But the γ-matrices are traceless, and hence the eigenvalues add up to 0. Therefore the eigenvalues of $i\gamma^0$ are $-1, -1, +1, +1$. Thus P can be cast in the form

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} .$$

We conclude that there are two independent degrees of freedom for a fermion; similar to the case of light one speaks of two polarizations. For a particular choice of the sign of ω_k we can thus specialise the expansion of the fermion to

$$\psi = \int \frac{d^3k}{(2\pi)^3} \left(v_+(k) e^{i\omega_k t - \mathbf{k}\cdot x} + v_-(k) e^{-i\omega_k t + \mathbf{k}\cdot x}\right) ,$$

where $\omega_k = \sqrt{\mathbf{k}\cdot\mathbf{k} + m^2c^2/\hbar^2}$ and where the $v_\pm(k)$ are linear combinations of the two basis polarization vectors u_1 and u_2:

$$v_\pm(k) = \alpha_\pm(k) u_1 + \beta_\pm(k) u_2 \,.$$

5.6 Light rays and gamma rays

Lasers produce light of a high intensity and with almost only one frequency. That is, the light of a laser is almost **monochromatic**. We assume that the laser is perfect and thus emits only radiation of one particular wavelength. Also we consider 'general lasers', which can radiate electrons, α-particles, $\beta^{\pm}$-radiation and so on. We shortly comment on the nature of the different kinds of radiation and see how the modes come into play. To make life easy for us, we imagine the laser is placed such that the medium through which the beam is shot, is the vacuum.

First we consider the common situation where light is radiated. Light waves are particular solutions to the **Maxwell equations** in vacuum, or any other homogeneous medium. The Maxwell equations in vacuum are given by

$$\nabla \cdot \mathbf{E} = 0\,, \quad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}\,,$$
$$\nabla \cdot \mathbf{B} = 0\,, \quad \nabla \times \mathbf{B} = \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}\,,$$

where $\mathbf{E}$ is the electric field strength, $\mathbf{B}$ is the magnetic field strength and t is the time, and c is again the speed of light. As usual in physics, boldface symbols denote 3-dimensional vectors, while their components are not written in bold;

$$\nabla \cdot \mathbf{A} = \operatorname{div} \mathbf{A} := \frac{\partial A_1}{\partial x_1} + \frac{\partial A_2}{\partial x_2} + \frac{\partial A_3}{\partial x_3}$$

and

$$\nabla \times \mathbf{A} = \operatorname{curl} \mathbf{A} := \begin{pmatrix} \dfrac{\partial A_3}{\partial x_2} - \dfrac{\partial A_2}{\partial x_3} \\ \dfrac{\partial A_1}{\partial x_3} - \dfrac{\partial A_3}{\partial x_1} \\ \dfrac{\partial A_2}{\partial x_1} - \dfrac{\partial A_1}{\partial x_2} \end{pmatrix}$$

denote the **divergence** and **curl** of a vector field A, respectively. Using the generally valid relation

$$\nabla \times (\nabla \times \mathbf{X}) = \nabla(\nabla \cdot \mathbf{X}) - \nabla^2 \mathbf{X}$$

and the fact that the divergence of $\mathbf{B}$ and $\mathbf{E}$ vanishes we obtain from the Maxwell equations the wave equations

$$\nabla^2 \mathbf{E} = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{E},\,, \quad \nabla^2 \mathbf{B} = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{B}\,.$$

To solve we use the ansatz

$$\mathbf{E}(x,t) = \mathbf{E} e^{i\omega t - i\mathbf{k}\cdot\mathbf{x}}\,, \quad \mathbf{B}(x,t) = \mathbf{B} e^{i\omega t - i\mathbf{k}\cdot\mathbf{x}}\,,$$

where $\mathbf{E}$ and $\mathbf{B}$ are now fixed vectors. The ansatz represents waves propagating in the $\mathbf{k}$-direction and at any fixed point in space the measured frequency is ω. From the wave equations we immediately find the **dispersion relations** for the Maxwell equations that relate ω and $\mathbf{k} = (k_x, k_y, k_z)^T$;

$$\omega = c|\mathbf{k}|,$$

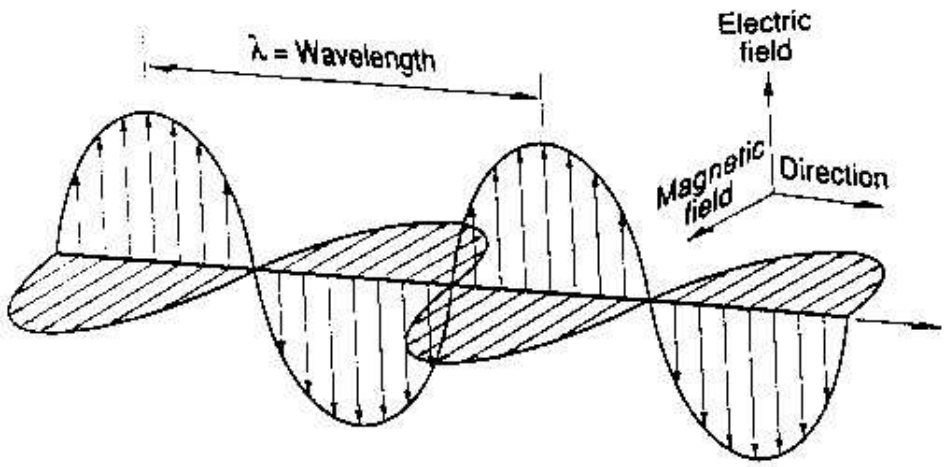


Figure 5.1: An image of a solution of the electromagnetic wave equations. The Poynting vector gives the direction of the wave and is perpendicular to the electric and the magnetic field.

where

$$|\mathbf{k}| := \mathbf{k} \cdot \mathbf{k} = k_x^2 + k_y^2 + k_z^2.$$

We compute

$$\nabla \cdot \mathbf{E}(x,t) = 0 \;\Rightarrow\; \mathbf{k} \cdot \mathbf{E} = 0\,,$$

and similarly $\mathbf{k} \cdot \mathbf{B} = 0$. Thus $\mathbf{k}$ is perpendicular to both $\mathbf{E}$ and $\mathbf{B}$. We find for the outer products

$$\nabla \times \mathbf{E}(x,t) = -i\mathbf{k} \times \mathbf{E}(x,t)\,, \quad \nabla \times \mathbf{B}(x,t) = -i\mathbf{k} \times \mathbf{B}(x,t)\,,$$

and thus it follows

$$\mathbf{k} \times \mathbf{E} = \omega \mathbf{B}\,, \quad \mathbf{k} \times \mathbf{B} = -\frac{\omega}{c^2}\mathbf{E}\,.$$

We see that $\mathbf{E}$ and $\mathbf{B}$ are perpendicular to each other, and $\mathbf{k}$ is perpendicular to $\mathbf{E}$ and $\mathbf{B}$, hence $\mathbf{k}$ is parallel to the so-called **Poynting vector** $\mathbf{P} = \mathbf{E} \times \mathbf{B}$. Figure 5.1 displays an image of a solution.

Without loss of generality we may change the coordinates so that $\mathbf{k}$ points into the z-direction; then $k_x = k_y = 0$ and only k_z is nonzero. Then, since $\omega\mathbf{B} = \mathbf{k} \times \mathbf{E}$ and $\mathbf{E}$ is orthogonal to $\mathbf{k}$, light is completely determined by giving the x- and y-components of $\mathbf{E}$. Thus light has two degrees of freedom; put in other words, light has two **polarizations**. Linearly polarized light is light where $\mathbf{E}$ oscillates in a constant direction orthogonal to the light ray. Circularly polarized light is light where $\mathbf{E}$ rotates along the path of light; this can be achieved by superimposing two linearly polarized light beams. Since the Maxwell equations are linear, any sum of solutions is again a solution. Note that to actually get the solution for $\mathbf{E}(x,t)$, one has to take the real part.

So we have seen that a light beam is determined by giving two polarizations. These polarizations can be interpreted as modes of an oscillator. One can write the general solution in

terms of coefficient functions $a(\mathbf{k})$ as[1]

$$\mathbf{E}(x,t) = \int d\mathbf{k} \left(a(\mathbf{k})\mathbf{u}_{\mathbf{k}}(\mathbf{x})e^{-i\omega_{\mathbf{k}}t} + a^*(\mathbf{k})\mathbf{u}_{\mathbf{k}}(\mathbf{x})^* e^{i\omega_{\mathbf{k}}t} \right), \tag{5.20}$$

where the frequency is given by the dispersion relation $\omega_{\mathbf{k}} = c|\mathbf{k}|$, and

$$\mathbf{u}_{\mathbf{k}}(\mathbf{x}) = \varepsilon_1(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}} + \varepsilon_2(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}\,,$$

where $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$ are **polarization vectors** chosen to satisfy

$$\varepsilon_1(\mathbf{k}) \cdot \varepsilon_2(\mathbf{k}) = \varepsilon_1(\mathbf{k}) \cdot \mathbf{k} = \varepsilon_2(\mathbf{k}) \cdot \mathbf{k} = 0\,,\ \varepsilon_1(\mathbf{k})^2 = \varepsilon_2(\mathbf{k})^2 = 1\,.$$

Note the similarity with the Maxwell equation. The main difference is in the dispersion relation. In addition, since now the fields functions are real, the coefficients of the positive frequency part and the negative frequency part are related. The positive frequency part

$$\widehat{\mathbf{E}} := \int d\mathbf{k} a^*(\mathbf{k})\mathbf{u}_k(\mathbf{x})^* \mathbf{e}^{i\omega_{\mathbf{k}}t}$$

of the solution (5.20) is called the **analytic signal** of $\mathbf{E}$; clearly $\mathbf{E} = \overline{\widehat{\mathbf{E}}} + \widehat{\mathbf{E}} = 2\,\mathrm{Re}\,\widehat{\mathbf{E}}$.

In the quantum theory one promotes the modes $a(\mathbf{k})$ and $a^*(\mathbf{k})$ to operators. We treat the transition from the classical theory to the quantum theory in detail only for the harmonic oscillator, corresponding to a single monochromatic mode; see Chapter 20.

To motivate the connection, we rewrite the Hamiltonian into a specific form that we will later recognize as the Hamiltonian of a harmonic oscillator, thereby showing that the Maxwell equations give rise to (an infinite set of) harmonic oscillators.

First we consider the system in a finite volume V to avoid some questions of finiteness. In that case (since one has to impose appropriate boundary conditions), the integral over wave vectors $\mathbf{k}$ for the electric field becomes a sum over a discrete (but infinite) set of wave vectors. To get a sum over finitely many terms, one also has to remove wave vectors with very large momentum; this corresponds to discretizing space[2].

The functions $\mathbf{u}_{\mathbf{k}}(\mathbf{x})$ can then be normalized as

$$\int_V d\mathbf{x}\ \mathbf{u}_{\mathbf{k}}(\mathbf{x})^* \mathbf{u}_{\mathbf{k}'}(\mathbf{x}) = \delta_{\mathbf{k}\mathbf{k}'}\,.$$

The energy density of the electromagnetic field is proportional to $\mathbf{E}^2 + \mathbf{B}^2$. Hence classically the Hamiltonian is given by

$$H = \frac{1}{2}\int_V d\mathbf{x}\ \left(\mathbf{E}^2 + \mathbf{B}^2\right)\,.$$

[1]We are not taking all details into account here, since we only want to convey the general picture of what is happening and don't use the material outside this section.

[2]Getting a proper limit is the subject of renormalization theory, which is beyond the scope of our presentation. The mathematical details for interactive fields are still obscure; indeed, whether **quantum electrodynamics** (QED) exists as a mathematically well-defined theory is one of the big open questions in mathematical physics.

Inserting the expansions (5.20) of $\mathbf{E}$ and $\mathbf{B}$ into the expression for the Hamiltonian and taking into account the normalization of the $\mathbf{u_k}$ one obtains after shifting the ground state energy to zero and performing the so-called thermodynamic limit $V \to \infty$ a Hamiltonian of the form

$$H = \tfrac{1}{2} \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \left(a^*_{\mathbf{k}} a_{\mathbf{k}} + a_{\mathbf{k}} a^*_{\mathbf{k}} \right) .$$

In Chapter 20 we will show that the quantum mechanical Hamiltonian of the harmonic oscillator is given by $H = \hbar\omega a^* a$ for some constant ω and operators a and a^*. For light we thus obtain for each possible $\mathbf{k}$-vector a quantum oscillator. In practice, a laser admits only a selection of possible $\mathbf{k}$-vectors. In the ideal case that there is only one possible $\mathbf{k}$-vector, that is, the Poynting vector can only point in one direction and only one wavelength is allowed, the Hamiltonian reduces to the Hamiltonian of one harmonic oscillator.

Chapter 6

Spectral analysis

In this chapter we show that the spectrum of a quantum Hamiltonian (defining the admissible energy levels) contains very useful information about a conservative quantum system. It not only allows one to solve the Heisenberg equations of motion but also has a direct link to experiment, in that the differences of the energy levels are directly observable, since they can be probed by coupling the system to a harmonic oscillator with adjustable frequency.

6.1 The quantum spectrum

In quantum mechanics the classical Hamiltonian becomes an operator on some Hilbert space. Formally, instead of a function of q and p defined by a formal expression $H(q.p)$ defining a classical N-particle Hamiltonian as a function of position q and momentum p, one has a similar expression where now q and p are vectors whose components are linear operators on the Hilbert space $\mathbb{R}^{3N}$. The main difference is the lack of commutativity; so the order of operators in the expressions matters.

Which operators are used to encode the components of q and p depends on the representation used. In the **position representation**, the components of q act as multiplication by position coordinates, while the components of p are multiples of the differentiation operators with respect to the position coordinates; in the **momentum representation**, this also holds but with position and momentum interchanged. Both representations are equivalent.

The collection of eigenvalues of the Hamiltonian H of a quantum system is referred to as the spectrum of H (or of the system). Formally, the **spectrum** of a linear operator H is the set of all $E \in \mathbb{C}$ such that $H - E$ is *not* invertible. In finite dimensions, this implies the nontrivial solvability of the equation $(H - E)\psi = 0$, and hence of the existence of an eigenvector $\psi \neq 0$ satisfying the **time-independent Schrödinger equation**

$$H\psi = E\psi. \tag{6.1}$$

In infinite dimensions, things are a bit more complicated and require the spectral theorem

from functional analysis. If the spectrum of H is, however, discrete then (6.1) remains valid.

As we shall show in Section 20.3, the Hamiltonian of a quantum harmonic oscillator in normal mode form is given by $H = E_0 + \hbar\omega n$, where n is the so-called **number operator** whose spectrum consists of the nonnegative integers. Hence the eigenvectors of H (also called **eigenfunctions** if, as here, the Hilbert space consists of functions) are eigenvectors of n, and the eigenvalues E_k of H are related to the eigenvalues $k \in \mathbb{N}_0$ of n by the formula

$$E_k = E_0 + k\hbar\omega.$$

This shows that the eigenvalues of the quantum harmonic oscillator are quantized, and the eigenvalue differences are integral multiples of the energy quantum $\hbar\omega$. That the spectrum of the Hamiltonian is discrete is sometimes rephrased as 'H is quantized'.

In this and the next section we investigate the experimental meaning of the spectrum of the Hamiltonian of an arbitrary quantum system. Since the Hamiltonian describes the evolution of the system via the quantum Heisenberg equation (1.17), i.e.,

$$\dot{f} = H\angle f = \frac{i}{\hbar}[H, f]\,,$$

one expects that the spectrum will be related to the time dependence of $f(t)$. To solve the Heisenberg equation, we need to find a representation where the Hamiltonian acts diagonally.

In the case where the Hilbert space $\mathbb{H}$ is finite-dimensional, we can always diagonalize H, since H is Hermitian. There is an orthonormal basis of eigenvectors of H, and fixing such a basis we may represent all $\psi \in \mathbb{H}$ by their components ψ_k in this basis, thus identifying $\mathbb{H}$ with $\mathbb{C}^n$ with the standard inner product. In this representation, H acts as a diagonal matrix whose diagonal entries are the eigenvalues corresponding to the basis of eigenvectors;

$$(H\psi)_k = E_k\psi_k\,.$$

In the case where the Hilbert space is infinite-dimensional and H is self-adjoint, an analogous representation is possible, using the **Gel'fand–Maurin theorem**, also known under the name **nuclear spectral theorem**. The theorem asserts that if H is self-adjoint, then H can be extended into the dual space of the domain of definition of H; there it has a complete family of eigenfunctions, which can be used to coordinatize the Hilbert space. The situation is slightly complicated by the fact that the spectrum may be partially or fully continuous, in which case the concept of a basis of eigenvectors no longer makes sense since the eigenvectors corresponding to points in the continuous spectrum are no longer square integrable and hence lie outside the Hilbert space.

In the physics literature, the rigorous mathematical exposition is usually abandoned at this stage, and one simply proceeds by analogy, choosing a set Ω of labels of the eigenstates and treating them "formally" as if they form a discrete set. Often, the discreteness of the spectrum is enforced verbally by artificially "putting the particles in a finite box" and

going to an infinite volume limit at the very end of the computations. The justification for the approach is that most experiments are indeed very well localized; in letting two protons collide in CERN we do not take interaction with particles on Jupiter into account. Mathematically we thus put our system in a box. Since we do not want our system to interact too much with the walls of the box we take the box large enough. Having met the final requirement one observes that the physical quantities do not depend on the precise form and size of the box. To simplify the equations one then takes the size of the box to infinity. Making this mathematically precise is quite difficult, though well-understood for nonrelativiastic systems. In particular, for the part of the spectrum that becomes continuous in this limit, the limits of the eigenvectors become **generalized eigenvectors** lying no longer in the Hilbert space itself but in a distributional extension of the Hilbert space which must be discussed in the setting of a so-called **Gelfand triple** or **rigged Hilbert space**; cf. Section 20.4.

In many cases of physical interest, these generalized eigenvectors come in two flavors, depending on the boundary conditions imposed, resulting in two families of **in-eigenstates** $|k\rangle_-$ and **out-eigenstates** $|k\rangle_+$ labelled by a set Ω which in the case of the harmonic oscillator is $\Omega = \mathbb{N}_0$. (The bra-ket notation used here informally is made precise in Section 20.4.) The in- and out-states are called so because they have a natural geometric interpretation in scattering experiments (see Section 6.4). In addition to these eigenstates, there is a measure $d\mu(k)$ on Ω, and a **spectral density** $\rho(k)$ with real positive values such that every vector in the Hilbert space has a unique representation in the form

$$\psi = \int_\Omega d\mu(k)\psi_+(k)|k\rangle_+ = \int_\Omega d\mu(k)\psi_-(k)|k\rangle_- \,.$$

For any fixed choice of the sign in $\psi(k) := \psi_\pm(k)$, the inner product is given by

$$\phi^*\psi = \int_\Omega d\mu(k)\rho(k)\overline{\phi}(k)\psi(k)\,. \tag{6.2}$$

The spectral measure $d\mu(k)$ may also have a discrete part corresponding to square integrable eigenstates, in which case $|k\rangle_+ = |k\rangle_-$. If all eigenvectors are square integrable, the spectrum is completely discrete. In particular, this is the case for the harmonic oscillator, for which we construct the diagonal representation explicitly in Section 20.

Since the $|k\rangle_\pm$ are eigenvectors with corresponding eigenvalue $E(k) = E_k$, that is, the Hamiltonian satisfies

$$(H\psi)(k) = E(k)\psi(k)\,, \tag{6.3}$$

we say that H **acts diagonally** in the representation defined by the $\psi(k)$. Thus one can identify the Hilbert space with the space $L^2(\Omega)$ of coefficient functions $\psi_\pm$ with finite $\int_\Omega d\mu(k)\rho(k)|\psi_\pm(k)|^2$; the Hamiltonian is then determined by (6.3). The in- and out-states are related by the so-called **S-matrix**, a unitary matrix $S \in \operatorname{Lin} L^2(\Omega)$ such that

$$\psi_+(k) = (S\psi_-)(k)\,.$$

As a consequence of the time-symmetric nature of conservative quantum dynamics and the time-asymmetry of scattering eigenstates, the in-representation and the out-representation

are both equivalent to the original representation on which the Hamiltonian is defined. In many cases of interest, one can then rigorously prove existence and uniqueness of the S-matrix.

The transformation from an arbitrary Hilbert space representation to the equivalent representation in terms of which H is diagonal, is an analogue of a Fourier transformation; the latter corresponds to the special case where $\mathbb{H} = L^2(\mathbb{R})$ and H is a differential operator with constant coefficients.

In general, the Gel'fand–Maurin theorem guarantees the existence of a topological space Ω and a Borel measurable spectral density function $\rho : \Omega \to \mathbb{R}_+$ such that the original Hilbert space is $L^2(\Omega, \rho)$ with inner product (6.2) and such that (6.3) holds. Indeed, Ω can be constructed as the set of **characters**, that is, $*$-homomorphisms into the complex numbers, of a maximal commutative C*-algebra of bounded linear operators containing the bounded operators e^{itH} ($t \in \mathbb{R}$). (Since we don't use this construction further, the concepts involved will not be explained in detail.)

The above reasoning is completely parallel to the finite-dimensional case, where $\mathbb{H} = \mathbb{C}^n$. There one would write $\psi = \sum_k \psi_k |k\rangle$ and have $(H\psi)_k = E_k \psi_k$. An arbitrary quantity $f \in \operatorname{Lin} \mathbb{H} = \mathbb{C}^{n\times n}$ would then be represented by a matrix, acting as $(f\psi)_k = \sum_l f_{kl}\psi_l$. In the infinite-dimensional setting, k takes values in the label space Ω. The quantities of primary interest are represented by integral operators defined by a kernel function

$$(f\psi)(k) := \int_\Omega d\mu(l) f(k,l)\psi(l)\,;$$

the $f(k,l)$ are the analogues of the matrix entries f_{kl}.

Finding a diagonal representation for a given quantum system (i.e., given a Hilbert space and a Hamiltonian) is in general quite difficult; succeeding is virtually equivalent with "solving" the theory of the system. Indeed, in terms of the diagonal representation, we can obtain a full solution of the Heisenberg dynamics. We have

$$\begin{aligned}
\int_\Omega d\mu(l)\dot{f}(k,l,t)\psi(l) &= \frac{i}{\hbar}\Big((Hf\psi)(k) - (fH\psi)(k)\Big) \\
&= \frac{i}{\hbar}\Big(E(k)\int_\Omega d\mu(l)(f\psi)(l) - \int_\Omega d\mu f(k,l,t)E(l)\psi(l)\Big) \\
&= \frac{i}{\hbar}\int_\Omega d\mu(l) f(k,l,t)\Big(E(k) - E(l)\Big)\psi(l)\,,
\end{aligned}$$

from which it follows that

$$\dot{f}(k,l,t) = \frac{i}{\hbar}\Big(E(k) - E(l)\Big) f(k,l,t)\,. \tag{6.4}$$

In (6.4) we recognize a linear differential equation with constant coefficients, whose general solution is

$$f(k,l,t) = e^{\frac{i}{\hbar}(E(k)-E(l))t} f(k,l,0)\,.$$

Thus the kernel function of the operator f has oscillatory behavior with frequencies

$$\omega_{kl} = \frac{E(k) - E(l)}{\hbar}\,. \tag{6.5}$$

This relation, the modern form of the **Rydberg–Ritz combination principle** found in 1908 by Walter Ritz [236], may be expressed in the form

$$\Delta E = \hbar\omega, \tag{6.6}$$

The formula (6.6) appears first in Planck's famous paper [219] from 1900 where he explained the radiation spectrum of a black body. Planck wrote it in the form $\Delta E = h\nu$, where $h = 2\pi\hbar$ and $\nu = \omega/2\pi$ is the linear frequency. The symbol for the quotient $\hbar = h/2\pi$, which translates this into our formula was invented much later, in 1930, by Dirac in his famous book[1] on quantum mechanics [74].

6.2 Probing the spectrum of a system

All physical systems exhibit small (and sometimes large) oscillations of various frequencies, collectively referred to as the **spectrum** of the system. By observing the size of these oscillations and their dependence on the frequency, valuable information can be obtained about intrinsic properties of the system. Indeed, the resulting science of **spectroscopy** is today one of the indispensable means for obtaining experimental information on the structure of chemical materials and the presence of traces of chemical compounds.

To probe the spectrum of a quantum system, we bring it into contact with a macroscopically observable (hence classical) weakly damped harmonic oscillator. That we treat just a single harmonic oscillator is for convenience only. In practice, one often observes many oscillators simultaneously, e.g., by observing the oscillations of the electromagnetic field in the form of electromagnetic radiation – light, X-rays, or microwaves. However, the oscillators do not interact that strongly in most cases and in the case of electromagnetic radiation not at all. In that case the result of probing a system with multiple oscillators results in a linear superposition of the results of probing with a single oscillator. This is a special case of the general fact that solutions of linear differential equations depend linearly on the right hand side.

From the point of view of the macroscopically observable classical oscillator, the probed quantum system appears simply as a time-dependent external force $F(t)$ that modifies the dynamics of the free harmonic oscillator. Instead of the equation $m\ddot{q} + c\dot{q} + kq = 0$ we get the differential equation describing the **forced harmonic oscillator**, given by

$$m\ddot{q} + c\dot{q} + kq = F(t)\,.$$

[1]The book contains the Dirac equation but also Dirac's famous mistake (cf. Section 6.3) – he had wrongly interpreted the antiparticle of the electron predicted by his equation (later named the positron) to be the proton.

The external force F is usually the value

$$F(t) = \langle f(t) \rangle$$

of a quantity f from the algebra of quantities of the probed system, as discussed in more detail in Part II. This follows from the general principles of Section 19.2 for modeling interactions of a quantum system with a classical, macroscopic system (only the latter are directly measurable). How classical measurements are to be interpreted in a pure quantum context will be discussed in Section 10.4.

If the measurement is done far from the probed system, such as a measurement of light (electromagnetic radiation) emitted by a far away source (e.g., a star, but also a Bunsen flame observed by the eye), the back reaction of the classical oscillator on the probed system can be neglected. Then the probed system can be considered as a Hamiltonian system and evolves according to the Heisenberg equation (1.13). In particular, the analysis of Section 6.1 applies, and since expectations are linear, the external force F evolves as a superposition of exponentials $e^{i\omega t}$, where the ω are differences of eigenvalues of H. In the quantum case the spectrum may have a discrete part, leading to a sum of different exponentials $e^{i\omega t}$ that, as we shall see, leads to conspicuous spikes in the Fourier transform of the response and a continuous part that leads to an integral over such terms which typically provide a smooth background response. In the following, we shall assume for simplicity a purely discrete spectrum, and hence an expansion of F of the form

$$F(t) = \sum_l F_l e^{i\omega_l t} \,,$$

with distinct, real and nonzero frequencies. However, the analysis holds with obvious changes also for a (partly or fully) continuous spectrum if the sums are replaced by appropriate integrals.

The solution to the differential equation consists of a particular solution and a solution to the homogeneous equation. Due to damping, the latter is transient and decays to zero. To get a particular solution, we note that common experience shows that forced oscillations typically have the same frequency as the force. We therefore make the ansatz

$$q(t) = \sum_l q_l e^{i\omega_l t} \,.$$

Inserting both sums into the differential equation, we obtain the relation

$$\sum_l \Big(-m\omega_l^2 + ic\omega_l + k\Big) q_l e^{i\omega_l t} = \sum_l F_l e^{i\omega_l t} \,,$$

from which we conclude that we have a solution precisely when

$$q_l = \frac{F_l}{k - m\omega_l^2 + ic\omega_l} \,, \qquad \text{for all } l.$$

Since the frequencies are real and distinct, the denominator cannot vanish. The energy in the lth mode is therefore proportional to

$$|q_l|^2 = \frac{|F_l|^2}{(k - m\omega_l^2)^2 + (c\omega_l)^2} \,. \tag{6.7}$$

Now first imagine that the system under study has only one frequency, that is, $F_l \neq 0$ for only one l. For example, the system under study is also an oscillator that is swinging with a certain frequency. In this case the oscillator with which we probe the system will also swing with that same frequency as the probed system, but with an amplitude given by (6.7). We see that for $\omega = \sqrt{\frac{k}{m}}$ close to ω_l the oscillator responds most to the force it feels from the probed system. The frequency $\omega = \sqrt{\frac{k}{m}}$ is called the **resonance frequency** of the oscillator. The above we know from phenomena of daily (or not so daily) life, as pushing a swing (or riding a car with a defect shock absorber); if you push with the 'right' frequency the result will be that the swing goes higher and higher, pushing with another frequency results in a seemingly chaotic incoherent swinging.

Returning to the case that there are more F_l nonzero, we see that the oscillator will swing with the same frequencies as the probed system. But the intensity with which the oscillator swings depends on the positions of the ω_l relative to the resonance frequencies. Suppose that c is relatively small, so that we can ignore the term $c\omega$ in the denominator of (6.7). Then the q_l for which ω_l is close to ω show a higher intensity.

Looking for resonances with an oscillator that has an adjustable frequency ω therefore gives a way to experimentally find the frequencies in the force incident to the oscillator. If the frequency ω passes over one of the frequencies of the probed system, the oscillator will swing more intensively.

The resonances occur around a natural frequency but also the width of the interval in which the system shows a resonance has information. If the interval is small, one speaks of a **sharp resonance** and this corresponds to a discrete or nearly discrete spectrum of the frequencies. If the resonance is not sharp, the response corresponds to a continuous spectrum. The graph that shows the absorbed energy (which is proportional to $|q_l|^2$) as a function of the frequency ($\sim \omega_l$) for a system with one resonance frequency typically has a **Lorentz shape**, according to the formula (6.7): There is a peak around $\omega_0 = \sqrt{k/m}$ with a certain width, and on both sides of the peak the function tends to zero at plus and minus infinity. In Figure 6.1 we displayed a graph of a Lorentz shape for a harmonic oscillator with varying frequency ω in contact with a probed system that has one F_l nonzero for the frequency ω_0.

For general systems with more resonance frequencies, the graph is a superposition of such curves and the peaks around the resonance frequencies can have different widths and different heights. This graph is recorded by typical spectrometers, and the shapes and positions of characteristic pieces of the graph contain important information about the system. We shall assume that the peaks have already been translated into resonance frequencies (a non-trivial task in case of overlapping resonances), and concentrate on relating these frequencies to the Hamiltonian of the system. This is done in Section 6.4.

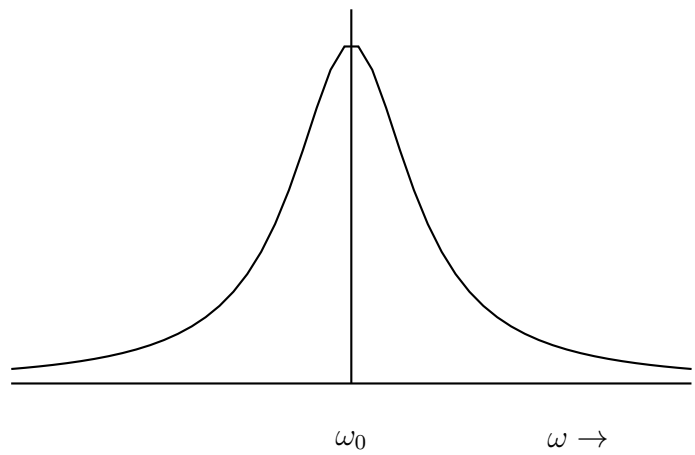


Figure 6.1: Lorentz-shape. The absorbed energy of the oscillator with varying frequency ω.

6.3 The early history of quantum mechanics

In this section we remark on some important aspects of the history of quantum mechanics. We focus on the physics of the atom, which was one of the main reasons to develop quantum mechanics. In Section 6.5 we discuss the physics of the black body and the history of the formula of Planck, which describes black body radiation. For an interesting historical account we refer to for example VAN DER WAERDEN[276] or ZEIDLER [299].

The importance of the spectrum in quantum physics is not only due to the preceding analysis, which allows a complete solution of the dynamics, but also to the fact that the spectrum can easily be probed experimentally. Indeed, spectral data (from black body radiation and the spectral absorption and emission lines of hydrogen) were historically the trigger for the development of modern quantum theory. Even the name spectrum for the set of eigenvalues was derived from this connection to experiment.

Probing the spectrum through contact with a damped harmonic oscillator has been discussed in Section 6.2. Note that the observed frequencies give the spectrum of the force, not the spectrum of the Hamiltonian. As derived above, the spectrum of the force consists of the spectral differences of the Hamiltonian spectrum. This is in accordance with the fact that (in nonrelativistic mechanics) absolute energy is meaningless and only energy differences are observable.

In case of the harmonic oscillator, the spectrum of the Hamiltonian H is discrete (see Chapter 20 for the details and derivation), consisting of the nonnegative integral multiples $k\omega$ of the base frequency ω. Thus the set of labels for the eigenvectors $|k\rangle$ is discrete, $\Omega = \mathbb{N}_0$. The number of allowed frequencies is thus countable and the external force may be expanded into a sum of the form

$$F(t) = \sum e^{i\omega_{kl}t} F_{kl} \,.$$

Explicitly, the frequencies are given by $\omega_{kl} = \omega(k-l) \in \mathbb{Z}\omega$. Thus quantum mechanics produces overtones. This is not an authentic quantum mechanical feature; in classical

mechanics one finds overtones in a similar setting – for example, in the pitching of a guitar string.

A historically more interesting system is the hydrogen atom, where the energies are given by an equation of the form

$$E_k = E_0 - \frac{C}{k^2}\,,$$

for some constant C. Then the frequencies are given by the **Rydberg formula**

$$\omega_{kl} = R_H\Big(\frac{1}{k^2} - \frac{1}{l^2}\Big)\,, \tag{6.8}$$

where $R_H \sim 1.1 \cdot 10^7 m^{-1}$ is the Rydberg constant. The Rydberg formula correctly gives the observed spectral lines of the hydrogen atom. The formula was discovered by Rydberg in 1889 (Martinson and Curtis [187]) after preliminary work of Balmer, who found the formula for the **Balmer series** of spectral lines (given by $k = 2$). Schrödinger derived this formula using the theoretical framework of quantum mechanics.

Let us review the situation of the time where quantum mechanics was conceived. Around 1900 physicists were experimentally exploring the atom, which until then was (since antiquity) only a philosophically disputable part of Nature. The experiments clearly indicated that atoms existed and that matter was built up from atoms. The physicist Boltzmann had argued that atoms existed, but his point of view had not been accepted; only after his death in 1906, the existence of atoms was unarguably proved by experiments by Perrin around 1909. This lead to the problem of finding the constituents of the atom and its structure. In 1897 Thompson had discovered the electron as a subatomic particle. Since the atom is electrically neutral, the atom has to contain positively charged particles. Thompson thought of a model in which the atom was a positively charged sphere with the electrons being in this "plum pudding" of positive charge. But then in 1911 Rutherford put Thompson's model to the test; Marsden and Geiger, who were working under the supervision of Rutherford, shot α-particles at a thin foil of gold and looked at the scattering pattern [115]. The experiment is therefore called the **Geiger–Marsden experiment**. At that time, α-particles were considered a special radiation emitted by some 'radio-active' elements; now we know that these are the nuclei of Helium with the electrons being stripped off.

Since the α-particles are positive, they have a particular kind of interaction with the positively charged sphere of Thompson's model. But since the electrons swim around in the positive charge, the net charge is zero and most interaction is screened off. Therefore it was expected that the α-particles would be only slightly deflected. However, the pattern was not at all like that! It rather looked as if almost all α-particles went straight through and a small percentage was deflected by a concentrated positive charge. Most α-particles that were deflected were scattered backwards, implying that they had an almost head-on collision with a positive charge.

The very small percentage of scattered α-particles indicated that the chance that an α-particle meets a positively charged nucleus on its way is very small, which implies that the nucleus is very small compared to the atom. Therefore Rutherford (who wrote a paper to explain the results of the Geiger–Marsden experiment) concluded that the nucleus of an

atom is positively charged and the electrons circle around the nucleus, and furthermore, the size of the nucleus is very small compared to the radii at which the electrons circle around the atom [245]. If one imagines the atomic nucleus to have the size of a pea and one would place it at the top of the Eiffel tower, the closest electrons would circle around in an orbit that touches the ground; the atom is mostly empty.

In 1918 it was again Rutherford who performed an important experiment from which he concluded that the electric charge of the atomic nucleus was carried by little particles, called protons. The hydrogen atom was found to be the simplest atom; it consists of a proton and one electron circling around the proton. Because of this experiment the discovery of the proton is attributed to Rutherford.

Classically, if an electron circles around in an electric field it radiates and thus loses energy. The question thus arises why the hydrogen atom is stable. Again classically, an electron can circle around a positive charge with arbitrary energy. If the electron changes its orbit, this happens gradually, hence the energy changes continuously and the absorption or emissions patterns of the hydrogen atom should be continuous. But experiments done by Rydberg in 1888 and Balmer in 1885 showed that hydrogen absorbed or emitted light at well-defined frequencies, visible as lines in the spectrum obtained by refraction. For the atomic model this implies that the electron can only have well-defined energies separated by gaps (forbidden energies). In 1913 Bohr wrote a series of papers [40, 41, 42, 43] in which he postulated a model to account for this. Bohr postulated that angular momentum is quantized (if p is the momentum of the electron and r the radius, then the angular momentum is $L = r \times p$, where the cross denotes the vector product) and that the electron does not lose energy continuously. With these assumptions he could explain the spectrum observed by Rydberg.

The model of Bohr did not explain the behavior of atoms, it only gave rules the atom had to obey. In 1925 Werner Heisenberg wrote a paper [123] where he tried to give a fundamental basis for the rules of quantum mechanics. Heisenberg described the dynamics of the transitions of an electron in an atom by using the 'states' of the electron as labels. For example, he wrote the frequency emitted by an electron jumping from a state n to a state $n - \alpha$ as $\nu(n, n - \alpha)$. Just two months later Max Born and Pascal Jordan wrote a paper [47] about the paper of Heisenberg, in which they made clear that what Heisenberg actually did was promoting observables to matrices. The three of them, Born, Jordan and Heisenberg, wrote in the same year a paper [179] where they elaborated on the formalism they developed. Also in the same year 1925 Paul Dirac wrote a paper in response to the paper of Heisenberg, in which the remarkable relation $q_r p_s - p_s q_r = \delta_{rs} i\hbar$ appeared. Dirac tried to find the relation between a classical theory and the corresponding quantum theory. In fact, Dirac postulated this equation: "we make the fundamental assumption that the difference between the Heisenberg product of two quantum quantities is equal to $ih/2\pi$ times their Poisson bracket expression".

So, in the beginning years of quantum mechanics, the dynamics of the observables was described by a kind of matrix mechanics. (A modern version of this is the view presented in the present book.) Based on work of de Broglie, Schrödinger came up with a differential equation for the nonrelativistic electron [249]. A probability interpretation for Schrödinger's wave function was found by Born. In 1927, Pauli reformulated his exclusion principle in

terms of spin and antisymmetry. In 1928, Dirac discovered the Dirac equation for the relativistic electron. In 1932, the early years concluded with the discovery of the positron by Anderson and the neutron by Chadwick, which were enough to explain the behavior of ordinary matter and radioactivity. But the forces that hold the nucleus together were still unknown, and already in 1934, Yukawa predicted the existence of new particles, the mesons. Since then the particle zoo has increased further and further.

A number of Nobel prizes (most of them in physics, but one in chemistry – early research on atoms was interdisciplinary) for the pioneers accompanied the early development of quantum mechanics[2]:

- 1908 Ernest Rutherford, (Nobel prize in chemistry) for his investigations into the disintegration of the elements, and the chemistry of radioactive substances
- 1918 Max Planck, in recognition of the services he rendered to the advancement of physics by his discovery of energy quanta
- 1921 Albert Einstein, for his services to theoretical physics, and especially for his discovery of the law of the photoelectric effect
- 1922 Niels Bohr, for his services in the investigation of the structure of atoms and of the radiation emanating from them
- 1929 Louis de Broglie, for his discovery of the wave nature of electrons
- 1932 Werner Heisenberg for the creation of quantum mechanics, the application of which has led among others to the discovery of the allotropic forms of hydrogen
- 1933 Erwin Schrödinger and Paul A.M. Dirac, for the discovery of new productive forms of atomic theory
- 1935 James Chadwick, for the discovery of the neutron
- 1936 Carl D. Anderson, for his discovery of the positron

and belatedly, but still for work done before 1935,

- 1945 Wolfgang Pauli, for the discovery of the exclusion principle, also called the Pauli principle
- 1949 Hideki Yukawa, for his prediction of the existence of mesons on the basis of theoretical work on nuclear forces
- 1954 Max Born, for his fundamental research in quantum mechanics, especially for his statistical interpretation of the wave function

[2]The remarks to each Nobel laureate are the official wordings in the announcements of the Nobel prizes. For press announcements, Nobel lectures of the laureates, and their biographies, see the web site `http://nobelprize.org/physics/laureates`.

The story of the discovery of antimatter is interesting. Though Dirac called it a prediction in his Nobel lecture, *"There is one other feature of these equations which I should now like to discuss, a feature which led to the prediction of the positron",* it was only a postdiction. Yes, he had a theory in which there were antiparticles. But before the positron was discovered, Dirac thought the antiparticles had to be protons (though there was a problem with the mass) since new particles were inconceivable at that time. Official history seems to have followed Dirac's lead in his Nobel lecture, and tells the story as it should have happened from the point of the theorist, namely that he (i.e., theory) actually predicted the positron. The truth is a little different.

Anderson discovered and named the positron in 1932. He wrote the announcement of his discovery in Science [11], "with due reserve in interpretation". The proper publication [13], where he also predicted "negative protons" (now called antiprotons), was still without any awareness of Dirac's theory. It is in the subsequent paper [12] that Anderson relates the positron to Dirac's theory.

Heisenberg, Dirac, and Anderson were all 31 years old when they got the Nobel prize. The fact that Anderson's paper [13] is very rarely cited[3] should cast some doubt on the relevance of citation counts for actual impact in science.

6.4 The spectrum of many-particle systems

To give a better intuition for what kind of spectra quantum systems can be expected to have, we discuss here the spectrum of many-particle systems from an informal point of view.

There are **bound states**, where all particles of the system stay together, and there are **scattering states**, where the system is broken up into several fragments moving independently but possibly influencing each other. The nomenclature comes from the scattering experiments in physics; shooting particles at each other can result in the formation of a system where the particles are bound together or where the particles scatter off from each other. In the case of a scattering process, different **arrangements**, (i.e., partitions of the set of individual particles into fragments which form a subsystem moving together) describe the combination of particles before a collision and their recombination in the debris after a collision.

The discrete spectrum of a Hamiltonian H corresponds to the bound states; each discrete eigenvalue to a different mode of the bound system. The study of the discrete spectrum of compound systems is the domain of **spectroscopy**. We shall return to this topic in Chapter 23, when the machinery to understand a spectrum is fully developed.

The continuous part of the spectrum corresponds to the scattering states. In general, the spectrum is discrete till a certain energy level, called the **dissociation threshold**, and

[3] `http//www.prola.aps.org/` lists only 37 citations, and only 5 before 1954. The paper [12] is cited 35 times.

after the dissociation threshold the spectrum is continuous. For the hydrogen atom, the dissociation threshold is $13.6eV$. For the harmonic oscillator, the dissociation threshold is infinite. In such a case, where the dissociation threshold is infinite, there is no continuous spectrum and the system is always bound; we call this **confinement**. For example, three quarks always form a bound state, that is, they are confined. A single quark can not get loose from its partners. It may also be the case that there is no bound state; for example, the atoms in inert gases don't form bound states, hence a system consisting of more than one of such atoms has only a continuous spectrum.

In scattering experiments the ingoing particles and the outgoing particles can be different. Hence one needs to keep track of what precisely went where. After the scattering the particles separate from each other in different clusters. The constituents in cluster i form a bound state, which can be in an excited state, which we denote E_i. If the cluster i is moving with a momentum, the total kinetic energy of cluster i is $p_i^2/2m_i$, where m_i is the mass of cluster i. If there are N clusters after a collision (scattering), the resulting total energy is

$$E = \sum_{i=1}^{N} \Big(\frac{p_i^2}{2m_i} + E_i \Big) .$$

In scattering experiments a possible outcome of clusters and their constituents is called a **channel**. It is very common in particle physics that a single reaction – like shooting two protons at each other – has more than one channel. We see that in each channel, there is a continuous spectrum above a certain energy level Δ, which is the sum of the ground state energies of the different clusters. To theoretically disentangle the spectrum, one uses an analytic continuation of the scattering amplitudes. We thus view the spectrum as a subset of the complex plane. When multiplying the momenta with a complex phase that has a nonzero imaginary part, the continuous part of the spectrum becomes imaginary and is tilted away from the real axis. The bound states still appear on the real line as isolated points, that is, discrete. But now at each bound state with energy above Δ there is a line connected representing the continuously varying momentum of the corresponding cluster. The technique of disentangling the spectrum using analytic continuation is called **complex scaling**. For more background and rigorous mathematical arguments, see, e.g., Simon [253], Moiseyev [191], or Bohm [39].

Dissipation. If we admit dissipation, the Hamiltonian is no longer Hermitian, since there is typically an antihermitian contribution to the potential, generally called an **optical potential** since it was first used in optics. Also, the dynamics need no longer be governed by the Heisenberg equation, but can be both in the classical and in the quantum case of the more general form

$$\dot{f} = H \angle f + \sum_{j,k} L_j^* \angle G_{jk} (L_k \angle f) \tag{6.9}$$

with **Lindblad operators** L_j encoding interactions with the unmodelled environment into which the lost energy dissipates, and complex coefficients G_{jk} forming a symmetric, positive definite matrix. Remembering that $\angle$ acts as a derivation, the additional terms can be viewed as generalized diffusion terms; indeed, the dynamics (6.9) describes classically for example reaction-diffusion equations, and its quantum version is the quantum equivalent of stochastic differential equations, which model systems like Brownian motion and give

microscopic models of diffusion processes. For details, see, e.g., Gardiner [99], Breuer & Petruccione [50].

Assuming that the terms in the sum of (6.9) are negligible, the dynamics satisfies the Heisenberg equation, and the above analysis applies with small changes. However, since H is no longer Hermitian, the energy levels typically acquire a possibly nonzero (and then positive) imaginary part. Isolated eigenvalues with positive imaginary parts are called **resonances**. The oscillation frequencies are still of of the form $\hbar\omega = \Delta E$, but since the energies have a positive imaginary part, the oscillations will be damped, as can be seen by looking at the form of $e^{i\omega t}$. That this does not lead to a decay of the response of the oscillator is due to stochastic contributions modelled by the Lindblad terms and neglected in our simplified analysis.

Resonances with tiny imaginary parts behave almost like bound states, and represent **unstable particles**, which decay in a stochastic manner; the value $\Gamma = 2\,\mathrm{Im}\,\omega$ gives their **lifetime**, defined as the time where (in a large sample of unstable particles) the number of undecayed particles left is reduced by a factor of e, the basis of the exponential function.

Thus the spectrum of a Hamiltonian contains valuable experimentally observable information about a quantum system.

6.5 Black body radiation

In the remainder of this chapter, we discuss the spectrum of a black body and some of its consequences.

In the history the 'black body' plays an important role. Applying some basic concepts of quantum mechanics and statistical mechanics one arrives at the distribution formula first derived by Max Planck in December 1900 [220]. According to Van der Waerden in his (partially autobiographical) book [276] the presentation of Planck in December 1900 was the birth of quantum mechanics.

What is a black body? A body that looks black does not reflect any light, it absorbs all incoming light. Hence if some radiation comes from a perfectly black body, it needs to be due to the interaction of the internal degrees of freedom with light. It is hard to experimentally construct a black body. The theoretical idea is to have a hollow box with a single little hole, through which the box can emit radiation outwards. Since the hole is assumed to be very small, no light will fall inwards and then be reflected through the hole again. Thus no light will be reflected (or at least almost no light). In practice many objects behave like black bodies above a certain temperature. The sun does not reflect a substantial amount of light (where should it come from?) compared to the amount it radiates. Therefore one of the best black bodies is the sun.

Given a black body, there is a positive integrable function $f(\omega)$ of the frequency ω, such

that the amount of energy radiated in the frequency interval $[\omega_1, \omega_2]$ is

$$E([\omega_1, \omega_2]) = \int_{\omega_1}^{\omega_2} d\omega \; f(\omega) \, .$$

The function $f(\omega)$ is the radiation-energy density. The main object of this section is the function $f(\omega)$. The importance of the black body lies in the fact that the radiation emitted is only due to its internal energy and its interaction with light. In practice a system has always interaction with the environment and light falling onto it (since we want to 'see' where the black body is, the latter is often inevitable). What would we expect from the radiation-energy density? First, since $\omega = 0$ means that the energy of the photons emitted is $\hbar\omega = 0$ and $\omega < 0$ is not a possibility, we have $f(0) = 0$. Second, the function f has to be integrable, hence $\lim_{\omega\to\infty} f(\omega) = 0$. The total integral $\int_0^\infty d\omega f(\omega)$ represents the total energy of the body. Therefore we certainly want f to be integrable, i.e., $f \in L^1(\mathbb{R}^+)$.

We know from experience that black bodies (like dark metals) do not radiate any thermal energy when they are at room temperature, but heating them up makes them glow red. When we rise the temperature, the color shifts more and more in the blue direction. This phenomenon can also be seen in flames; the outer, cooler side is red while more inwards, the flame gets lighter, reaches white and goes over to blue, and then becomes invisible. Empirically one concludes that the function $f(\omega)$ has a maximum at a frequency ω_{max}, where ω_{max} is temperature dependent; the larger the temperature T, the larger ω_{max}. Before 1900 it was already found that the fraction ω_{max}/T was almost independent of the body that was heated up. In 1893 the physicist Wilhelm Wien[4] used the statistical mechanics developed by Maxwell and Boltzmann to the laws of thermodynamics to derive **Wien's displacement law** [290]

$$\frac{\omega_{max}}{T} = \frac{2\pi c}{b} \, ,$$

where c is the speed of light and b is a constant whose numerical value is approximately $2.9 \cdot 10^{-3} m \cdot K$. In 1896 Wien derived a formula, called **Wien's approximation** for the radiation density

$$f(\omega) = a\omega^3 e^{-b\frac{\omega}{T}} \, , \tag{6.10}$$

for some parameters $a, b > 0$. It is clear that the proposed f is integrable and satisfies $f(0) = 0$. For large ω the radiation-energy density matches the observed densities, however, for small ω the radiation density of Wien does not match the experiments.

On the other hand, there were other radiation laws. First, there was **Stefan's law** (or Stefan–Boltzmann law) derived on basis of empirical results in 1879 [259]. The statement of Stefan's law is that the total energy radiated per second of a hot radiating body is proportional to the fourth power of the temperature:

$$\frac{dE}{dt} = \sigma A T^4 \, ,$$

where A is the area of the body and σ is a constant. In 1884 Boltzmann gave a theoretical derivation of Stefan's law using the theoretical tools of statistical mechanics [44]. The

[4]His real name is rather long: Wilhelm Carl Werner Otto Fritz Franz Wien.

second radiation law known in 1900 was **Rayleigh's law**. Lord Rayleigh used classical mechanics to derive a better description of the radiation density for low values of ω [229]. He proposed

$$f(\omega) = \gamma\omega^2 \,,$$

which is clearly wrong for large ω and is not even integrable. Later in 1905, Lord Rayleigh improved the derivation of his proposal in a collaboration with Sir James Jeans, again based on purely classical arguments. Although their discovery was interesting, it did not match the experiments for high ω. In December 1900, Max Planck had given a seminar and gave a derivation of $f(\omega)$ that resulted in a radiation-energy density that matched the experiments both for low and for high ω. Even more was true, the formula of Planck reproduced Wien's displacement law, Wien's approximation, Rayleigh's proposal and Stefan's law. The formula Planck derived was giving the energy density of a black body in thermal equilibrium, from which one obtains the radiation-energy density

$$f(\omega) = \frac{\hbar V}{\pi^2 c^3} \frac{\omega^3}{e^{\hbar\omega\beta} - 1} \,,$$

where V is the volume of the black body (the cavity actually) and $\beta = 1/kT$, k is Boltzmann's constant. Indeed for low ω we get an expression that is quadratic in ω, for high ω we get Wien's law and integrating the expression over ω one sees that the integral is proportional to T^4. The accordance with Wien's displacement law will be shown later – we will also remark on the agreement of Planck's law later.

So what precisely did Planck do that the others did wrong? The key ingredient in Planck's derivation is to consider the constituents of the black body as follows: the black body is just a cavity where the inner walls can have an interaction with light. The walls of the cavity are made of molecules that behave like compounds of harmonic oscillators. Planck assumed that the energies of the molecules take values in some discrete set: the states of the molecules do not vary continuously but are discrete. Hence we can put the states in bijection with the natural numbers. Furthermore he assumed that the light inside the cavity induces transitions in the molecules by absorbing or emitting radiation. A transition from a state labelled with n and with energy E_n and a state labelled with m and with energy E_m is only possible if the energy differences and the frequencies are related by $|E_n - E_m| = \hbar\omega$. Thus by discretizing the states of the interior of the black body the interaction with light varies over a discrete set of frequencies. Planck at the moment saw the discretization as a purely theoretical and mathematical tool that would bear no relation with reality. It just reproduced the correct results, which was most important: it gave a formula that fitted all experiments. Very puzzling at the time was the necessary assumption that the energy was quantized – an assumption that marked the start of the quantum era. It took some time until the derivation of Planck's law was given a clear meaning.

6.6 Derivation of Planck's law

In 1905 Einstein gave a comprehensible derivation, which we shall present below. In modern textbooks one can find a one-page-derivation and we will present such a proof below as well.

For both derivations we need a basic fact from statistical mechanics, called the Boltzmann distribution.

Suppose that we have a physical system consisting of many identical molecules (or atoms, or any other smaller subsystems). Each molecule can attain different states that are labelled with integers $n = 0, 1, 2, \ldots$. In a modern treatment, these states are identified with the eigenstates of the quantum Hamiltonian, and we shall use this terminology, though it was not available when Einstein wrote his paper. We thus assume that the spectrum of the molecules is discrete and there is a bijection between the eigenstates of the molecule and the natural numbers. Each eigenstate n of the molecule corresponds to an eigenvalue E_n of the Hamiltonian, giving the energy the molecule has in eigenstate n. The Boltzmann distribution gives the relative frequency of eigenstates of the molecules. Writing $N(n)$ for the number of molecules in state n, the **Boltzmann distribution** dictates that

$$\frac{N(n)}{N(m)} = e^{-\frac{(E_n - E_m)}{kT}} . \tag{6.11}$$

when the system is in thermal equilibrium with itself and with the surrounding system. Thus, the temperature T has to be constant. Such a 'mixed' state, where the volume, the temperature, and the number of particles are kept constant and in thermal equilibrium with its environment is called a **canonical ensemble**. A derivation of the Boltzmann distribution can be found in many elementary textbooks on statistical physics, e.g., Reichl [230], Mandl [182], Huang [129], or Kittel [153].

The probability p_n of measuring an arbitrary molecule to be in state n is

$$p_n = \frac{e^{-\frac{E_n}{kT}}}{Z} ,$$

where Z is the **partition function**

$$Z = \sum_n e^{-\frac{E_n}{kT}} .$$

One can thus rewrite

$$p_n = e^{-\frac{(E_n - F)}{kT}} ,$$

where we defined the **Helmholtz free energy** F as

$$F = -kT \ln Z .$$

One often regroups the states into states that have equal energy. Then to each natural number corresponds an energy E_n, and a natural number g_n counting the number of states with energy E_n. The number g_n is called the **degeneracy** of the energy E_n. Thus we have

$$Z = \sum_n g_n e^{-\frac{E_n}{kT}} ,$$

and the probability p_n of measuring a molecule with energy E_n is

$$p_n = g_n e^{-\frac{(E_n - F)}{kT}} .$$

The constant $\beta = 1/kT$ is called the **inverse temperature** and plays a fundamental role; in statistical physics, it is customary to express all quantities in terms of β. The average of the energy, denoted $\bar{E}$, is found by

$$\bar{E} = \sum_{E_n} E_n p_n = -\frac{\partial}{\partial \beta} \ln Z(\beta)\,.$$

Einstein's derivation. We now focus on two energies in the molecule, n and m with $E_m > E_n$ and degeneracies g_n and g_m, and assume the molecules have interaction with light. There are three types of processes that might happen: (i) A molecule in state m might decay to state n while omitting light with the frequency

$$\hbar\omega = E_m - E_n; \tag{6.12}$$

this process is called **spontaneous decay**. (ii) A molecule might jump from n to m by absorbing light with the right frequency (6.12). (iii) A molecule decays from m to n by being kicked by light having the right frequency (6.12); this process is called **induced emission**. Thus, there is one transition which happens even in the absence of light: in a spontaneous emission the molecule may jump from m to n, thereby emitting light. The other two transitions take place under the influence of light; they are therefore dependent of how much light is present and thus depends on the radiation-energy density $f(\omega)$.

The probabilities of transitions are given as transition rates dW/dt; dW is the infinitesimal difference in molecules in a certain state and dt is an infinitesimal time interval. Now spontaneous emission is independent of the presence of light and only depends on the characteristics of the molecule and the number of molecules in state m. Therefore,

$$dW_1 = N(m)A_{mn}dt\,,$$

where dW_1 is the number of molecules undergoing spontaneous emission from m to n during a time interval dt, and where A_{mn} is some number depending on the states n and m (not on temperature in particular). We denote dW_2 the amount of molecules absorbing light and jumping from n to m during a time interval dt and dW_3 the number of molecules jumping from m to n under influence of light (getting the right kick). The probabilities are determined by some constants B_{mn} and C_{mn}, which are characteristic for the states m and n and the amount of light that has the right frequency. Thus dW_2 and dW_3 are proportional to $f(\omega)$;

$$dW_2 = N(n)B_{mn}f dt\,, \quad dW_3 = N(m)C_{mn}f dt\,.$$

Now we consider we have an enclosed system of molecules that are in equilibrium with the light in the system. Being in equilibrium means

$$dW_1 + dW_3 = dW_2\,.$$

Using the Boltzmann distribution we get

$$g_m e^{-\frac{E_m}{kT}}(A_{mn} + fC_{mn}) = g_n e^{-\frac{E_n}{kT}} f B_{mn}\,. \tag{6.13}$$

Now comes a basic assumption that Einstein does; if T becomes larger the system gets very hot and transitions will be more and more frequent. Therefore one assumes that as $T \to \infty$ that also $f \to \infty$. In this case the exponentials in (6.13) become 1 and the term with A can be neglected and we obtain

$$g_m C_{mn} = g_n B_{mn} \,. \tag{6.14}$$

From another point of view the assumption Einstein makes is natural. The relation $g_m C_{mn} = g_n B_{mn}$ is representing that the processes $m \to n$ under induced emission, or $n \to m$ under absorption are symmetric; the numbers C_{mn} and B_{mn} only differ by the ratio of number of states with energy E_n to the number of states with energy E_m. Indeed, taking $g_m = g_n = 1$, the process of induced emission is the time-reversed process of absorption. Since the equations in nature show a **time-reversal symmetry** (in this case) we find in this case $C_{mn} = B_{mn}$. If now g_n and g_m are not equal one has to correct for this and multiply the probabilities with the corresponding multiplicities to get (6.14). With the assumption (6.14) we find

$$f = \frac{A_{mn}/C_{mn}}{e^{(E_m - E_n)/kT} - 1} \,.$$

Inserting now $E_m - E_n = \hbar\omega$ and requiring that Wien's law (6.10) holds in the limit where ω is large we obtain

$$f(\omega) = \frac{a\omega^3}{e^{\hbar\omega/kT} - 1} \,.$$

In particular we find that $A_{mn}/C_{mn} = a\omega^3$, which relates the constants A_{mn} and C_{mn} to the energy difference $E_m - E_n$. The constant a does not depend on the frequency and the temperature.

Modern derivation. We now discuss a relatively fast derivation that in addition gives a value for the constant a in Wien's law (6.10). We consider a box with the shape of a cube with sides L. Later we then require that the precise shape of the box is not relevant in the limit where the typical sizes are much larger then the wavelength. Then the only relevant parameter is the volume $V = L^3$. We assume the walls of the box can absorb and emit light; we furthermore assume that the walls are made of a conducting material. Away from the walls light satisfies Maxwell equations, but at the walls the perpendicular components of the electric field have to vanish; if the electric field would not vanish, the electrons in the material of the wall would be accelerated, but then the system is not in equilibrium. A plane wave solution to the Maxwell equations is of the form

$$e^{i\omega t - ik_x x - ik_y y - ik_z z} \,, \quad \omega^2 = c^2(k_x^2 + k_y^2 + k_z^2) \,.$$

We can always chose a coordinate system that is aligned with the box. Then the boundary conditions imply $e^{ik_x L} = 0$ and thus $k_x = \frac{\pi n_x}{L}$ for some integer n_x. The wave functions with negative n_x are identical to the corresponding wave functions with positive n_x; they just differ by a phase. Therefore we may assume $n_x \geq 0$. For the other coordinate directions the discussion is similar.

Thus we find that for each triple of integer numbers $\mathbf{n} = (n_x, n_y, n_z)$ we have a harmonic oscillator with frequency

$$\omega_n = \frac{c\pi}{L} n, \quad n = \sqrt{\mathbf{n} \cdot \mathbf{n}} \,.$$

We now use the fact (proved below in Section 20.3) that for each harmonic oscillator the energies are $E_n(r) = \hbar\omega_n(r + \frac{1}{2})$. Since energy is defined only up to a constant shift, we subtract the zero-point energy $E_0 = \frac{1}{2}\hbar\omega_n$ and take $E_n(r) = \omega_n r$. The partition function is then

$$Z(\mathbf{n}, \beta) = \sum_{r=0}^{\infty} e^{r\hbar\omega_n\beta} = \frac{1}{e^{\hbar\omega_n\beta} - 1}\,.$$

Therefore the average energy in the mode corresponding to $\mathbf{n}$ is

$$\begin{aligned} \bar{E}_n &= -\frac{\partial}{\partial\beta}\ln(1 - e^{\hbar\omega_n\beta}) \\ &= \frac{\hbar\omega_n}{e^{\hbar\omega_n\beta} - 1}\,. \end{aligned}$$

We now have to sum up all the energies for all modes. Since we are interested in the behavior of $f(\omega)$ in the regime where the number L is much larger than the wavelength we replace the sum over $\vec{n}$ by an integral. We have to integrate over the positive octant where $n_x \geq 0$, $n_y \geq 0$ and $n_z \geq 0$. Since all expressions are rotationally symmetric in $\mathbf{n}$, we can also integrate over all of $\mathbb{R}^3$ and divide by 8. We have not yet taken into account that light has two polarizations. Therefore, for each $\mathbf{n}$ there are two harmonic oscillators. The total energy enclosed in the box is thus

$$E = \frac{2}{8}\int_{\mathbb{R}^3} dn_x dn_y dn_z\, \bar{E}_n = \pi\int_0^{\infty} n^2 dn \frac{\hbar\omega_n}{e^{\hbar\omega_n\beta} - 1}\,.$$

Here we transformed to polar coordinates and wrote $\omega_n = \frac{c\pi}{L}\sqrt{n_x^2 + n_y^2 + n_z^2}$.

We now exchange the integral over n to an integral over ω. We have

$$\omega = \frac{c\pi n}{L} \;\Rightarrow\; n^2 dn = \left(\frac{L}{\pi c}\right)^3 \omega^2 d\omega\,,$$

from which we find

$$E = \frac{L^3\hbar}{\pi^2 c^3}\int_0^{\infty} \frac{\omega^3}{e^{\hbar\omega\beta} - 1} d\omega\,.$$

With $L^3 = V$ being the volume we thus find

$$f(\omega) = \frac{V\hbar}{\pi^2 c^3}\frac{\omega^3}{e^{\hbar\omega\beta} - 1}\,. \tag{6.15}$$

Of course, this f only represents the radiation-energy density inside the black body. However, up to some overall constants the above f is the radiation-energy density of a black body since the emitted radiation is proportional to the energy density.

In the following section we shall derive Stefan's law.

6.7 Stefan's law and Wien's displacement law

From the calculated density (6.15) we can draw some conclusions, which we now shortly treat.

To calculate the total radiation that is emitted, we first calculate the total energy by integrating (6.15) over all ω. We get for the total energy of the light inside the black body

$$E = \frac{Vk^4T^4}{\pi^2c^3\hbar^3}\int_0^\infty \frac{x^3dx}{e^x-1}\,.$$

But we have

$$\int_0^\infty \frac{x^3dx}{e^x-1} = \frac{\pi^4}{15}\,,$$

and thus the energy density $u(T)$ is given by

$$u(T) = \frac{E}{V} = \frac{\pi^2k^4T^4}{15\hbar^3c^3}\,.$$

We see that the energy density is expressible by fundamental constants and the fourth power of the temperature. Since the energy density determines the total radiation emitted per time interval we see that the total energy a black body radiates per time interval is proportional to T^4. This already explains Stefan's law, but in order to derive Stefan's law we have to be a bit more careful.

In order to see how much a black body will radiate, we pinch a small hole in the black body. Let us say that the area of the hole is dA. Now the question is how many photons will hit the hole from inside out? We fix a time t and a small time interval dt. Only the photons that are within a distance between ct and $ct + cdt$ away from the hole are eligible to pass through the hole in a time interval dt after time t. We thus consider a thin shell of a half sphere inside the black body a distance ct away from the hole and of thickness cdt. Light however spreads in all directions and so not all the photons inside the shell are going in the direction of the hole. Our task is to find the ratio of the total that does go through the hole. This is a purely geometric question.

We introduce spherical coordinates around the hole; an angle φ ranging from 0 to 2π that goes around the hole, and a polar angle θ ranging from 0 to $\pi/2$ (values below zero correspond to points outside the black body). We cut the half sphere of radius ct in little stripes by cutting for fixed θ along the angle φ; each stripe is a thin band of thickness $ctd\vartheta$ and of length $2\pi\sin\theta$. Consider a little 'cube' of size $dV = (ct)^2\sin\theta d\theta d\varphi cdt$ in the shell. The fraction of radiation going in the right direction is given by the solid angle $d\Omega$ that dA describes seen from the little cube. But $d\Omega$ is given by the projection of the surface dA onto the surface of the sphere of radius ct around the little cube:

$$d\Omega = \frac{dA\cos\theta}{4\pi c^2t^2}\,.$$

The cube of volume emits all the radiation present in the cube (since the light waves just pass through), and that amounts to an energy $dE = u(T)dV$. From the little cube under consideration the amount of radiation going in the right direction is thus

$$ud\Omega dV = u(T)\frac{cdA\cos\theta\sin\theta}{4\pi}d\theta d\varphi dt\,.$$

Note that the amount of radiation is independent of the radius of the half sphere. Since the question is of a purely geometric nature, that is to be expected. We now get the total

amount of radiation from summing up all the $d\Omega$ contributions: Denoting by dU the energy that leaves the hole during the time interval dt, we have

$$\begin{aligned}\frac{dU}{dt} &= \int_0^{\pi/2} d\theta \int_0^{2\pi} d\varphi\, u(T) \frac{cdA\cos\theta\sin\theta}{4\pi} \\ &= \frac{c}{4} u(T) dA\,.\end{aligned}$$

For a black body that radiates over all its surface, and not only through one little hole, we sum up the contributions over all little surfaces dA. In order that the above analysis still holds the shape of the black body needs to be such that radiation that exits the black body does not enter again. If the black body is convex this requirement is met, e.g., we could take a sphere. We then find Stefan's law in the form given by

$$\frac{dU}{dt} = \frac{\pi^2 k^4 T^4 A}{60\hbar^3 c^2} = \sigma A T^4\,,$$

with **Stefan's constant**

$$\sigma = \frac{\pi^2 k^4}{60\hbar^3 c^2} \sim 5.7 \cdot 10^{-8} J.s^{-1}.m^{-2} K^{-4}\,.$$

We now turn to Wien's displacement law. We write the radiation-energy density as

$$f(\omega) = A \frac{\omega^3}{e^{\hbar\omega\beta} - 1}\,.$$

Differentiation with respect to ω and putting the result to zero to obtain the position of the maximum gives the equations

$$3 - x = 3e^{-x}\,, \quad x = \hbar\omega_{max}\beta\,.$$

We discard the trivial solution $x = 0$ since this corresponds to the behavior at $\omega = 0$. One finds the other solution by solving the equation $3 - x = 3e^{-x}$ with numerical methods and finds $x \sim 2.82$. Hence we have

$$\omega_{max} \sim \frac{2.82\,T}{\hbar k}\,.$$

Part II

Statistical mechanics

Chapter 7

Phenomenological thermodynamics

Part II discusses statistical mechanics from an algebraic perspective, concentrating on thermal equilibrium but discussing basic things in a more general framework. A treatment of equilibrium statistical mechanics and the kinematic part of nonequilibrium statistical mechanics is given which derives from a single basic assumption (Definition 9.1.1) the full structure of phenomenological thermodynamics and of statistical mechanics, except for the third law which requires an additional quantization assumption.

This chapter gives a concise description of standard phenomenological equilibrium thermodynamics for single-phase systems in the absence of chemical reactions and electromagnetic fields. From the formulas provided, it is an easy step to go to various examples and applications discussed in standard textbooks such as Callen [55] or Reichl [230]. A full discussion of global equilibrium would also involve the equilibrium treatment of multiple phases and chemical reactions. Since their discussion offers no new aspects compared with traditional textbook treatments, they are not treated here.

Our phenomenological approach is similar to that of Callen [55], who introduces the basic concepts by means of a few postulates from which everything else follows. The present setting is a modified version designed to match the more fundamental approach based on statistical mechanics. By specifying the kinematical properties of states outside equilibrium, his informal thermodynamic stability arguments (which depend on a dynamical assumption close to equilibrium) can be replaced by rigorous mathematical arguments.

7.1 Standard thermodynamical systems

We discuss here the special but very important case of thermodynamic systems describing the single-phase global equilibrium of matter composed of one or several kinds of substances in the absence of chemical reactions and electromagnetic fields. We call such systems **standard thermodynamic systems**; they are ubiquitous in applications. In particular,

a standard system is considered to be uncharged, homogeneous, and isotropic, so that each finite region looks like any other and is very large in microscopic units.

The substances of fixed chemical composition are labeled by an index $j \in J$. A standard thermodynamic system is completely characterized by[1] the **mole number** N_j of each substance j, the corresponding **chemical potential** μ_j of substance j, the **volume** V, the **pressure** P, the **temperature** T, the **entropy** S, and the **Hamilton energy** H. These variables, the **extensive** variables N_j, V, S, H and the **intensive** variables μ_j, P, T, are jointly called the **basic thermodynamic variables**. We group the N_j and the μ_j into vectors N and μ indexed by J and write $\mu \cdot N = \sum_{j\in J} \mu_j N_j$. In the special case of a **pure substance**, there is just a single kind of substance; then we drop the indices and have $\mu \cdot N = \mu N$. In this section, all numbers are real.

The mathematics of thermodynamics makes essential use of the concept of convexity. A set $X \subseteq \mathbb{R}^n$ is called **convex** if $tx + (1-t)y \in X$ for all $x, y \in X$ and all $t \in [0,1]$. A real-valued function ϕ is called **convex** on the convex set $X \subseteq \mathbb{R}^n$ if ϕ is defined on X and, for all $x, y \in X$,

$$\phi(tx + (1-t)y) \le t\phi(x) + (1-t)\phi(y) \quad \text{for } 0 \le t \le 1.$$

Clearly, ϕ is convex iff for all $x, y \in X$, the function $\mu : [0,1] \to \mathbb{R}$ defined by

$$\mu(t) := \phi(x + t(y-x))$$

is convex. It is well-known that, for twice continuously differentiable ϕ, this is the case iff the second derivative $\mu''(t)$ is nonnegative for $0 \le t \le 1$. Note that by a theorem of Aleksandrov (see Aleksandrov [6], Alberti & Ambrosio [4], Rockafellar [238]), convex functions are almost everywhere twice continuously differentiable: For almost every $x \in X$, there exist a unique vector $\partial\phi(x) \in \mathbb{R}^n$, the **gradient** of ϕ at x, and a unique symmetric, positive semidefinite matrix $\partial^2\phi(x) \in \mathbb{R}^{n\times n}$, the **Hessian** of ϕ at x, such that

$$\phi(x+h) = \phi(x) + h^T\partial\phi(x) + \frac{1}{2}h^T\partial^2\phi(x)h + o(\|h\|^2)$$

for sufficiently small $h \in \mathbb{R}^n$. A function ϕ is called **concave** if $-\phi$ is convex. Thus, for a twice continuously differentiable function ϕ of a single variable τ, ϕ is concave iff $\mu''(\tau) \le 0$ for $0 \le \tau \le 1$.

7.1.1 Proposition. *If ϕ is convex on the convex set X then the function ψ defined by*

$$\psi(s,x) := s\phi(x/s)$$

is convex in the set $\{(s,x) \in \mathbb{R}\times X \mid s > 0\}$ and concave in the set $\{(s,x) \in \mathbb{R}\times X \mid s < 0\}$.

[1] In the terminology, we mainly follow the IUPAC convention (Alberty [5, Section 7]), except that we use the letter H to denote the Hamilton energy, as customary in quantum mechanics. In equilibrium, H equals the internal energy U. The Hamilton energy should not be confused with the enthalpy which is usually denoted by H but here is given in equilibrium by $H + PV$. For a history of thermodynamics notation, see Battino et al. [29].

Proof. It suffices to show that $\mu(t) := \psi(s+tk, x+th)$ is convex (concave) for all s, x, h, k such that $s + tk > 0$ (resp. < 0). Let $z(t) := (x+th)/(s+tk)$ and $c := sh - kx$. Then

$$z'(t) = \frac{c}{(s+tk)^2}, \quad \mu(t) = (s+tk)\phi(z(t)),$$

hence

$$\mu'(t) = k\phi(z(t)) + \phi'(z(t))\frac{c}{s+tk},$$

$$\mu''(t) = k\phi'(z(t))\frac{c}{(s+tk)^2} + \frac{c^T}{(s+tk)^2}\phi''(z(t))\frac{c}{s+tk} + \phi'(z(t))\frac{-ck}{(s+tk)^2} = \frac{c^T\phi''(z(t))c}{(s+tk)^3},$$

which has the required sign. □

Equilibrium thermodynamics is about characterizing so-called equilibrium states in terms of intensive and extensive variables and their relations, and comparing them with similar nonequilibrium states. In a nonequilibrium state, only extensive variables have a well-defined meaning; but these are not sufficient to characterize system behavior completely.

All valid statements in the equilibrium thermodynamics of standard systems can be deduced from the following definition.

7.1.2 Definition. (Phenomenological thermodynamics)
(i) Temperature T, pressure P, and volume V are positive, mole numbers N_j are nonnegative. The **extensive variables** H, S, V, N_j are additive under the composition of disjoint subsystems. We combine the N_j into a column vector with these components.

(ii) There is a convex **system function** Δ of the **intensive variables** T, P, μ which is monotone increasing in T and monotone decreasing in P. The intensive variables are related by the **equation of state**

$$\Delta(T, P, \mu) = 0. \tag{7.1}$$

The set of (T, P, μ) satisfying $T > 0$, $P > 0$ and the equation of state is called the **state space**.

(iii) The Hamilton energy H satisfies the **Euler inequality**

$$H \geq TS - PV + \mu \cdot N \tag{7.2}$$

for all (T, P, μ) in the state space.

(iv) **Equilibrium states** have well-defined intensive and extensive variables satisfying equality in (7.2). A system is in **equilibrium** if it is completely characterized by an equilibrium state.

This is the complete list of assumptions defining phenomenological equilibrium thermodynamics for standard systems; the system function Δ can be determined either by fitting to experimental data, or by calculation from a more fundamental description, cf. Theorem

9.2.1. All other properties follow from the system function. Thus, all equilibrium properties of a material are characterized by the system function Δ.

Surfaces where the system function is not differentiable correspond to so-called **phase transitions**. The equation of state shows that, apart from possible phase transitions, the state space has the structure of an $(s-1)$-dimensional manifold in $\mathbb{R}^s$, where s is the number of intensive variables; in case of a standard system, the manifold dimension is therefore one higher than the number of kinds of substances.

Standard systems describe only a single phase of a substance (typically the solid, liquid, or gas phase), and changes between these as some thermodynamic variable(s) change. Thermodynamic systems with multiple phases (e.g., boiling water, or water containing ice cubes) are only piecewise homogeneous. Each phase may be described separately as a standard thermodynamic system. But discussing the equilibrium at the interfaces between different phases needs some additional effort. (This is described in all common textbooks on thermodynamics.) Therefore, we consider only regions of the state space where the system function Δ is twice continuously differentiable.

Each equilibrium instance of the material is characterized by a particular state (T, P, μ), from which all equilibrium properties can be computed:

7.1.3 Theorem.

(i) In any equilibrium state, the extensive variables are given by

$$S = \Omega \frac{\partial \Delta}{\partial T}(T, P, \mu), \quad V = -\Omega \frac{\partial \Delta}{\partial P}(T, P, \mu), \quad N = \Omega \frac{\partial \Delta}{\partial \mu}(T, P, \mu), \tag{7.3}$$

and the ***Euler equation***

$$H = TS - PV + \mu \cdot N. \tag{7.4}$$

Here Ω is a positive number called the ***system size****.*

(ii) In equilibrium, we have the ***Maxwell reciprocity relations***

$$-\frac{\partial V}{\partial T} = \frac{\partial S}{\partial P}, \quad \frac{\partial N_j}{\partial T} = \frac{\partial S}{\partial \mu_j}, \quad \frac{\partial N_j}{\partial P} = -\frac{\partial V}{\partial \mu_j}, \quad \frac{\partial N_j}{\partial \mu_k} = \frac{\partial N_k}{\partial \mu_j}, \tag{7.5}$$

and the ***stability conditions***

$$\frac{\partial S}{\partial T} \geq 0, \quad \frac{\partial V}{\partial P} \leq 0, \quad \frac{\partial N_j}{\partial \mu_j} \geq 0. \tag{7.6}$$

Proof. At fixed S, V, N, inequality (7.2) holds in equilibrium with equality, by definition. Therefore the triple (T, P, μ) is a maximizer of $TS - PV + \mu \cdot N$ under the constraints $\Delta(T, P, \mu) = 0$, $T > 0$, $P > 0$. A necessary condition for a maximizer is the stationarity of the Lagrangian

$$L(T, P, \mu) = TS - PV + \mu \cdot N - \Omega \Delta(T, P, \mu)$$

for some Lagrange multiplier Ω. Setting the partial derivatives to zero gives (7.3), and since the maximum is attained in equilibrium, the Euler equation (7.4) follows. The system size Ω is positive since $V > 0$ and Δ is decreasing in P. Since the Hessian matrix of Δ,

$$\Sigma = \begin{pmatrix} \frac{\partial^2\Delta}{\partial T^2} & \frac{\partial^2\Delta}{\partial P\partial T} & \frac{\partial^2\Delta}{\partial\mu\partial T} \\ \frac{\partial^2\Delta}{\partial T\partial P} & \frac{\partial^2\Delta}{\partial P^2} & \frac{\partial^2\Delta}{\partial\mu\partial P} \\ \frac{\partial^2\Delta}{\partial T\partial\mu} & \frac{\partial^2\Delta}{\partial P\partial\mu} & \frac{\partial^2\Delta}{\partial\mu^2} \end{pmatrix} = \Omega^{-1} \begin{pmatrix} \frac{\partial S}{\partial T} & \frac{\partial S}{\partial P} & \frac{\partial S}{\partial\mu} \\ -\frac{\partial V}{\partial T} & -\frac{\partial V}{\partial P} & -\frac{\partial V}{\partial\mu} \\ \frac{\partial N}{\partial T} & \frac{\partial N}{\partial P} & \frac{\partial N}{\partial\mu} \end{pmatrix},$$

is symmetric, the Maxwell reciprocity relations follow. Since Δ is convex, Σ is positive semidefinite; hence the diagonal elements of Σ are nonnegative, giving the stability conditions. □

Note that there are further stability conditions since the determinants of all principal submatrices of Σ must be nonnegative. In addition, since $N_j \geq 0$, (7.3) implies that Δ is monotone increasing in each μ_j.

7.1.4 Example. The equilibrium behavior of electrically neutral gases at sufficiently low pressure can be modelled as ideal gases. An **ideal gas** is defined by a system function of the form

$$\Delta(T, P, \mu) = \sum_{j\in J} \pi_j(T) e^{\mu_j/RT} - P, \tag{7.7}$$

where the $\pi_j(T)$ are positive functions of the temperature,

$$R \approx 8.31447\, JK^{-1}\mathrm{mol}^{-1} \tag{7.8}$$

is the **universal gas constant**[2], and we use the bracketing convention $\mu_j/RT = \mu_j/(RT)$. Differentiation with respect to P shows that $\Omega = V$ is the system size, and from (7.1), (7.3), and (7.4), we find that, in equilibrium,

$$P = \sum_j \pi_j(T) e^{\mu_j/RT}, \quad S = V \sum_j \Big(\frac{\partial}{\partial T}\pi_j(T) - \frac{\mu_j \pi_j(T)}{RT^2}\Big) e^{\mu_j/RT},$$

$$N_j = \frac{V\pi_j(T)}{RT} e^{\mu_j/RT}, \quad H = V \sum_j \Big(T\frac{\partial}{\partial T}\pi_j(T) - \pi_j(T)\Big) e^{\mu_j/RT}.$$

Expressed in terms of T, V, N, we have

$$PV = RT \sum_j N_j, \quad \mu_j = RT \log \frac{RTN_j}{V\pi_j(T)},$$

[2]For the internationally recommended values of this and other constants, their accuracy, determination, and history, see CODATA [67].

$$H = \sum_j h_j(T) N_j, \quad h_j(T) = RT\Big(T\frac{\partial}{\partial T}\log \pi_j(T) - 1\Big),$$

from which S can be computed by means of the Euler equation (7.4). In particular, for one **mole** of a single substance, defined by $N = 1$, we get the **ideal gas law**

$$PV = RT \tag{7.9}$$

discovered by Clapeyron [64]; cf. Jensen [141].

In general, the difference $h_j(T) - h_j(T')$ can be found experimentally by measuring the energy needed for raising or lowering the temperature of pure substance j from T' to T while keeping the N_j constant. In terms of infinitesimal increments, the **heat capacities**

$$C_j(T) = dh_j(T)/dT,$$

we have

$$h_j(T) = h_j(T') + \int_{T'}^{T} dT\, C_j(T).$$

From the definition of $h_j(T)$, we find that

$$\pi_j(T) = \pi_j(T') \exp \int_{T'}^{T} \frac{dT}{T}\Big(1 + \frac{h_j(T)}{RT}\Big).$$

Thus there are two undetermined integration constants for each kind of substance. These cannot be determined experimentally as long as we are in the range of validity of the ideal gas approximation. Indeed, if we pick arbitrary constants α_j and γ_j and replace $\pi_j(T), \mu_j, H$, and S by

$$\pi'_j(T) := e^{\alpha_j - \gamma_j/RT}\pi_j(T), \quad \mu'_j = \mu_j + \gamma_j - RT\alpha_j,$$

$$H' = H + \sum_j \alpha_j N_j, \quad S' = S + R\sum_j \gamma_j N_j,$$

all relations remain unchanged. Thus, the Hamilton energy and the entropy of an ideal gas are only determined up to an arbitrary linear combination of the mole numbers. This is an instance of the deeper problem to determine under which conditions thermodynamic variables are controllable; cf. the discussion in the context of Example 10.1.1 below.

This gauge freedom (present only in the ideal gas) can be fixed by choosing a particular **standard temperature** T_0 and setting arbitrarily $h_j(T_0) = 0$, $\mu_j(T_0) = 0$. Alternatively, at sufficiently large temperature T, heat capacities are usually nearly constant, and making use of the gauge freedom, we may simply assume that

$$h_j(T) = h_{j0}T, \quad \pi_j(T) = \pi_{j0}T \quad \text{for large } T.$$

7.2 The laws of thermodynamics

In global equilibrium, all thermal variables are constant throughout the system, except at phase boundaries, where the extensive variables may exhibit jumps and only the intensive variables remain constant. This is sometimes referred to as the **zeroth law of thermodynamics** (Fowler & Guggenheim[89]) and characterizes global equilibrium; it allows one to measure intensive variables (like temperature) by bringing a calibrated instrument that is sensitive to this variable (for temperature a thermometer) into equilibrium with the system to be measured.

For example, the ideal gas law (7.9) can be used as a basis for the construction of a **gas thermometer**: The amount of expansion of volume in a long, thin tube can easily be read off from a scale along the tube. We have $V = aL$, where a is the cross section area and L is the length of the filled part of the tube, hence $T = (aP/R)L$. Thus, at constant pressure, the temperature of the gas is proportional to L. For the history of temperature, see Roller [240] and Truesdell [270].

We say that two thermodynamic systems are brought in good **thermal contact** if the joint system tends after a short time to an equilibrium state. To measure the temperature of a system, one brings it in thermal contact with a thermometer and waits until equilibrium is established. The system and the thermometer will then have the same temperature, which can be read off from the thermometer. If the system is much larger than the thermometer, this temperature will be essentially the same as the temperature of the system before the measurement. For a survey of the problems involved in defining and measuring temperature outside equilibrium, see Casas-Vásquez & Jou [58].

To be able to formulate the first law of thermodynamics we need the concept of a reversible change of states, i.e., changes preserving the equilibrium condition. For use in later sections, we define the concept in a slightly more general form, writing α for P and μ jointly. We need to assume that the system under study is embedded into its environment in such a way that, at the boundary, certain thermodynamic variables are kept constant (and independent of position). This determines the **boundary conditions** of the thermodynamic system; see the discussion in Section 7.3.

7.2.1 Definition. A **state variable** is an almost everywhere continuously differentiable function $\phi(T, \alpha)$ defined on the state space (or on a subset of it). Temporal changes in a state variable that occur when the boundary conditions are kept fixed are called **spontaneous changes**. A **reversible transformation** is a continuously differentiable mapping

$$\lambda \to (T(\lambda), \alpha(\lambda))$$

from a real interval into the state space; thus $\Delta(T(\lambda), \alpha(\lambda)) = 0$. The **differential**

$$d\phi = \frac{\partial \phi}{\partial T} dT + \frac{\partial \phi}{\partial \alpha} \cdot d\alpha, \tag{7.10}$$

obtained by multiplying the chain rule by $d\lambda$, describes the change of a state variable ϕ under arbitrary (infinitesimal) reversible transformations. In formal mathematical terms, differentials are exact linear forms on the state space manifold; cf. Chapter 17.

Reversible changes per se have nothing to do with changes in time. However, by sufficiently slow, quasistatic changes of the boundary conditions, reversible changes can often be realized approximately as temporal changes. The degree to which this is possible determines the efficiency of thermodynamic machines. The analysis of the efficiency by means of the so-called **Carnot cycle** was the historical origin of thermodynamics.

The state space is often parameterized by different sets of state variables, as required by the application. If $T = T(\kappa, \lambda)$, $\alpha = \alpha(\kappa, \lambda)$ is such a parameterization then the state variable $g(T, \alpha)$ can be written as a function of (κ, λ),

$$g(\kappa, \lambda) = g(T(\kappa, \lambda), \alpha(\kappa, \lambda)). \tag{7.11}$$

This notation, while mathematically ambiguous, is common in the literature; the names of the argument decide which function is intended. When writing partial derivatives without arguments, this leads to serious ambiguities. These can be resolved by writing $\left(\frac{\partial g}{\partial \lambda}\right)_\kappa$ for the partial derivative of (7.11) with respect to λ; it can be evaluated using (7.10), giving the **chain rule**

$$\left(\frac{\partial g}{\partial \lambda}\right)_\kappa = \frac{\partial g}{\partial T}\left(\frac{\partial T}{\partial \lambda}\right)_\kappa + \frac{\partial g}{\partial \alpha} \cdot \left(\frac{\partial \alpha}{\partial \lambda}\right)_\kappa. \tag{7.12}$$

Here the partial derivatives in the original parameterization by the intensive variables are written without parentheses.

Differentiating the equation of state (7.1), using the chain rule (7.10), and simplifying using (7.3) gives the **Gibbs-Duhem equation**

$$0 = SdT - VdP + N \cdot d\mu \tag{7.13}$$

for reversible changes. If we differentiate the Euler equation (7.4), we obtain

$$dH = TdS + SdT - PdV - VdP + \mu \cdot dN + N \cdot d\mu,$$

and using (7.13), this simplifies to the **first law of thermodynamics**

$$dH = TdS - PdV + \mu \cdot dN. \tag{7.14}$$

Historically, the first law of thermodynamics took on this form only gradually, through work by Mayer [188], Joule [143], Helmholtz [125], and Clausius [65].

Considering global equilibrium from a fundamental point of view, the extensive variables are the variables that are conserved or at least change so slowly that they may be regarded as time independent on the time scale of interest. In the absence of chemical reactions, the mole numbers, the entropy, and the Hamilton energy are conserved; the volume is a system size variable which, in the fundamental view, must be taken as infinite (thermodynamic limit) to exclude the unavoidable interaction with the environment. However, real systems are always in contact with their environment, and the conservation laws are approximate only. In thermodynamics, the description of the system boundary is generally reduced to the degrees of freedom observable at a given resolution.

The result of this reduced description (for derivations, see, e.g., Balian [20], Grabert [109], Rau & Müller [228]) is a dynamical effect called **dissipation** (Thomson [268]). It

is described by the **second law of thermodynamics**, which was discovered by (CLAUSIUS [66]. The Euler inequality (7.2) together with the Euler equation (7.4) only express the nondynamical part of the second law since, in equilibrium thermodynamics, dynamical questions are ignored: Parts (iii)-(iv) of Definition 7.1.2 say that if S, V, N are conserved (thermal, mechanical and chemical isolation) then the **internal energy**,

$$U := TS - PV + \mu \cdot N \tag{7.15}$$

is minimal in equilibrium; if T, V, N are conserved (mechanical and chemical isolation of a system at constant temperature T) then the **Helmholtz (free) energy**,

$$F := U - TS = -PV + \mu \cdot N$$

is minimal in equilibrium; and if T, P, N are conserved (chemical isolation of a system at constant temperature T and pressure P) then the **Gibbs (free) energy**,

$$G := F + PV = \mu \cdot N$$

is minimal in equilibrium.

The **third law of thermodynamics**, due to NERNST [201], says that entropy is nonnegative. In view of (7.3), this is equivalent to the monotonicity of $\Delta(T, P, \mu)$.

7.3 Consequences of the first law

The first law of thermodynamics describes the observable energy balance in a reversible process. The total energy flux dH into the system is composed of the **thermal energy flux** or **heat flux** TdS, the **mechanical energy flux** $-PdV$, and the **chemical energy flux** $\mu \cdot dN$.

The Gibbs-Duhem equation (7.13) describes the energy balance necessary to compensate the changes $d(TS) = TdS + SdT$ of thermal energy, $d(PV) = PdV + VdP$ of mechanical energy, and $d(\mu \cdot N) = \mu \cdot dN + N \cdot d\mu$ of chemical energy in the energy contributions to the Euler equation to ensure that the Euler equation remains valid during a reversible transformation. Indeed, both equations together imply that $d(TS - PV + \mu \cdot N - H)$ vanishes, which expresses the preservation of the Euler equation.

Related to the various energy fluxes are the **thermal work**

$$Q = \int T(\lambda) dS(\lambda),$$

the **mechanical work**

$$W_{\text{mech}} = -\int P(\lambda) dV(\lambda),$$

and the **chemical work**

$$W_{\text{chem}} = \int \mu(\lambda) \cdot dN(\lambda)$$

performed in a reversible transformation. The various kinds of work generally depend on the path through the state space; however, the mechanical work depends only on the end points if the associated process is conservative.

As is apparent from the formulas given, thermal work is done by changing the entropy of the system, mechanical work by changing the volume, and chemical work by changing the mole numbers. In particular, in case of thermal, mechanical, or chemical **isolation**, the corresponding fluxes vanish identically. Thus, constant S characterizes thermally isolated, **adiabatic** systems, constant V characterizes mechanically isolated, systems, and constant N characterizes chemically isolated, **closed**[3] or **impermeable** systems. Note that this constancy only holds when all assumptions for a standard system are valid: global equilibrium, a single phase, and the absence of chemical reactions. Of course, these boundary conditions are somewhat idealized situations, which, however, can be approximately realized in practice and are of immense scientific and technological importance.

The first law shows that, in appropriate units, the temperature T is the amount of energy needed to increase in a mechanically and chemically isolated system the entropy S by one unit. The pressure P is, in appropriate units, the amount of energy needed to decrease in a thermally and chemically isolated system the volume V by one unit. In particular, increasing pressure decreases the volume; this explains the minus sign in the definition of P. The chemical potential μ_j is, in appropriate units, the amount of energy needed to increase in a thermally and mechanically isolated system the mole number N_j by one. With the traditional units, temperature, pressure, and chemical potentials are no longer energies.

We see that the entropy and the volume behave just like the mole number. This analogy can be deepened by observing that mole numbers are the natural measure of the amounts of "matter" of each kind in a system, and chemical energy flux is accompanied by adding or removing matter. Similarly, volume is the natural measure of the amount of "space" a system occupies, and mechanical energy flux in a standard system is accompanied by adding or removing space. Thus we may regard entropy as the natural measure of the amount of "heat" contained in a system[4], since thermal energy flux is accompanied by adding or removing heat. Looking at other extensive quantities, we also recognize energy as the natural measure of the amount of "power" (colloquial), momentum as the natural measure of the amount of "force" (colloquial), and mass as the natural measure of the amount of "inertia" (colloquial) of a system. In each case, the notions in quotation marks are the colloquial terms which are associated in ordinary life with the more precise, formally

[3]Note that the terms 'closed system' has also a much more general interpretation – which we do *not* use in this chapter –, namely as a conservative dynamical system.

[4]Thus, entropy is the modern replacement for the historical concepts of **phlogiston** and **caloric**, which failed to give a correct account of heat phenomena. Phlogiston turned out to be "missing oxygen", an early analogue of the picture of positrons as holes, "missing electrons", in the Dirac sea. Caloric was a massless substance of heat which had almost the right properties, explained many effects correctly, and fell out of favor only after it became known that caloric could be generated in arbitrarily large amounts from mechanical energy, thus discrediting the idea of heat being a substance. (For the precise relation of entropy and caloric, see Kuhn [163, 164], Walter [283], and the references quoted there.) In the modern picture, the extensivity of entropy models the substance-like properties of the colloquial term "heat". But as there are no particles of space whose mole number is proportional to the volume, so there are no particles of heat whose mole number is proportional to the entropy. Nevertheless, the introduction of heat particles on a formal level has some uses; see, e.g., Streater [263].

defined physical quantities. For historical reasons, the words heat, power, and force are used in physics with a meaning different from the colloquial terms "heat", "power", and "force".

7.4 Consequences of the second law

The second law is centered around the impossibility of perpetual motion machines due to the inevitable loss of energy by dissipation such as friction (see, e.g., Bowden & Leben [49]), uncontrolled radiation, etc.. This means that – unless continually provided from the outside – energy is lost with time until a metastable state is attained, which usually is an equilibrium state. Therefore, the energy at equilibrium is minimal under the circumstances dictated by the boundary conditions. In a purely kinematic setting as in our treatment, the approach to equilibrium cannot be studied, and only the minimal energy principles – one for each set of boundary conditions – remain.

Traditionally, the second law is often expressed in the form of an extremal principle for some thermodynamic potential. We derive here the extremal principles for the Hamilton energy, the Helmholtz energy, and the Gibbs energy[5], which give rise to the **Hamilton potential**

$$U(S,V,N) := \max_{T,P,\mu} \{TS - PV + \mu \cdot N \mid \Delta(T,P,\mu) = 0; T > 0; P > 0\},$$

the **Helmholtz potential**

$$F(T,V,N) := \max_{P,\mu} \{-PV + \mu \cdot N \mid \Delta(T,P,\mu) = 0; T > 0; P > 0\},$$

and the **Gibbs potential**

$$G(T,P,N) := \max_{\mu} \{\mu \cdot N \mid \Delta(T,P,\mu) = 0; T > 0; P > 0\}.$$

The Gibbs potential is of particular importance for everyday processes since the latter frequently happen at approximately constant temperature, pressure, and mole number. (For other thermodynamic potentials used in practice, see Alberty [5]; for the maximum entropy principle, see Section 10.7.)

7.4.1 Theorem. ***(Extremal principles)***
(i) In an arbitrary state,

$$H \geq U(S,V,N), \tag{7.16}$$

with equality iff the state is an equilibrium state. The remaining thermodynamic variables are then given by

$$T = \frac{\partial}{\partial S} U(S,V,N), \quad P = -\frac{\partial}{\partial V} U(S,V,N), \quad \mu = \frac{\partial}{\partial N} U(S,V,N), \quad H = U(S,V,N).$$

[5]The different potentials are related by so-called Legendre transforms; cf. Rockafellar [239] for the mathematical properties of Legendre transforms, Arnol'd [16] for their application in mechanics, and Alberty [5] for their application in chemistry.

In particular, an equilibrium state is uniquely determined by the values of S, V, and N.

(ii) In an arbitrary state,

$$H - TS \geq F(T, V, N), \tag{7.17}$$

with equality iff the state is an equilibrium state. The remaining thermodynamic variables are then given by

$$S = -\frac{\partial F}{\partial T}(T, V, N), \quad P = -\frac{\partial F}{\partial V}(T, V, N), \quad \mu = \frac{\partial F}{\partial N}(T, V, N),$$

$$H = F(T, V, N) + TS.$$

In particular, an equilibrium state is uniquely determined by the values of T, V, and N.

(iii) In an arbitrary state,

$$H - TS + PV \geq G(T, P, N), \tag{7.18}$$

with equality iff the state is an equilibrium state. The remaining thermodynamic variables are then given by

$$S = -\frac{\partial G}{\partial T}(T, P, N), \quad V = \frac{\partial G}{\partial P}(T, P, N), \quad \mu = \frac{\partial G}{\partial N}(T, P, N),$$

$$H = G(T, P, N) + TS - PV.$$

In particular, an equilibrium state is uniquely determined by the values of T, P, and N.

Proof. We prove (ii); the other two cases are entirely similar. (7.17) and the statement about equality is a direct consequence of Axiom 7.1.2(iii)–(iv). Thus, the difference $H - TS - F(T, V, N)$ takes its minimum value zero at the equilibrium value of T. Therefore, the derivative with respect to T vanishes, which gives the formula for S. To get the formulas for P and μ, we note that for constant T, the first law (7.14) implies

$$dF = d(H - TS) = dH - TdS = -PdV + \mu \cdot dN.$$

For the reversible transformation which only changes P or μ_j, we conclude that $dF = -PdV$ and $dF = \mu \cdot dN$, respectively. Solving for P and μ_j, respectively, implies the formulas for P and μ_j. □

The above results imply that one can regard each thermodynamic potential as a complete alternative way to describe the manifold of thermal states and hence all equilibrium properties. This is very important in practice, where one usually describes thermodynamic material properties in terms of the Helmholtz or Gibbs potential, using models like NRTL (Renon & Prausnitz [231], Prausnitz et al. [223]) or SAFT (Chapman et al. [59, 60]).

The additivity of extensive quantities is reflected in the corresponding properties of the thermodynamic potentials:

7.4.2 Theorem. *The potentials $U(S,V,N)$, $F(T,V,N)$, and $G(T,P,N)$ satisfy, for real $\lambda, \lambda^1, \lambda^2 \geq 0$,*

$$U(\lambda S, \lambda V, \lambda N) = \lambda U(S,V,N), \tag{7.19}$$

$$F(T, \lambda V, \lambda N) = \lambda F(T,V,N), \tag{7.20}$$

$$G(T,P,\lambda N) = \lambda G(T,P,N), \tag{7.21}$$

$$U(\lambda^1 S^1 + \lambda^2 S^2, \lambda^1 V^1 + \lambda^2 V^2, \lambda^1 N^1 + \lambda^2 N^2) \leq \lambda^1 U(S^1,V^1,N^1) + \lambda^2 U(S^2,V^2,N^2), \tag{7.22}$$

$$F(T, \lambda^1 V^1 + \lambda^2 V^2, \lambda^1 N^1 + \lambda^2 N^2) \leq \lambda^1 F(T,V^1,N^1) + \lambda^2 F(T,V^2,N^2), \tag{7.23}$$

$$G(T,P,\lambda^1 N^1 + \lambda^2 N^2) \leq \lambda^1 G(T,P,N^1) + \lambda^2 G(T,P,N^2). \tag{7.24}$$

In particular, these potentials are convex in S, V, and N.

Proof. The first three equations express homogeneity and are a direct consequence of the definitions. Inequality (7.23) holds since, for suitable P and μ,

$$\begin{aligned} F(T, \lambda^1 V^1 + \lambda^2 V^2, \lambda^1 N^1 + \lambda^2 N^2) &= -P(\lambda^1 V^1 + \lambda^2 V^2) + \mu \cdot (\lambda^1 N^1 + \lambda^2 N^2) \\ &= \lambda^1(-PV^1 + \mu \cdot N^1) + \lambda^2(-PV^2 + \mu \cdot N^2) \\ &\leq \lambda^1 F(T,V^1,N^1) + \lambda^2 F(T,V^2,N^2); \end{aligned}$$

and the others follow in the same way. Specialized to $\lambda^1 + \lambda^2 = 1$, the inequalities express the claimed convexity. □

For a system at constant temperature T, pressure P, and mole number N, consisting of a number of parts labeled by a superscript k which are separately in equilibrium, the Gibbs energy is extensive, since

$$\begin{aligned} G &= H - TS + PV = \sum H^k - T \sum S^k + P \sum V^k \\ &= \sum (H^k - TS^k + PV^k) = \sum G^k. \end{aligned}$$

Equilibrium requires that $\sum G^k$ is minimal among all choices with $\sum N^k = N$, and by introducing a Lagrange multiplier vector μ^* for the constraints, we see that in equilibrium, the derivative of $\sum (G(T,P,N^k) - \mu^* \cdot N^k)$ with respect to each N^k must vanish. This implies that

$$\mu^k = \frac{\partial G}{\partial N^k}(T,P,N^k) = \mu^*.$$

Thus, in equilibrium, all μ^k must be the same. At constant T, V, and N, one can apply the same argument to the Helmholtz potential, and at constant S, V, and N to the Hamilton potential. In each case, the equilibrium is characterized by the constancy of the intensive parameters.

The degree to which macroscopic space and time correlations are absent characterizes the amount of **macroscopic disorder** of a system. Global equilibrium states are therefore macroscopically highly uniform; they are the most ordered macroscopic states in the universe rather than the most disordered ones. A system not in global equilibrium is characterized by macroscopic local inhomogeneities, indicating that the space-independent global

equilibrium variables alone are not sufficient to describe the system. Its intrinsic complexity is apparent only in a microscopic treatment; cf. Section 10.6 below. The only macroscopic shadow of this complexity is the critical opalescence of fluids near a critical point (Andrews [14], Forster [88]). The contents of the second law of thermodynamics for global equilibrium states may therefore be phrased informally as follows: *In global equilibrium, macroscopic order (homogeneity) is perfect and microscopic complexity is maximal.* In particular, the traditional interpretation of entropy as a measure of disorder is often misleading. Much more carefully argued support for this statement, with numerous examples from teaching practice, is in Lambert [167].

7.4.3 Theorem. *(**Entropy form of the second law**)*
In an arbitrary state of a standard thermodynamic system

$$S \leq S(H,V,N) := \min\{T^{-1}(H + PV - \mu \cdot N) \mid \Delta(T,P,\mu) = 0\},$$

with equality iff the state is an equilibrium state. The remaining thermal variables are then given by

$$T^{-1} = \frac{\partial S}{\partial H}(H,V,N), \quad T^{-1}P = \frac{\partial S}{\partial V}(H,V,N), \quad T^{-1}\mu = -\frac{\partial S}{\partial N}(H,V,N), \tag{7.25}$$

$$U = H = TS(T,V,N) - PV + \mu \cdot N. \tag{7.26}$$

Proof. This is proved in the same way as Theorem 7.4.1. □

This result implies that when a system in which H, V and N are kept constant reaches equilibrium, the entropy must have increased. Unfortunately, the assumption of constant H, V and N is unrealistic; such constraints are not easily realized in nature. Under different constraints[6], the entropy is no longer maximal.

In systems with several phases, a naive interpretation of the second law as moving systems towards increasing disorder is even more inappropriate: A mixture of water and oil spontaneously separates, thus "ordering" the water molecules and the oil molecules into separate phases!

Thus, while the second law in the form of a maximum principle for the entropy has some theoretical and historical relevance, it is not the extremal principle ruling nature. The irreversible nature of physical processes is instead manifest as **energy dissipation** which, in a microscopic interpretation, indicates the loss of energy to the unmodelled microscopic

[6]For example, if one pours milk into a cup of coffee, stirring mixes coffee and milk, thus increasing complexity. Macroscopic order is restored after some time when this increased complexity has become macroscopically inaccessible. Since T, P and N are constant, the cup of coffee ends up in a state of minimal Gibbs energy, and not in a state of maximal entropy! More formally, the first law shows that, for standard systems at fixed value of the mole number, the value of the entropy decreases when H or V (or both) decrease reversibly; this shows that the value of the entropy may well decrease if accompanied by a corresponding decrease of H or V. The same holds out of equilibrium (though our equilibrium argument no longer applies); for example, the reaction $2\,H_2 + O_2 \to 2\,H_2O$ (if catalyzed) may happen spontaneously at constant $T = 25\,°C$ and $P = 1$ atm, though it decreases the entropy.

degrees of freedom. Macroscopically, the global equilibrium states are therefore states of least free energy, the correct choice of which depends on the boundary condition, with the least possible freedom for change. This macroscopic immutability is another intuitive explanation for the maximal macroscopic order in global equilibrium states.

7.5 The approach to equilibrium

Using only the present axioms, one can say a little bit about the behavior of a system close to equilibrium in the following, idealized situation. Suppose that a system at constant S, V, and N which is close to equilibrium at some time t reaches equilibrium at some later time t^*. Then the second law implies

$$0 \leq H(t) - H(t^*) \approx (t - t^*)\frac{dH}{dt},$$

so that $dH/dt \leq 0$. We assume that the system is composed of two parts, which are both in equilibrium at times t and t^*. Then the time shift induces on both parts a reversible transformation, and the first law can be applied to them. Thus

$$dH = \sum_{k=1,2} dH^k = \sum_{k=1,2} (T^k dS^k - P^k dV^k + \mu^k \cdot dN^k).$$

Since S, V, and N remain constant, we have $dS^1 + dS^2 = 0$, $dV^1 + dV^2 = 0$, $dN^1 + dN^2 = 0$, and since for the time shift $dH \leq 0$, we find the inequality

$$0 \geq (T^1 - T^2)dS^1 - (P^1 - P^2)dV^1 + (\mu^1 - \mu^2) \cdot dN^1.$$

This inequality gives information about the direction of the flow in case that all but one of the extensive variables are known to be fixed.

In particular, at constant V^1 and N^1, we have $dS^1 \leq 0$ if $T^1 > T^2$; i.e., "heat" (entropy) flows from the hotter part towards the colder part. At constant S^1 and N^1, we have $dV^1 \leq 0$ if $P^1 < P^2$; i.e., "space" (volume) flows from lower pressure to higher pressure: the volume of the lower pressure part decreases and is compensated by a corresponding increase of the volume in the higher pressure part. And for a pure substance at constant S^1 and V^1, we have $dN^1 \leq 0$ if $\mu^1 > \mu^2$; i.e., "matter" (mole number) flows from higher chemical potential towards lower chemical potential. These qualitative results give temperature, pressure, and chemical potential the familiar intuitive interpretation.

This glimpse on nonequilibrium properties is a shadow of the far reaching fact that, in nonequilibrium thermodynamics, the intensive variables behave like potentials whose gradients induce forces that tend to diminish these gradients, thus enforcing (after the time needed to reach equilibrium) agreement of the intensive variables of different parts of a system. In particular, temperature acts as a thermal potential, whose differences create thermal forces which induce thermal currents, a flow of "heat" (entropy), in a similar way

as differences in electrical potentials create electrical currents, a flow of "electricity" (electrons)[7]. While these dynamical issues are outside the scope of the present work, they motivate the fact that one can control some intensive parameters of the system by controlling the corresponding intensive parameters of the environment and making the walls permeable to the corresponding extensive quantities. This corresponds to standard procedures familiar to everyone from ordinary life, such as: heating to change the temperature; applying pressure to change the volume; immersion into a substance to change the chemical composition; or, in the more general thermal models discussed in Section 10.1, applying forces to displace an object.

The stronger nonequilibrium version of the second law says that (for suitable boundary conditions) equilibrium is actually attained after some time (strictly speaking, only in the limit of infinite time). This implies that the energy difference

$$\delta E := H - U(S,V,N) = H - TS - F(S,V,N) = H - TS + PV = G(S,V,N)$$

is the amount of energy that is dissipated in order to reach equilibrium. In an equilibrium setting, we can only compare what happens to a system prepared in a nonequilibrium state assuming that, subsequently, the full energy difference δE is dissipated so that the system ends up in an equilibrium state. Since few variables describe everything of interest, this constitutes the power of equilibrium thermodynamics. But this power is limited, since equilibrium thermodynamics is silent about when – or whether at all – equilibrium is reached. Indeed, in many cases, only metastable states are reached, which change too slowly to ever reach equilibrium on a human time scale. Typical examples of this are crystal defects, which constitute nonglobal minima of the free energy – the globasl minimum would be a perfect crystal.

7.6 Description levels

As we have seen, extensive and intensive variables play completely different roles in equilibrium thermodynamics. Extensive variables such as mass, charge, or volume depend additively on the size of the system. The conjugate intensive variables act as parameters defining the state.

A system composed of many small subsystems, each in equilibrium, needs for its complete characterization the values of the extensive and intensive variables in each subsystem. Such a system is in global equilibrium only if its intensive variables are independent of the subsystem. On the other hand, the values of the extensive variables may jump at phase space boundaries, if (as is the case for multi-phase systems) the equations of state allow multiple values for the extensive variables to correspond to the same values of the intensive variables. If the intensive variables are not independent of the subsystem then, by the second law, the differences in the intensive variables of adjacent subsystems give rise to thermodynamic forces trying to move the system towards equilibrium.

[7] See Table 10.1 for more parallels in other thermodynamic systems, and Fuchs [94] for a thermodynamics course (and for a German course Job [142]) thoroughly exploiting these parallels.

A real nonequilibrium system does not actually consist of subsystems in equilibrium; however, typically, smaller and smaller pieces behave more and more like equilibrium systems. Thus we may view a real system as the continuum limit of a larger and larger number of smaller and smaller subsystems, each in approximate equilibrium. As a result, the extensive and intensive variables become fields depending on the continuum variables used to label the subsystems. For extensive variables, the integral of their fields over the label space gives the bulk value of the extensive quantity; thus the fields themselves have a natural interpretation as a density. For intensive variables, an interpretation as a density is physically meaningless; instead, they have a natural interpretation as field strengths. The gradients of their fields have physical significance as the sources for thermodynamic forces.

From this field theory perspective, the extensive variables in the single-phase global equilibrium case have constant densities, and their bulk values are the densities multiplied by the system size (which might be mass, or volume, or another additive parameter), hence scale linearly with the size of the system, while intensive variables are invariant under a change of system size. We do *not* use the alternative convention to call extensive any variable that scales linearly with the system size, and intensive any variable that is invariant under a change of system size.

We distinguish four nested levels of thermal descriptions, depending on whether the system is considered to be in global, local, microlocal, or quantum equilibrium. The highest and computationally simplest level, **global equilibrium**, is concerned with macroscopic situations characterized by finitely many space- and time-independent variables. The next level, **local equilibrium**, treats macroscopic situations in a continuum mechanical description, where the equilibrium subsystems are labeled by the space coordinates. Therefore the relevant variables are finitely many space- and time-dependent fields. The next deeper level, **microlocal**[8] **equilibrium**, treats mesoscopic situations in a kinetic description, where the equilibrium subsystems are labeled by phase space coordinates. The relevant variables are now finitely many fields depending on time, position, and momentum; cf. Balian [18]. The bottom level is the microscopic regime, where we must consider **quantum equilibrium**. This no longer fits a thermodynamic framework but must be described in terms of quantum dynamical semigroups; see Section 10.2.

The relations between the different description levels are discussed in Section 10.2. Apart from descriptions on these clear-cut levels, there are also various hybrid descriptions, where some part of a system is described on a more detailed level than the remaining parts, or where, as for stirred chemical reactions, the fields are considered to be spatially homogeneous and only the time-dependence matters.

What was said at the beginning of Section 7.2 about measuring intensive variables like temperature applies in principle also in local or microlocal equilibrium, but with fields in place of variables. The extensive variables are now densities represented by distributions that can be meaningfully integrated over bounded regions (the domains of contact with a measuring instrument), whereas intensive variables are nonsingular fields (e.g., pressure) whose integrals denote – after divistion by the size of the domain of contact with an instrument –

[8]The term microlocal for a phase space dependent analysis is taken from the literature on partial differential equations; see, e.g., Martinez [1].

a local mean value of the fields.

Chapter 8

Quantities, states, and statistics

When considered in sufficient detail, no physical system is truly in global equilibrium; one can always find smaller or larger deviations. To describe these deviations, extra variables are needed, resulting in a more complete but also more complex model. At even higher resolution, this model is again imperfect and an approximation to an even more complex, better model. This refinement process may be repeated in several stages. At the most detailed stages, we transcend the frontier of current knowledge in physics, but even as this frontier recedes, deeper and deeper stages with unknown details are imaginable.

Therefore, it is desirable to have a meta-description of thermodynamics that, starting with a detailed model, allows to deduce the properties of each coarser model, in a way that all description levels are consistent with the current state of the art in physics. Moreover, the results should be as independent as possible of unknown details at the lower levels. This meta-description is the subject of **statistical mechanics**.

This chapter introduces the technical machinery of statistical mechanics, Gibbs states and the partition function, in a uniform way common to classical mechanics and quantum mechanics. As in the phenomenological case, the intensive variables determine the state (which now is a more abstract object), whereas the extensive variables now appear as values of other abstract objects called quantities. This change of setting allows the natural incorporation of quantum mechanics, where quantities need not commute, while values are numbers observable in principle, hence must satisfy the commutative law.

The operational meaning of the abstract concepts of quantities, states and values introduced in the following becomes apparent once we have recovered the phenomenological results of Chapter 7 from the abstract theory developped in this and the next chapter. Chapter 10 discusses in more detail how the theory relates to experiment.

8.1 Quantities

Any fundamental description of physical systems must give account of the numerical values of quantities observable in experiments when the system under consideration is in a specified state. Moreover, the form and meaning of states, and of what is observable in principle, must be clearly defined. We consider an axiomatic conceptual foundation on the basis of quantities[1] and their values, consistent with the conventions adopted by the International System of Units (SI) [265], who declare: "*A quantity in the general sense is a property ascribed to phenomena, bodies, or substances that can be quantified for, or assigned to, a particular phenomenon, body, or substance. [...] The value of a physical quantity is the quantitative expression of a particular physical quantity as the product of a number and a unit, the number being its numerical value.*"

In different states, the quantities of a given system may have different values; the state (equivalently, the values determined by it) characterizes an individual system at a particular time. Theory must therefore define what to consider as quantities, what as states, and how a state assigns values to a quantity. Since quantities can be added, multiplied, compared, and integrated, the set of all quantities has an elaborate structure whose properties we formulate after the discussion of the following motivating example.

8.1.1 Example. As a simple example satisfying the axioms to be introduced, the reader may think of an N-level quantum system. The **quantities** are the elements of the algebra $\mathbb{E} = \mathbb{C}^{N\times N}$ of square complex $N \times N$ matrices, the **constants** are the multiples of the identity matrix, the **conjugate** f^* of f is given by conjugate transposition, and the **integral** $\int g = \operatorname{tr} g$ is the **trace**, the sum of the diagonal entries or, equivalently, the sum of the eigenvalues. The standard basis consisting of the N **unit vectors** e^k with a one in component k and zeros in all other component corresponds to the N levels of the quantum systems. The Hamiltonian H is represented by a diagonal matrix $H = \operatorname{Diag}(E_1, \dots, E_N)$ whose diagonal entries E_k are the **energy levels** of the system. In the nondegenerate case, all E_k are distinct, and the diagonal matrices comprise all functions of H. Quantities given by arbitrary nondiagonal matrices are less easy to interpret. However, an important class of quantities are the matrices of the form $P = \psi\psi^*$, where ψ is a vector of norm 1; they satisfy $P^2 = P = P^*$ and are the quantities observed in binary measurements such as detector clicks; see Section 10.5. The **states** of the N-level system are mappings defined by a **density matrix** $\rho \in \mathbb{E}$, a positive semidefinite Hermitian matrix with trace one, assigning to each quantity $f \in \mathbb{E}$ the **value** $\langle f\rangle = \operatorname{tr}\rho f$ of f in this state. The diagonal entries $p_k := \rho_{kk}$ represent the probability for obtaining a response in a binary test for the kth quantum level; the off-diagonal entries ρ_{jk} represent deviations from a classical mixture of quantum levels.

8.1.2 Definition.

[1] Quantities are formal, numerical properties associated to a given system in a given state. We deliberately avoid the notion of observables, since it is not clear on a fundamental level what it means to 'observe' something, and since many things (such as the fine structure constant, neutrino masses, decay rates, scattering cross sections) which can be observed in nature are only indirectly related to what is traditionally called an 'observable' in quantum mechanics. The related problem of how to interpret measurements is discussed in Section 10.4.

(i) A $*$**-algebra** is a set $\mathbb{E}$ whose elements are called **quantities**, together with operations on $\mathbb{E}$ defining for any two quantities $f, g \in \mathbb{E}$ the **sum** $f + g \in \mathbb{E}$, the **product** $fg \in \mathbb{E}$, and the **conjugate** $f^* \in \mathbb{E}$, such that the following axioms (Q1)–(Q4) hold for all $\alpha \in \mathbb{C}$ and all $f, g, h \in \mathbb{E}$:

(Q1) $\mathbb{C} \subseteq \mathbb{E}$, i.e., complex numbers are special elements called **constants**, for which addition, multiplication and conjugation have their traditional meaning.

(Q2) $(fg)h = f(gh), \quad \alpha f = f\alpha, \quad 0f = 0, \quad 1f = f.$

(Q3) $(f + g) + h = f + (g + h), \quad f(g + h) = fg + fh, \quad f + 0 = f.$

(Q4) $f^{**} = f, \quad (fg)^* = g^* f^*, \quad (f + g)^* = f^* + g^*.$

(ii) A $*$-algebra $\mathbb{E}$ is called **commutative** if $fg = gf$ for all $f, g \in \mathbb{E}$, and **noncommutative** otherwise. The $*$-algebra $\mathbb{E}$ is called **nondegenerate** if

(Q5) $f^* f = 0 \quad \Rightarrow \quad f = 0.$

(iii) We introduce the notation

$$-f := (-1)f, \quad f - g := f + (-g), \quad [f, g] := fg - gf,$$
$$f^0 := 1, \quad f^l := f^{l-1} f \quad (l = 1, 2, \ldots),$$
$$\operatorname{Re} f := \frac{1}{2}(f + f^*), \quad \operatorname{Im} f := \frac{1}{2i}(f - f^*),$$

for $f, g \in \mathbb{E}$. $[f, g]$ is called the **commutator** of f and g, and $\operatorname{Re} f$, $\operatorname{Im} f$ are referred to as the **real part** (or **Hermitian part**) and **imaginary part** of f, respectively. $f \in \mathbb{E}$ is called **Hermitian** if $f^* = f$.

(iv) A $*$-homomorphism is a mapping ϕ from a $*$-algebra $\mathbb{E}$ with unity to another (or the same) $*$-algebra $\mathbb{E}'$ with unity such that

$$\phi(f + g) = \phi(f) + \phi(g), \quad \phi(fg) = \phi(f)\phi(g), \quad \phi(\alpha f) = \alpha\phi(f),$$
$$\phi(f^*) = \phi(f)^*, \quad \phi(1) = 1.$$

for all f, g in $\mathbb{E}$ and $\alpha \in \mathbb{C}$.

Note that we assume commutativity only for the product of complex numbers and elements of $\mathbb{E}$. In general, the product of two elements of $\mathbb{E}$ is indeed noncommutative. However, general commutativity of the addition is a consequence of our other assumptions. We prove this together with some other useful relations.

8.1.3 Proposition.
(i) For all f, g, $h \in \mathbb{E}$,

$$(f + g)h = fh + gh, \quad f - f = 0, \quad f + g = g + f \tag{8.1}$$

$$[f, f^*] = -2i[\operatorname{Re} f, \operatorname{Im} f]. \tag{8.2}$$

(ii) For all $f \in \mathbb{E}$, $\operatorname{Re} f$ and $\operatorname{Im} f$ are Hermitian. f is Hermitian iff $f = \operatorname{Re} f$ iff $\operatorname{Im} f = 0$. If f, g are commuting Hermitian quantities then fg is Hermitian, too.

Proof. (i) The right distributive law follows from

$$\begin{aligned}(f+g)h &= ((f+g)h)^{**} = (h^*(f+g)^*)^* = (h^*(f^*+g^*))^* \\ &= (h^*f^* + h^*g^*)^* = (h^*f^*)^* + (h^*g^*)^* \\ &= f^{**}h^{**} + g^{**}h^{**} = fh + gh.\end{aligned}$$

It implies $f - f = 1f - 1f = (1-1)f = 0f = 0$. From this, we may deduce that addition is commutative, as follows. The quantity $h := -f + g$ satisfies

$$-h = (-1)((-1)f + g) = (-1)(-1)f + (-1)g = f - g,$$

and we have

$$f + g = f + (h - h) + g = (f + h) + (-h + g) = (f - f + g) + (f - g + g) = g + f.$$

This proves (8.1). If $u = \operatorname{Re} f$, $v = \operatorname{Im} f$ then $u^* = u, v^* = v$ and $f = u + iv, f^* = u - iv$. Hence

$$[f, f^*] = (u + iv)(u - iv) - (u - iv)(u + iv) = 2i(vu - uv) = -2i[\operatorname{Re} f, \operatorname{Im} f],$$

giving (8.2).

(ii) The first two assertions are trivial, and the third holds since $(fg)^* = g^*f^* = gf = fg$ if f, g are Hermitian and commute. □

8.1.4 Definition.
(i) The $*$-algebra $\mathbb{E}$ is called **partially ordered** if there is a partial order $\geq$ satisfying the following axioms (Q6)–(Q9) for all $f, g, h \in \mathbb{E}$:

(Q6) $\geq$ is reflexive ($f \geq f$), antisymmetric ($f \geq g \geq f \Rightarrow f = g$), and transitive ($f \geq g \geq h \Rightarrow f \geq h$).

(Q7) $f \geq g \Leftrightarrow f + h \geq g + h$.

(Q8) $f \geq 0 \quad \Rightarrow \quad f = f^*$ and $g^*fg \geq 0$.

(Q9) $1 \geq 0$.

We introduce the notation

$$f \leq g :\Leftrightarrow g \geq f,$$

$$\|f\| := \inf\{\alpha \in \mathbb{R} \mid f^*f \leq \alpha^2, \alpha \geq 0\},$$

where the infimum of the empty set is taken to be ∞. The number $\|f\|$ is referred to as the **(spectral) norm** of f. An element $f \in \mathbb{E}$ is called **bounded** if $\|f\| < \infty$. The **uniform topology** is the topology induced on $\mathbb{E}$ by declaring as open sets arbitrary unions of finite intersections of the **open balls** $\{f \in \mathbb{E} \mid \|f - f_0\| < \varepsilon\}$ for some $\varepsilon > 0$ and some $f_0 \in \mathbb{E}$.

8.1.5 Proposition.
(i) For all quantities f, g, $h \in \mathbb{E}$ and $\lambda \in \mathbb{C}$,

$$f^*f \geq 0, \quad ff^* \geq 0, \tag{8.3}$$

$$f^*f \leq 0 \quad \Rightarrow \quad \|f\| = 0 \quad \Rightarrow \quad f = 0, \tag{8.4}$$

$$f \leq g \quad \Rightarrow \quad h^*fh \leq h^*gh, \ |\lambda|f \leq |\lambda|g, \tag{8.5}$$

$$f^*g + g^*f \leq 2\|f\| \ \|g\|, \tag{8.6}$$

$$\|\lambda f\| = |\lambda|\|f\|, \quad \|f \pm g\| \leq \|f\| \pm \|g\|, \tag{8.7}$$

$$\|fg\| \leq \|f\| \ \|g\|. \tag{8.8}$$

(ii) Among the complex numbers, precisely the nonnegative real numbers λ satisfy $\lambda \geq 0$.

Proof. (i) (8.3) follows from the case $f = 1$ of (Q8) by substituting then f or f^* for g. (8.4) follows from (8.3), the definition of the norm, and (Q5). To prove (8.5), we deduce from $f \leq g$ and (Q7) that $g - f \geq 0$, then use (Q8) to find $h^*gh - h^*fh = h^*(g-f)h \geq 0$, hence $h^*fh \leq h^*gh$. Specializing to $g = sqrt|\lambda|$ then gives $|\lambda|f \leq |\lambda|g$.

To prove (8.5), let $\alpha = \|f\|$, $\beta = \|g\|$. Then $f^*f \leq \alpha^2$ and $g^*g \leq \beta^2$. Since

$$\begin{aligned} 0 \leq (\beta f - \alpha g)^*(\beta f - \alpha g) &= \beta^2 f^*f - \alpha\beta(f^*g + g^*f) + \alpha^2 g^*g \\ &\leq \beta^2\alpha^2 - \alpha\beta(f^*g + g^*f) + \alpha^2\beta^2, \end{aligned}$$

$f^*g + g^*f \leq 2\alpha\beta$ if $\alpha\beta \neq 0$, and for $\alpha\beta = 0$, the same follows from (8.4). Therefore (8.6) holds. The first half of (8.7) is trivial, and the second half follows for the plus sign from

$$(f+g)^*(f+g) = f^*f + f^*g + g^*f + g^*g \leq \alpha^2 + 2\alpha\beta + \beta^2 = (\alpha+\beta)^2,$$

and then for the minus sign from the first half. Finally, by (8.5),

$$(fg)^*(fg) = g^*f^*fg \leq g^*\alpha^2 g = \alpha^2 g^*g \leq \alpha^2\beta^2.$$

This implies (8.8).

(ii) If λ is a nonnegative real number then $\lambda = f^*f \geq 0$ with $f = \sqrt{\lambda}$. If λ is a negative real number then $\lambda = -f^*f \leq 0$ with $f = \sqrt{-\lambda}$, and by antisymmetry, $\lambda \geq 0$ is impossible. If λ is a nonreal number then $\lambda \neq \lambda^*$ and $\lambda \geq 0$ is impossible by (Q8). □

8.1.6 Definition. A **Euclidean $*$-algebra** is a nondegenerate, partially ordered $*$-algebra $\mathbb{E}$, whose elements are called **quantities**, together with a complex-valued **integral** $\int$ defined on a subspace $\mathbb{S}$ of $\mathbb{E}$, whose elements are called **strongly integrable**, satisfying the following axioms (EA1)–(EA6) for all bounded $g \in \mathbb{E}$, all strongly integrable $h, h', h_l \in \mathbb{E}$, and all $\alpha, \beta \in \mathbb{C}$:

(EA1) h^*, αh, gh, and hg are strongly integrable,

(EA2) $\int(\alpha h + \beta h') = \alpha\int h + \beta\int h'$, $\quad \int gh = \int hg$, $\quad (\int h)^* = \int h^*$,

(EA3) $\int h^* h > 0$ if $h \neq 0$,

(EA4) $\int h^* g h = 0$ for all strongly integrable $h \quad \Rightarrow \quad g = 0$ **(nondegeneracy)**,

(EA5) $\int h_l^* h_l \to 0 \quad \Rightarrow \quad \int g h_l \to 0, \ \int h_l^* g h_l \to 0$,

(EA6) $h_l \downarrow 0 \quad \Rightarrow \quad \inf \int h_l = 0$ **(Dini property)**.

Here, integrals extend over the longest following product or quotient (in contrast to differential operators, which act on the shortest syntactically meaningful term), the **monotonic limit** is defined by $g_l \downarrow 0$ iff, for every strongly integrable h, the sequence (or net) $\int h^* g_l h$ consists of real numbers converging monotonically decreasing to zero.

Note that the integral can often be naturally extended from strongly integrable quantities to a significantly larger space of integrable quantities.

8.1.7 Proposition.

$$g \in \mathbb{E}, \quad \int g f = 0 \quad \textit{for all } f \in \mathbb{E} \quad \Rightarrow \quad g = 0. \tag{8.9}$$

For strongly integrable f, g,

$$\int (gh)^*(gh) \leq \int g^* g \int h^* h. \quad \textbf{(Cauchy-Schwarz inequality)} \tag{8.10}$$

In particular, every strongly integrable quantity is bounded.

Proof.

If $\int g f = 0$ for all $f \in \mathbb{E}$ then this holds in particular for $f = hh^*$. Thus $0 = \int g h h^* = \int h^* g h$ by (EA2), and (EA4) gives the desired conclusion (8.9). (8.10) holds since by (EA3), $\int g^* h$ defines a positive definite inner product on $\mathbb{S}$, and directly implies the final statement. □

We now describe the basic Euclidean $*$-algebras relevant in nonrelativistic physics. However, the remainder is completely independent of details how the axioms are realized; a specific realization is needed only when doing specific quantitative calculations.

8.1.8 Examples.
(i) **(N-level quantum systems)** The simplest family of Euclidean $*$-algebras is the algebra $\mathbb{E} = \mathbb{C}^{N \times N}$ of square complex $N \times N$ matrices; cf. Example 8.1.1. Here the quantites are square matrices, the constants are the multiples of the identity matrix, the conjugate is conjugate transposition, and the integral is the trace, the sum of the diagonal entries or, equivalently, the sum of the eigenvalues. In particular, all quantities are strongly integrable.

(ii) **(Nonrelativistic classical mechanics)** An atomic N-particle system is described in classical mechanics by the phase space $\mathbb{R}^{6N}$ with six coordinates – position $x^a \in \mathbb{R}^3$ and momentum $p^a \in \mathbb{R}^3$ – for each particle. The algebra

$$\mathbb{E}_N := C^\infty(\mathbb{R}^{6N})$$

of smooth complex-valued, arbitrarily often differentiable functions $g(x^{1:N}, p^{1:N})$ of 3-dimensional positions and momenta is a commutative Euclidean $*$-algebra with complex conjugation as conjugate and the **Liouville integral**

$$\int g = C^{-1} \int dp^{1:N} dx^{1:N} g_N(x^{1:N}, p^{1:N}),$$

where C is a positive constant. Strongly integrable quantities are the Schwartz functions in $\mathbb{E}$.[2] The axioms are easily verified.

(iii) **(Classical fluids)** A fluid is classically described by an atomic system with an indefinite number of particles. The appropriate Euclidean $*$-algebra for a single species of monatomic particles is the direct sum $\mathbb{E} = \oplus_{N\geq 0}\mathbb{E}_N$ whose quantities are infinite sequences $g = (g_0, g_1, ...)$ of $g_N \in \mathbb{E}_N^{\text{sym}}$, with $\mathbb{E}_N^{\text{sym}}$ consisting of all permutation-invariant functions functions form $\mathbb{E}_N$ as in (ii), and weighted Liouville integral

$$\int g = \sum_{N\geq 0} C_N^{-1} \int dp^{1:N} dx^{1:N} g_N(x^{1:N}, p^{1:N}).$$

Here C_N is a symmetry factor for the symmetry group of the N-particle systen, which equals $h^{3N}N!$ for indistinguishable particles; $h = 2\pi\hbar$ is Planck's constant. This accounts for the Maxwell statistics and gives the correct entropy of mixing. Classical fluids with monatomic particles of several different kinds require a tensor product of several such algebras, and classical fluids composed of molecules require additional degrees of freedom to account for the rotation and vibration of the molecules.

(iv) **(Nonrelativistic quantum mechanics)** Let $\mathbb{H}$ be a Euclidean space, a dense subspace of a Hilbert space. Then the algebra $\mathbb{E} := \operatorname{Lin}\mathbb{H}$ of continuous linear operators on $\mathbb{H}$ is a Euclidean $*$-algebra with the adjoint as conjugate and the **quantum integral**

$$\int g = \operatorname{tr} g,$$

given by the trace of the quantity in the integrand. Strongly integrable quantities are the operators $g \in \mathbb{E}$ which are trace class; this includes all linear operators of finite rank. Again, the axioms are easily verified. In the quantum context, Hermitian quantities f are often referred to as **observables**; but we do not use this term here.

We end this section by stating some results needed later. The exposition in this and the next chapter is fully rigorous if the statements of Proposition 8.1.9 and Proposition 8.1.10 are assumed in addition to (EA1)–(EA6). We prove these propositions only in case that $\mathbb{E}$ is finite-dimensional[3]. But they can also be proved if the quantities involved are smooth functions, or if they have a spectral resolution; cf., e.g., Thirring [267] (who works in the framework of C^*-algebras and von Neumann algebras).

[2] A **Schwartz function** of n variables $z \in \mathbb{R}^n$ is a function $f \in C^\infty(\mathbb{R}^n)$ such that the expressions $z_1^{k_1} \dots z_n^{k_n} \frac{\partial^{l_1+\dots+l^n} f(z)}{\partial z_1^{l_1} \dots \partial z_n^{l_n}}$ are bounded in z for any choice of nonnegative integers $k_1, \dots, k_n, l_1, \dots, l_n$.

[3] We'd appreciate to be informed about possible proofs in general that only use the properties of Euclidean $*$-algebras (and perhaps further, elementary assumptions).

8.1.9 Proposition. *For arbitrary quantities f, g,*

$$e^{\alpha f}e^{\beta f} = e^{(\alpha+\beta)f} \quad (\alpha, \beta \in \mathbb{R}),$$
$$(e^f)^* = e^{f^*},$$
$$e^f g = g e^f \quad \text{if } f \text{ and } g \text{ commute},$$
$$f^* = f \quad \Rightarrow \quad \log e^f = f,$$
$$f \geq 0 \quad \Rightarrow \quad \sqrt{f} \geq 0, \quad (\sqrt{f})^2 = f,$$

For any quantity $f = f(s)$ depending continuously on $s \in [a, b]$,

$$\int_a^b ds \int f(s) = \int \Big(\int_a^b ds f(s) \Big),$$

and for any quantity $f = f(\lambda)$ depending continuously differentiably on a parameter vector λ,

$$\frac{d}{d\lambda} \int f = \int df/d\lambda.$$

Proof. In finite dimensions, the first five assertions are standard matrix calculus, and the remaining two statements hold since $\int f$ must be a finite linear combination of the components of f. □

8.1.10 Proposition. *Let f, g be quantities depending continuously differentiably on a parameter or parameter vector λ, and suppose that*

$$[f(\lambda), g(\lambda)] = 0 \text{ for all } \lambda. \tag{8.11}$$

Thus, for any continuously differentiable function F of two variables,

$$\frac{d}{d\lambda} \int F(f, g) = \int \partial_1 F(f, g) \frac{df}{d\lambda} + \int \partial_2 F(f, g) \frac{dg}{d\lambda} \ . \tag{8.12}$$

Here $\partial_1 F$ and $\partial_2 f$ denote differentiation by the first and second argument of F, respectively.

Proof. We prove the special case $F(x, y) = x^m y^n$, where (8.12) reduces to

$$\frac{d}{d\lambda} \int f^m g^n = \int m f^{m-1} g^n \frac{df}{d\lambda} + \int n f^m g^{n-1} \frac{dg}{d\lambda}. \tag{8.13}$$

The general case then follows for polynomials $F(x, y)$ by taking suitable linear combinations, and for arbitrary F by a limiting procedure. To prove (8.13), we note that, more generally,

$$\begin{aligned}
\frac{d}{d\lambda} \int f_1 \dots f_{m+n} &= \int \tfrac{d}{d\lambda} (f_1 \dots f_{m+n}) \\
&= \int \sum_{j=1}^{m+n} f_1 \dots f_{j-1} \frac{df_j}{d\lambda} f_{j+1} \dots f_{m+n} \\
&= \sum_{j=1}^{m+n} \int f_1 \dots f_{j-1} \frac{df_j}{d\lambda} f_{j+1} \dots f_{m+n} \\
&= \sum_{j=1}^{m+n} \int f_{j+1} \dots f_{m+n} f_1 \dots f_{j-1} \frac{df_j}{d\lambda} \ ,
\end{aligned}$$

using the cyclic commutativity (EA2) of the integral. If we specialize to $f_j = f$ if $j \leq m$, $f_j = g$ if $j > m$, and use (8.11), we arrive at (8.13). □

Of course, the proposition generalizes to families of more than two commuting quantities; but more important is the special case $g = f$:

8.1.11 Corollary. *For any quantity f depending continuously differentiably on a parameter vector λ, and any continuously differentiable function F of a single variable,*

$$\frac{d}{d\lambda}\int F(f) = \int F'(f)\frac{df}{d\lambda}. \tag{8.14}$$

8.2 Gibbs states

Our next task is to specify the formal properties of the value of a quantity.

8.2.1 Definition. A **state** is a mapping $^-$ that assigns to all quantities f from a subspace of $\mathbb{E}$ containing all bounded quantities its **value** $\langle f\rangle \in \mathbb{C}$ such that for all $f, g \in \mathbb{E}$, $\alpha \in \mathbb{C}$,

(E1) $\langle 1\rangle = 1, \quad \langle f^*\rangle = \langle f\rangle^*, \quad \langle f+g\rangle = \langle f\rangle + \langle g\rangle$,

(E2) $\langle \alpha f\rangle = \alpha\langle f\rangle$,

(E3) If $f \geq 0$ then $\langle f\rangle \geq 0$,

(E4) If $f_l \in \mathbb{E},\ f_l \downarrow 0$ then $\langle f_l\rangle \downarrow 0$.

Note that this formal definition of a state – always used in the remainder of the book – differs from the phenomenological thermodynamic states defined in Section 7.1. The connection between the two notions will be made in Section 9.2.

Statistical mechanics essentially originated with Josiah Willard Gibbs, whose 1902 book Gibbs [102] on (at that time of course only classical) statistical mechanics is still readable. See Uffink [273] for a history of the subject.

All states arising in thermodynamics have the following particular form.

8.2.2 Definition. A **Gibbs state** is defined by assigning to any $g \in \mathbb{E}$ the value

$$\langle g\rangle := \int e^{-S/\hbar} g, \tag{8.15}$$

where S, called the **entropy** of the state, is a Hermitian quantity with strongly integrable $e^{-S/\hbar}$, satisfying the normalization condition

$$\int e^{-S/\hbar} = 1, \tag{8.16}$$

and $\hbar$ is the Boltzmann constant

$$\hbar \approx 1.38065 \cdot 10^{-23} J/K. \tag{8.17}$$

Theorem 8.2.3 below implies that a Gibbs state is indeed a state.

The Boltzmann constant defines the units in which the entropy is measured. In analogy[4] with Planck's constant $\hbar$, we write $\bar{k}$ in place of the customary k or k_B, in order to be free to use the letter k for other purposes. By a change of units one can enforce any value of $\bar{k}$. Chemists use instead of particle number N the corresponding **mole number**, which differs by a fixed numerical factor, the **Avogadro constant**

$$N_A = R/\bar{k} \approx 6.02214 \cdot 10^{23}\text{mol}^{-1},$$

where R is the universal gas constant (7.8). As a result, all results from statistical mechanics may be translated to phenomenological thermodynamics by setting $\bar{k} = R$, corresponding to setting $1\,\text{mol} = 6.02214 \cdot 10^{23}$, the number of particles in one mole of a pure substance.

What is here called entropy has a variety of alternative names in the literature on statistical mechanics. For example, Gibbs [102], who first noticed the rich thermodynamic implications of states defined by (8.15), called $-S$ the *index of probability*; Alhassid & Levine [7] and Balian [18] use the name *surprisal* for S. Our terminology is close to that of Mrugala et al. [196], who call S the *microscopic entropy*, and Hassan et al. [122], who call S the *information(al) entropy operator*. What is traditionally (and in Section 7.1) called entropy and denoted by S is in the present setting the value $\overline{S} = \langle S \rangle = \int e^{-S/\bar{k}} S$.

8.2.3 Theorem.
(i) A Gibbs state determines its entropy uniquely.

(ii) For any Hermitian quantity f with strongly integrable e^{-f}, the mapping $\langle \cdot \rangle_f$ defined by

$$\langle g \rangle_f := Z_f^{-1} \int e^{-f} g, \quad \text{where } Z_f := \int e^{-f}, \tag{8.18}$$

is a state. It is a Gibbs state with entropy

$$S_f := \bar{k}(f + \log Z_f). \tag{8.19}$$

*(iii) The **KMS condition** (cf. Kubo [161], Martin & Schwinger [186])*

$$\langle gh \rangle_f = \langle h Q_f g \rangle \quad \text{for bounded } g, h \tag{8.20}$$

holds. Here Q_f is the linear mapping defined by

$$Q_f g := e^{-f} g e^{f}.$$

Proof. (i) If the entropies S and S' define the same Gibbs state then

$$\int (e^{-S/\bar{k}} - e^{-S'/\bar{k}}) g = \langle g \rangle - \langle g \rangle = 0$$

for all g, hence (8.9) gives $e^{-S/\bar{k}} - e^{-S'/\bar{k}} = 0$. This implies that $e^{-S/\bar{k}} = e^{-S'/\bar{k}}$, hence $S = S'$ by Proposition 8.1.9.

[4] As we shall see in (20.20) and (9.43), $\hbar$ and $\bar{k}$ play indeed analogous roles in quantum mechanical and thermodynamic uncertainty relations.

(ii) The quantity $d := e^{-f/2}$ is nonzero and satisfies $d^* = d$, $e^{-f} = d^*d \geq 0$. Hence $Z_f > 0$ by (EA3), and $\rho := Z_f^{-1}e^{-f}$ is Hermitian and nonnegative. For $h \geq 0$, the quantity $g = \sqrt{h}$ is Hermitian (by Proposition 8.1.9) and satisfies $g\rho g^* = Z_f^{-1}(gd)(gd)^* \geq 0$, hence by (EA2),

$$\langle h\rangle_f = \langle g^*g\rangle_f = \int \rho g^* g = \int g\rho g^* \geq 0.$$

Moreover, $\langle 1\rangle_f = Z_f^{-1}\int e^{-f} = 1$. Similarly, if $g \geq 0$ then $g = h^*h$ with $h = \sqrt{g} = h^*$ and with $k := e^{-f/2}h$, we get

$$Z_f\langle g\rangle_f = \int e^{-f}hh^* = \int h^*e^{-f}h = \int k^*k \geq 0.$$

This implies (E3). the other axioms (E1)–(E4) follow easily from the corresponding properties of the integral. Thus $\langle\cdot\rangle_f$ is a state. Finally, with the definition (8.19), we have

$$Z_f^{-1}e^{-f} = e^{-f-\log Z_f} = e^{-S_f/\hbar},$$

whence $\langle\cdot\rangle_f$ is a Gibbs state.

(iii) By (EA2), $\langle hQ_fg\rangle_f = \int e^{-f}hQ_fg = \int Q_fge^{-f}h = \int e^{-f}gh = \langle gh\rangle_f$. □

Note that the state (8.18) is unaltered when f is shifted by a constant. Q_f is called the **modular automorphism** of the state $\langle\cdot\rangle_f$ since $Q_f(gh) = Q_f(g)Q_f(h)$; for a classical system, Q_f is the identity. In the following, we shall not make use of the KMS condition; however, it plays an important role in the mathematics of the thermodynamic limit (cf. Thirring [267]).

Z_f is called the **partition function** of f; it is a function of whatever parameters appear in a particular form given to f in the applications. A large part of traditional statistical mechanics is concerned with the calculation, for given f, of the partition function Z_f and of the values $\langle g\rangle_f$ for selected quantities g. As we shall see, the basic results of statistical mechanics are completely independent of the details involved, and it is this basic part that we concentrate upon in this book.

8.2.4 Example. A **canonical ensemble**[5], is defined as a Gibbs state whose entropy is an affine function of a Hermitian quantity H, called the **Hamiltonian**:

$$S = \beta H + \text{const},$$

with a constant depending on β, computable from (8.19) and the partition function

$$Z = \int e^{-\beta H}$$

[5] Except in the traditional notions of a microcanonical, canonical, or grand canonical ensemble, we avoid the term **ensemble** which in statistical mechanics is de facto used as a synonym for state but often has the connotation of a large real or imagined collection of identical copies of a systems. The latter interpretation has well-known difficulties to explain why each single macroscopic system is described correctly by thermodynamics; see, e.g., Sklar [254].

of $f = \beta H$. In particular, in the quantum case, where $\int$ is the trace, the finiteness of Z implies that S and hence H must have a discrete spectrum that is bounded below. Hence the partition function takes the familiar form

$$Z = \operatorname{tr} e^{-\beta H} = \sum_{n \in \mathcal{N}} e^{-\beta E_n}, \tag{8.21}$$

where the E_n ($n \in \mathcal{N}$) are the **energy levels**, the eigenvalues of H. If the spectrum of H is known, this leads to explicit formulas for Z. For example, a **two level system** is defined by the energy levels $0, E$ (or E_0 and $E_0 + E$, which gives the same results), and has

$$Z = 1 + e^{-\beta E}. \tag{8.22}$$

It describes a single **Fermion mode**, but also many other systems at low temperature; cf. (9.57). In particular, it is the basis of laser-induced chemical reactions in photochemistry (see, e.g., Karlov [144], Murov et al. [198]), where only two electronic energy levels (the ground state and the first excited state) are relevant; cf. the discussion of (9.57) below.

For a **harmonic oscillator**, defined by the energy levels nE, $n = 0, 1, 2, \ldots$ and describing a single **Boson mode**, we have

$$Z = \sum_{n=0}^{\infty} e^{-n\beta E} = (1 - e^{-\beta E})^{-1}.$$

Independent modes are modelled by taking tensor products of single mode algebras and adding their Hamiltonians, leading to spectra which are obtained by summing the eigenvalues of the modes in all possible ways. The resulting partition function is the product of the single-mode partition functions.] From here, a thermodynamic limit leads to the properties of ideal gases. Then nonideal gases due to interactions can be handled using the cumulant expansion, as indicated at the end of Section 8.3. The details are outside the scope of this book.

Since the Hamiltonian can be any Hermitian quantity, the quantum partition function formula (8.21) can in principle be used to compute the partition function of arbitrary quantized Hermitian quantities.

8.3 Kubo product and generating functional

The negative logarithm of the partition function, the so-called generating functional, plays a fundamental role in statistical mechanics.

We first discuss a number of general properties, discovered by Gibbs [102], Peierls [213], Bogoliubov [37], Kubo [162], Mori [194], and Griffiths [112]. The somewhat technical setting involving the Kubo inner product is necessary to handle noncommuting quantities correctly; everything would be much easier in the classical case. On a first reading, the proofs in this section may be skipped.

8.3.1 Proposition. *Let f be Hermitian such that e^{sf} is strongly integrable for all $s \in [-1,1]$. Then*

$$\langle g; h\rangle_f := \langle gE_f h\rangle_f, \tag{8.23}$$

where E_f is the linear mapping defined for Hermitian f by

$$E_f h := \int_0^1 ds\, e^{-sf} h e^{sf},$$

defines a bilinear, positive definite inner product $\langle\cdot\,;\cdot\rangle_f$ on the algebra of quantities, called the ***Kubo*** *(or* ***Mori*** *or* ***Bogoliubov****)* ***inner product****. For all f, g, the following relations hold:*

$$\langle g; h\rangle_f^* = \langle h^*; g^*\rangle_f, \tag{8.24}$$

$$\langle g^*; g\rangle_f > 0 \quad \text{if } g \neq 0, \tag{8.25}$$

$$\langle g; h\rangle_f = g\langle h\rangle_f \quad \text{if } g \in \mathbb{C}, \tag{8.26}$$

$$\langle g; h\rangle_f = \langle gh\rangle_f \quad \text{if } g \text{ or } h \text{ commutes with } f, \tag{8.27}$$

$$E_f g = g \quad \text{if } g \text{ commutes with } f. \tag{8.28}$$

If $f = f(\lambda)$ depends continuously differentiably on the real parameter vector λ then

$$\frac{d}{d\lambda} e^{-f} = -\Big(E_f \frac{df}{d\lambda}\Big) e^{-f}. \tag{8.29}$$

Proof. (i) We have

$$\langle g; h\rangle_f^* = \langle (gE_f h)^*\rangle_f = \langle (E_f h)^* g^*\rangle_f = \Big\langle \int_0^1 ds\, e^{sf} h^* e^{-sf} g^* \Big\rangle_f = \int_0^1 ds \langle e^{sf} h^* e^{-sf} g^*\rangle_f.$$

The integrand equals

$$\textstyle\int e^{-f} e^{sf} h^* e^{-sf} g^* = \int e^{sf} e^{-f} h^* e^{-sf} g^* = \int e^{-f} h^* e^{-sf} g^* e^{sf} = \langle h^* e^{-sf} g^* e^{sf}\rangle_f$$

by (EA2), hence

$$\langle g; h\rangle_f^* = \int_0^1 ds \langle h^* e^{-sf} g^* e^{sf}\rangle_f = \Big\langle h^* \int_0^1 ds\, e^{-sf} g^* e^{sf} \Big\rangle_f = \langle h^* E_f g^*\rangle_f = \langle h^*; g^*\rangle_f.$$

Thus (8.24) holds.

(ii) Suppose that $g \neq 0$. For $s \in [0,1]$, we define $u = s/2, v = (1-s)/2$ and $g(s) := e^{-uf} g e^{vf}$. Since f is Hermitian, $g(s)^* = e^{vf} g^* e^{-uf}$, hence by (EA2) and (EA3),

$$\textstyle\int e^{-f} g^* e^{-sf} g e^{sf} = \int e^{vf} g e^{-2uf} g^* e^{vf} = \int g(s)^* g(s) > 0,$$

so that

$$\langle g^*; g\rangle_f = \langle g^* E_f g\rangle_f = \int_0^1 ds \textstyle\int e^{-f} g^* e^{-sf} g e^{sf} > 0.$$

This proves (8.25), and shows that the Kubo inner product is positive definite.

(iii) If f and g commute then $ge^{sf} = e^{sf}g$, hence

$$E_f g = \int_0^1 ds e^{-sf} e^{sf} g = \int_0^1 ds g = g,$$

giving (8.28). The definition of the Kubo inner product then implies (8.27), and taking $g \in \mathbb{C}$ gives (8.26).

(iv) The function q on $[0,1]$ defined by

$$q(t) := \int_0^t ds\, e^{-sf} \frac{df}{d\lambda} e^{sf} + \Big(\frac{d}{d\lambda} e^{-tf}\Big) e^{tf}$$

satisfies $q(0) = 0$ and

$$\frac{d}{dt} q(t) = e^{-tf} \frac{df}{d\lambda} e^{tf} + \Big(\frac{d}{d\lambda} e^{-tf}\Big) f e^{tf} + \frac{d}{d\lambda}(-e^{-tf} f) e^{tf} = 0.$$

Hence q vanishes identically. In particular, $q(1) = 0$, giving (8.29). □

As customary in thermodynamics, we use differentials to express relations involving the differentiation by arbitrary parameters. To write (8.29) in differential form, we formally multiply by $d\lambda$, and obtain the **quantum chain rule** for exponentials,

$$de^{-f} = (-E_f df) e^{-f}. \tag{8.30}$$

If the $f(\lambda)$ commute for all values of λ then the quantum chain rule reduces to the classical chain rule. Indeed, then f commutes also with $\frac{df}{d\lambda}$; hence $E_f \frac{df}{d\lambda} = \frac{df}{d\lambda}$, and $E_f df = df$.

The following theorem is central to the mathematics of statistical mechanics. As will be apparent from the discussion in the next chapter, part (i) is the abstract mathematical form of the second law of thermodynamics, part (ii) allows the actual computation of thermal properties from microscopic assumptions, and part (iii) is the abstract form of the first law.

8.3.2 Theorem. *Let f be Hermitian such that e^{sf} is strongly integrable for all $s \in [-1,1]$.*

(i) The ***generating functional***

$$W(f) := -\log \textstyle\int e^{-f} \tag{8.31}$$

is a concave function of the Hermitian quantity f. In particular,

$$W(g) \le W(f) + \langle g - f \rangle_f. \quad \textbf{(Gibbs-Bogoliubov inequality)} \tag{8.32}$$

Equality holds in (8.32) iff f and g differ by an additive constant.

(ii) For Hermitian g, we have

$$W(f + \tau g) = W(f) - \log \langle e^{-f-\tau g} e^{f} \rangle_f. \tag{8.33}$$

Moreover, the ***cumulant expansion***

$$W(f+\tau g) = W(f) + \tau\langle g\rangle_f + \frac{\tau^2}{2}(\langle g\rangle_f^2 - \langle g;g\rangle_f) + O(\tau^3) \tag{8.34}$$

holds if the coefficients are finite.

(iii) If $f = f(\lambda)$ and $g = g(\lambda)$ depend continuously differentiably on λ then the following ***differentiation formulas*** *hold:*

$$d\langle g\rangle_f = \langle dg\rangle_f - \langle g;df\rangle_f + \langle g\rangle_f\langle df\rangle_f, \tag{8.35}$$

$$dW(f) = \langle df\rangle_f. \tag{8.36}$$

(iv) The entropy of the state $\langle\cdot\rangle_f$ is

$$S = \hbar(f - W(f)). \tag{8.37}$$

Proof. We prove the assertions in reverse order.

(iv) Equation (8.31) says that $W(f) = -\log Z_f$, which together with (8.19) gives (8.37).

(iii) We have

$$\begin{aligned} d\textstyle\int ge^{-f} &= \textstyle\int dge^{-f} + \int gde^{-f} = \int dge^{-f} - \int gE_f df e^{-f} \\ &= \textstyle\int (dg - gE_f df)e^{-f} = Z_f\langle dg - gE_f df\rangle_f. \end{aligned}$$

On the other hand, $d\int ge^{-f} = d(Z_f\langle g\rangle_f) = dZ_f\langle g\rangle_f + Z_f d\langle g\rangle_f$, so that

$$dZ_f\langle g\rangle_f + Z_f d\langle g\rangle_f = Z_f\langle dg - gE_f df\rangle_f = Z_f\langle dg\rangle_f - Z_f\langle g;df\rangle_f. \tag{8.38}$$

In particular, for $g = 1$ we find by (8.26) that $dZ_f = -Z_f\langle 1;df\rangle_f = -Z_f\langle df\rangle_f$. Now (8.36) follows from $dW(f) = -d\log Z_f = -dZ_f/Z_f = \langle df\rangle_f$, and solving (8.38) for $d\langle g\rangle_f$ gives (8.35).

(ii) Equation (8.33) follows from

$$e^{-W(h)} = \textstyle\int e^{-h} = \int e^{-h}e^f e^{-f} = \int e^{-f}e^{-h}e^f = (\int e^{-f})\langle e^{-h}e^f\rangle_f = e^{-W(f)}\langle e^{-h}e^f\rangle_f$$

by taking logarithms and setting $h = f+\tau g$. To prove the cumulant expansion, we introduce the function ϕ defined by

$$\phi(\tau) := W(f+\tau g),$$

From (8.36), we find $\phi'(\tau) = \langle g\rangle_{f+\tau g}$ for f, g independent of τ, and by differentiating this again,

$$\phi''(\tau) = \frac{d}{d\tau}\langle g\rangle_{f+\tau g} = -\Big\langle g\frac{E_f d(f+\tau g)}{d\tau}\Big\rangle_{f+\tau g} + \langle g\rangle_{f+\tau g}^2.$$

In particular,

$$\phi'(0) = \langle g\rangle_f, \quad \phi''(0) = \langle g\rangle_f^2 - \langle gE_f g\rangle_f = \langle g\rangle_f^2 - \langle g;g\rangle_f. \tag{8.39}$$

A Taylor expansion now implies (8.34).

(i) Since the Cauchy-Schwarz equation for the Kubo inner product implies

$$\langle g\rangle_f^2 = \langle g;1\rangle_f^2 \le \langle g;g\rangle_f\langle 1;1\rangle_f = \langle g;g\rangle_f,$$

(8.39) implies that

$$\frac{d^2}{d\tau^2}W(f+\tau g)\Big|_{\tau=0} \le 0$$

for all f, g. This implies that $W(f)$ is concave. Moreover, replacing f by $f + sg$, we find that $\phi''(s) \le 0$ for all s. The remainder form of Taylor's theorem therefore gives

$$\phi(\tau) = \phi(0) + \tau\phi'(0) + \int_0^\tau ds(\tau - s)\phi''(s) \le \phi(0) + \tau\phi'(0),$$

and for $\tau = 1$ we get

$$W(f+g) \le W(f) + \langle g\rangle_f. \tag{8.40}$$

(8.32) follows for $\tau = 1$ upon replacing g by $g - f$.

By the derivation, equality holds in (8.40) only if $\phi''(s) = 0$ for all $0 < s < 1$. By (8.39), applied with $f + sg$ in place of f, this implies $\langle g\rangle_{f+sg}^2 = \langle g;g\rangle_{f+sg}$. Thus we have equality in the Cauchy-Schwarz argument, forcing g to be a multiple of 1. Therefore equality in the Gibbs-Bogoliubov inequality (8.32) is possible only if $g - f$ is constant. □

As a consequence of the Gibbs-Bogoliubov inequality, we derive an important inequality for the entropy in terms of that of a given reference state.

8.3.3 Theorem. *Let S_c be the entropy of a reference state. Then, for an arbitrary Gibbs state $\langle\cdot\rangle$ with entropy S,*

$$\langle S\rangle \le \langle S_c\rangle, \tag{8.41}$$

with equality only if $S_c = S$.

Proof. Let $f = S/\hbar$ and $g = S_c/\hbar$. Since S and S_c are entropies, $W(f) = W(g) = 0$, and the Gibbs-Bogoliubov inequality (8.32) gives $0 \le \langle g - f\rangle_f = \langle S_c - S\rangle/\hbar$. This implies (8.41). If equality holds then equality holds in (8.32), so that S_c and S differ only by a constant. But this constant vanishes since the values agree. □

The difference

$$\langle S_c - S\rangle = \langle S_c\rangle - \langle S\rangle \ge 0 \tag{8.42}$$

is known as **relative entropy**. In an information theoretical context (cf. Section 10.6), the relative entropy may be interpreted as the amount of information in a state $\langle\cdot\rangle$ which cannot be explained by the reference state. This interpretation makes sense since the relative entropy vanishes precisely for the reference state. A large relative entropy therefore indicates that the state contains some important information not present in the reference state.

Approximations. The cumulant expansion is the basis of a well-known approximation method in statistical mechanics. Starting from special reference states $\langle\cdot\rangle_f$ with explicitly known $W(f)$ and E_f (corresponding to so-called explicitly solvable models), one obtains inductively expressions for values in these states by applying the differentiation rules. (In the most important cases, the resulting formulas for the values are commonly referred to as a **Wick theorem**, cf. Wick [289], although in the classical case, the formulas are much older and were derived in 1918 by Isserlis [133]. For details, see textbooks on statistical mechanics, e.g., Huang [130], Reichl [230].)

From these, one can calculate the coefficients in the cumulant expansion; note that higher order terms can be found by proceeding as in the proof, using further differentiation. This gives approximate generating functions (and by differentiation associated values) for Gibbs states with an entropy close to the explicitly solvable reference state. From the resulting generating function and the differentiation formulas (8.35)–(8.36), one gets as before the values for the given state.

The best tractable reference state $\langle\cdot\rangle_f$ to be used for a given Gibbs state $\langle\cdot\rangle_g$ can be obtained by minimizing the upper bound in the Gibbs-Bogoliubov inequality (8.32) over all f for which an explicit generating function is known. Frequently, one simply approximates $W(g)$ by the minimum of this upper bound,

$$W(g) \approx W_m(g) := \inf_f \Big(W(f) + \langle g - f\rangle_f\Big). \tag{8.43}$$

Using $W_m(g)$ in place of $W(g)$ defines a so-called **mean field theory**; cf. Callen [55]. For computations from first principles (quantum field theory), see, e.g., the survey by Berges et al. [134].

8.4 Limit resolution and uncertainty

Definition 8.2.1 generalizes the expectation axioms of Whittle [288, Section 2.2] for classical probability theory. Indeed, the values of our quantities are traditionally called expectation values, and refer to the mean over an ensemble of (real or imagined) identically prepared systems.

In our treatment, we keep the notation with pointed brackets familiar from statistical mechanics, but use the more neutral term **value** for $\langle f\rangle$ to avoid any reference to probability or statistics. This keeps the formal machinery completely independent of controversial issues about the interpretation of probabilities. Statistics and measurements, where the probabilistic aspect enters directly, are discussed separately in Chapter 10.2.

Our analysis of the uncertainty inherent in the description of a system by a state is based on the following result.

8.4.1 Proposition. *For Hermitian g,*

$$\langle g\rangle^2 \le \langle g^2\rangle. \tag{8.44}$$

Equality holds if $g = \langle g \rangle$.

Proof. Put $\overline{g} = \langle g \rangle$. Then $0 \leq \langle (g - \overline{g})^2 \rangle = \langle g^2 - 2\overline{g}g + \overline{g}^2 \rangle = \langle g^2 \rangle - 2\overline{g}\langle g \rangle + \overline{g}^2 = \langle g^2 \rangle - \langle g \rangle^2$. This gives (8.44). If $g = \overline{g}$ then equality holds in this argument. □

8.4.2 Definition. The number

$$\mathrm{cov}(f, g) := \mathrm{Re}\langle (f - \overline{f})^*(g - \overline{g}) \rangle$$

is called the **covariance** of $f, g \in \mathbb{E}$. Two quantities f, g are called **uncorrelated** if $\mathrm{cov}(f, g) = 0$, and **correlated** otherwise. The number

$$\sigma(f) := \sqrt{\mathrm{cov}(f, f)}$$

is called the **uncertainty** of $f \in \mathbb{E}$ in the state $\langle \cdot \rangle$. The number

$$\mathrm{res}(g) := \sqrt{\langle g^2 \rangle / \langle g \rangle^2 - 1}, \tag{8.45}$$

is called the **limit resolution** of a Hermitian quantity g with nonzero value $\langle g \rangle$.

Note that (E3) and (8.44) ensure that $\sigma(f)$ and $\mathrm{res}(g)$ are nonnegative real numbers that vanish if f, g are constant, i.e., complex numbers, and $g \neq 0$. This definition is analogous to the definitions of elementary classical statistics, where $\mathbb{E}$ is a commutative algebra of random variables, to the present, more general situation; in a statistical context, the uncertainty $\sigma(f)$ is referred to as **standard deviation**.

There is no need to associate an intrinsic statistical meaning to the above concepts. We treat the uncertainty $\sigma(f)$ and the limit resolution $\mathrm{res}(g)$ simply as an absolute and relative uncertainty measure, respectively, specifying how accurately one can treat g as a sharp number, given by this value.

In experimental practice, the limit resolution is a lower bound on the relative accuracy with which one can expect $\langle g \rangle$ to be determinable reliably[6] from measurements of a single system at a single time. In particular, a quantity g is considered to be **significant** if $\mathrm{res}(g) \ll 1$, while it is **noise** if $\mathrm{res}(g) \gg 1$. If g is a quantity and $\widetilde{g}$ is a good approximation of its value then $\Delta g := g - \widetilde{g}$ is noise. Sufficiently significant quantities can be treated as **deterministic**; the analysis of noise is the subject of **statistics**.

8.4.3 Proposition. *For any state,*

(i) $f \leq g \quad \Rightarrow \quad \langle f \rangle \leq \langle g \rangle$.

[6]The situation is analogous to the limit resolution with which one can determine the longitude and latitude of a city such as Vienna. Clearly these are well-defined only up to some limit resolution related to the diameter of the city. No amount of measurements can reduce the uncertainty below about 10km. For an extended object, the uncertainty in its position is conceptual, not just a lack of knowledge or precision. Indeed, a point may be *defined* in these terms: It is an object in a state where the position has zero limit resolution.

(ii) For $f, g \in \mathbb{E}$,

$$\begin{aligned} \operatorname{cov}(f,g) &= \operatorname{Re}(\langle f^* g\rangle - \langle f\rangle^* \langle g\rangle), \\ \langle f^* f\rangle &= \langle f\rangle^* \langle f\rangle + \sigma(f)^2, \\ |\langle f\rangle| &\le \sqrt{\langle f^* f\rangle}. \end{aligned}$$

(iii) If f is Hermitian then $\bar{f} = \langle f\rangle$ is real and

$$\sigma(f) = \sqrt{\langle (f-\overline{f})^2\rangle} = \sqrt{\langle f^2\rangle - \langle f\rangle^2}.$$

(iv) Two commuting Hermitian quantities f, g are uncorrelated iff

$$\langle fg\rangle = \langle f\rangle\langle g\rangle.$$

Proof. (i) follows from (E1) and (E3).

(ii) The first formula holds since

$$\langle (f-\bar{f})^*(g-\bar{g})\rangle = \langle f^* g\rangle - \bar{f}^*\langle g\rangle - \langle f\rangle^*\bar{g} + \bar{f}^*\bar{g} = \langle f^* g\rangle - \langle f\rangle^*\langle g\rangle.$$

The second formula follows for $g = f$, using (E1), and the third formula is an immediate consequence.

(iii) follows from (E1) and (ii).

(iv) If f, g are Hermitian and commute then fg is Hermitian by Proposition 8.1.3(ii), hence $\langle fg\rangle$ is real. By (ii), $\operatorname{cov}(f,g) = \langle fg\rangle - \langle f\rangle\langle g\rangle$, and the assertion follows. □

Formally, the essential difference between classical mechanics and quantum mechanics in the latter's lack of commutativity. While in classical mechanics there is in principle no lower limit to the uncertainties with which we can prepare the quantities in a system of interest, the quantum mechanical uncertainty relation for noncommuting quantities puts strict limits on the uncertainties in the preparation of microscopic states. Here, *preparation* is defined informally as bringing the system into a state such that measuring certain quantities f gives numbers that agree with the values $\langle f\rangle$ to an accuracy specified by given uncertainties.

We now discuss the limits of the accuracy to which this can be done.

8.4.4 Proposition.
*(i) The **Cauchy–Schwarz inequality***

$$|\langle f^* g\rangle|^2 \le \langle f^* f\rangle\langle g^* g\rangle$$

holds for all $f, g \in \mathbb{E}$.

*(ii) The **uncertainty relation***

$$\sigma(f)^2\sigma(g)^2 \ge |\operatorname{cov}(f,g)|^2 + \left|\tfrac{1}{2}\langle f^* g - g^* f\rangle\right|^2$$

holds for all $f, g \in \mathbb{E}$.

(iii) For $f, g \in \mathbb{E}$,

$$\operatorname{cov}(f,g) = \operatorname{cov}(g,f) = \tfrac{1}{2}(\sigma(f+g)^2 - \sigma(f)^2 - \sigma(g)^2), \tag{8.46}$$

$$|\operatorname{cov}(f,g)| \le \sigma(f)\sigma(g), \tag{8.47}$$

$$\sigma(f+g) \le \sigma(f) + \sigma(g). \tag{8.48}$$

In particular,

$$|\langle fg\rangle - \langle f\rangle\langle g\rangle| \le \sigma(f)\sigma(g) \quad \textit{for commuting Hermitian } f, g. \tag{8.49}$$

Proof. (i) For arbitrary $\alpha, \beta \in \mathbb{C}$ we have

$$\begin{aligned} 0 &\le \langle(\alpha f - \beta g)^*(\alpha f - \beta g)\rangle \\ &= \alpha^*\alpha\langle f^*f\rangle - \alpha^*\beta\langle f^*g\rangle - \beta^*\alpha\langle g^*f\rangle + \beta\beta^*\langle g^*g\rangle \\ &= |\alpha|^2\langle f^*f\rangle - 2\operatorname{Re}(\alpha^*\beta\langle f^*g\rangle) + |\beta|^2\langle g^*g\rangle \end{aligned}$$

We now choose $\beta = \langle f^*g\rangle$, and obtain for arbitrary real α the inequality

$$0 \le \alpha^2\langle f^*f\rangle - 2\alpha|\langle f^*g\rangle|^2 + |\langle f^*g\rangle|^2\langle g^*g\rangle. \tag{8.50}$$

The further choice $\alpha = \langle g^*g\rangle$ gives

$$0 \le \langle g^*g\rangle^2\langle f^*f\rangle - \langle g^*g\rangle|\langle f^*g\rangle|^2.$$

If $\langle g^*g\rangle > 0$, we find after division by $\langle g^*g\rangle$ that (i) holds. And if $\langle g^*g\rangle \le 0$ then $\langle g^*g\rangle = 0$ and we have $\langle f^*g\rangle = 0$ since otherwise a tiny α produces a negative right hand side in (8.50). Thus (i) also holds in this case.

(ii) Since $(f-\bar{f})^*(g-\bar{g}) - (g-\bar{g})^*(f-\bar{f}) = f^*g - g^*f$, it is sufficient to prove the uncertainty relation for the case of quantities f, g whose value vanishes. In this case, (i) implies

$$(\operatorname{Re}\langle f^*g\rangle)^2 + (\operatorname{Im}\langle f^*g\rangle)^2 = |\langle f^*g\rangle|^2 \le \langle f^*f\rangle\langle g^*g\rangle = \sigma(f)^2\sigma(g)^2.$$

The assertion follows since $\operatorname{Re}\langle f^*g\rangle = \operatorname{cov}(f,g)$ and

$$i\operatorname{Im}\langle f^*g\rangle = \tfrac{1}{2}(\langle f^*g\rangle - \langle f^*g\rangle^*) = \tfrac{1}{2}\langle f^*g - g^*f\rangle.$$

(iii) Again, it is sufficient to consider the case of quantities f, g whose value vanishes. Then

$$\begin{aligned} \sigma(f+g)^2 &= \langle(f+g)^*(f+g)\rangle = \langle f^*f\rangle + \langle f^*g + g^*f\rangle + \langle g^*g\rangle \\ &= \sigma(f)^2 + 2\operatorname{cov}(f,g) + \sigma(g)^2, \end{aligned} \tag{8.51}$$

and (8.46) follows. (8.47) is an immediate consequence of (ii), and (8.48) follows easily from (8.51) and (8.47). Finally, (8.49) is a consequence of (8.47) and Proposition 8.4.3(iii). □

If we apply Proposition 8.4.4(ii) to scalar position q and momentum p variables satisfying the **canonical commutation relation**

$$[q, p] = i\hbar, \tag{8.52}$$

we obtain

$$\sigma(q)\sigma(p) \geq \tfrac{1}{2}\hbar, \tag{8.53}$$

the **uncertainty relation** of Heisenberg [123, 237]. It implies that no state exists where both position q and momentum p have arbitrarily small uncertainty.

Chapter 9

The laws of thermodynamics

This chapter rederives the laws of thermodynamics from statistical mechanics, thus putting the phenomenological discussion of Chapter 7 on more basic foundations.

We confine our attention to a restricted but very important class of Gibbs states, those describing thermal states. We introduce thermal states by selecting the quantities whose values shall act as extensive variables in a thermal model. On this level, we shall be able to reproduce the phenomenological setting of the present section from first principles; see the discussion after Theorem 9.2.3. If the underlying detailed model is assumed to be known then the system function, and with it all thermal properties, are computable in principle, although we only hint at the ways to do this numerically. We also look at a hierarchy of thermal models based on the same bottom level description and discuss how to decide which description levels are appropriate.

Although dynamics is important for systems not in global equilibrium, we completely ignore dynamical issues in this chapter. We take a strictly kinematic point of view, and look as before only at a single phase without chemical reactions. In principle, it is possible to extend the present setting to cover the dynamics of the nonequilibrium case and deduce quantitatively the dynamical laws of nonequilibrium thermodynamics (Beris & Edwards [33], Oettinger [209]) from microscopic properties, including phase formation, chemical reactions, and the approach to equilibrium; see, e.g., Balian [18], Grabert [109], Rau & Müller [228], Spohn [257].

9.1 The zeroth law: Thermal states

Thermal states are special Gibbs states, used in statistical mechanics to model macroscopic physical systems that are homogeneous on the (global, local, microlocal, or quantum) level used for modeling. They have all the properties traditionally postulated in thermodynamics. While we discuss the lower levels on an informal basis, we consider in the formulas for notational simplicity mainly the case of global equilibrium, where there are only finitely many extensive variables. Everything extends, however, with (formally trivial but from a

rigorous mathematical view nontrivial) changes to local and microlocal equilibrium, where extensive variables are fields, provided the sums are replaced by appropriate integrals; cf. Oettinger [209].

In the setting of statistical mechanics, the intensive variables are, as in Section 7.1, numbers parameterizing the entropy and characterizing a particular system at a particular time. To each admissible combination of intensive variables there is a unique thermal state providing values for all quantities. The extensive variables then appear as the values of corresponding extensive quantities.

A basic extensive quantity present in each thermal system is the **Hamilton energy** H; it is identical to the **Hamiltonian** function (or operator) in the underlying dynamical description of the classical (or quantum) system. In addition, there are further basic extensive quantities which we call X_j $(j \in J)$ and collect in a vector X, indexed by J. All other extensive quantities are expressible as linear combinations of these basic extensive quantities. The number and meaning of the extensive variables depends on the type of the system; typical examples are given in Table 10.1 in Section 10.2.

In the context of statistical mechanics (cf. Examples 8.1.8), the Euclidean $*$-algebra $\mathbb{E}$ is typically an algebra of functions (for classical physics) or linear operators (for quantum physics), and H is a particular function or linear operator characterizing the class of systems considered. The form of the operators X_j depends on the level of thermal modeling; for further discussion, see Section 10.2.

For qualitative theory and for deriving semi-empirical recipes, there is no need to know details about H or X_j; it suffices to treat them as primitive objects. The advantage we gain from such a less detailed setting is that to reconstruct all of phenomenological thermodynamics, a much simpler machinery suffices than what would be needed for a detailed model

It is intuitively clear from the informal definition of extensive variables in Section 7.5 that the only functions of independent extensive variables that are again extensive can be linear combinations, and it is a little surprising that *the whole machinery of equilibrium thermodynamics follows from a formal version of the simple assumption that in thermal states the entropy is extensive*. We take this to be the mathematical expression of the zeroth law and formalize this assumption in a precise mathematical definition.

9.1.1 Definition. A **thermal system** is defined by a family of Hermitian **extensive variables** H and X_j $(j \in J)$ from a Euclidean $*$-algebra. A **thermal state** of a thermal system is a Gibbs state whose entropy S is a linear combination of the basic extensive quantities of the form

$$S = T^{-1}\Big(H - \sum_{j\in J} \alpha_j X_j\Big) = T^{-1}(H - \alpha \cdot X) \quad \textbf{(zeroth law of thermodynamics)} \tag{9.1}$$

with suitable real numbers $T \neq 0$ and α_j $(j \in J)$. Here α and X are the vectors with components α_j $(j \in J)$ and X_j $(j \in J)$, respectively.

Thus the value of an arbitrary quantity g is

$$\overline{g} := \langle g \rangle = \int e^{-\beta(H-\alpha\cdot X)} g, \tag{9.2}$$

where

$$\beta = \frac{1}{\hbar T} \ . \tag{9.3}$$

The numbers α_j are called the **intensive variables conjugate to** X_j, the number T is called the **temperature**, and β the **coldness**. $\overline{S}, \overline{H}, \overline{X}, T$, and α are called the **thermal variables** of the system. Note that the extensive variables of traditional thermodynamics are in the present setting not represented by the extensive quantities S, H, X_j themselves but by their values $\overline{S}, \overline{H}, \overline{X}$.

Since we can write the zeroth law (9.1) in the form

$$H = TS + \alpha \cdot X, \tag{9.4}$$

called the **Euler equation**, the temperature T is considered to be the intensive variable conjugate to the entropy S.

9.1.2 Remarks. (i) As already discussed in Section 7.2 for the case of temperature, measuring intensive variables is based upon the empirical fact that two systems in contact where the free exchange of some extensive quantity is allowed tend to relax to a joint equilibrium state, in which the corresponding intensive variable is the same in both systems. If a small measuring device is brought into close contact with a large system, the joint equilibrium state will be only minimally different from the original state of the large system; hence the intensive variables of the measuring device will move to the values of the intensive variables of the large system in the location of the measuring device. This allows to read off their value from a calibrated scale.

(ii) Many treatises of equilibrium thermodynamics take the possibility of measuring temperature to be the contents of the zeroth law of thermodynamics. The present, different choice for the zeroth law has far reaching consequences. Indeed, as we shall see, the definition implies the first and second law, and (together with a quantization condition) the third law of thermodynamics. Thus these become theorems rather than separately postulated laws.

(iii) We emphasize that the extensive quantities H and X_j are independent of the intensive quantities T and α, while S, defined by (9.1), is an extensive quantity defined only when values for the intensive quantities are prescribed. From (9.1) it is clear that values also depend on the particular state a system is in. It is crucial to distinguish between the quantities H or X_j, which are part of the definition of the system but independent of the state (since they are independent of T and α), and their values $\overline{H} = \langle H \rangle$ or $\overline{X}_j = \langle X_j \rangle$, which change with the state.

(iv) In thermodynamics, the interest is restricted to the values of the thermal variables. In statistical mechanics, the values of the thermal variables determine a state of the microscopic system. In particular, the knowledge of the intensive variables allows one to compute the values (9.2) of *arbitrary* microscopic quantities, not only the extensive ones. Of course, these values don't give information about the position and momentum of individual particles but

only about their means. For example, the mean velocity of an ideal monatomic gas at temperature T turns out to be $\langle \mathbf{v} \rangle = 0$, and the mean velocity-squared is $\langle \mathbf{v}^2 \rangle = 3\hbar T$. (We don't derive these relations here; usually they are obtained from a starting point involving the Boltzmann equation.)

(v) A general Gibbs state has an incredibly high complexity. Indeed, in the classical case, the specification of an arbitrary Gibbs state for 1 mole of a pure, monatomic substance such as Argon requires specifying the entropy S, a function of $6N_A \approx 36 \cdot 10^{23}$ degrees of freedom. In comparison, a global equilibrium state of Argon is specified by three numbers T, p and μ, a local equilibrium state by three fields depending on four parameters (time and position) only, and a microlocal equilibrium state by three fields depending on seven parameters (time, position, and momentum). Thus global, local, and microlocal equilibrium states form a small minority in the class of all Gibbs states. It is remarkable that this small class of states suffices for the engineering accuracy description of all macroscopic phenomena.

(vi) Of course, the number of thermal variables or fields needed to describe a system depends on the true physical situation. For example, a system that is in local equilibrium only cannot be adequately described by the few variables characterizing global equilibrium. The problem of selecting the right set of extensive quantities for an adequate description is discussed in Section 10.2.

(vii) The formulation (9.1) is almost universally used in practice. However, an arbitrary linear combination

$$S = \gamma H + h_0 X_0 + \ldots + h_s X_s \tag{9.5}$$

can be written in the form (9.1) with $T = 1/\gamma$ and $\alpha_j = -h_j/\gamma$, provided that $\gamma \neq 0$; indeed, (9.5) is mathematically the more natural form, which also allows states of infinite temperature that are excluded in (9.1). This shows that the coldness β is a more natural variable than the temperature T; it figures prominently in statistical mechanics. Indeed, the formulas of statistical mechanics are continuous in β even for systems such as those considered in Example 9.2.5, where β may become zero or negative. The temperature T reaches in this case infinity, then jumps to minus infinity, and then continues to increase. According to Landau & Lifschitz [168, Section 73], states of negative temperature, i.e., negative coldness, must therefore be considered to be hotter, i.e., less cold, than states of any positive temperature. On the other hand, in the limit $T \to 0$, a system becomes infinitely cold, giving intuition for the unattainability of zero absolute temperature.

(viii) In mathematical statistics, there is a large body of work on *exponential families*, which is essentially the mathematical equivalent of the concept of a thermal state over a commutative algebra; see, e.g., Barndorff-Nielsen [25]. In this context, the values of the extensive quantities define a *sufficient statistic*, from which the whole distribution can be reconstructed (cf. Theorem 9.2.4 below and the remarks on objective probability in Section 8.4). This is one of the reasons why exponential families provide a powerful machinery for statistical inference; see, e.g., Bernardo & Smith [34]. For recent extensions to quantum statistical inference, see, e.g., Barndorff-Nielsen et al. [26] and the references there.

(ix) For other axiomatic settings for deriving thermodynamics, which provide different perspectives, see Carathéodory [57], Haken [119], Jaynes [139], Katz [147], Emch &

Liu [81], and Lieb & Yngvason [175].

9.2 The equation of state

Not every combination (T, α) of intensive variables defines a thermal state; the requirement that $\langle 1 \rangle = 1$ enforces a restriction of (T, α) to a manifold of admissible thermal states.

9.2.1 Theorem. *Suppose that $T > 0$.*

(i) For any $\kappa > 0$, the ***system function*** *Δ defined by*

$$\Delta(T, \alpha) := \kappa T \log \int e^{-\beta(H - \alpha \cdot X)} \tag{9.6}$$

is a convex function of T and α. It vanishes only if T and α are the intensive variables of a thermal state.

(ii) In a thermal state, the intensive variables are related by the ***equation of state***

$$\Delta(T, \alpha) = 0. \tag{9.7}$$

The ***state space*** *is the set of (T, α) satisfying (9.7).*

(iii) The values of the extensive variables are given by

$$\overline{S} = \Omega \frac{\partial \Delta}{\partial T}(T, \alpha), \quad \overline{X} = \Omega \frac{\partial \Delta}{\partial \alpha}(T, \alpha) \quad \text{for some } \Omega > 0, \tag{9.8}$$

and the ***phenomenological Euler equation***

$$\overline{H} = T\overline{S} + \alpha \cdot \overline{X}. \tag{9.9}$$

(iv) Regarding $\overline{S}$ and $\overline{X}$ as functions of T and α, the matrix

$$\Sigma := \begin{pmatrix} \dfrac{\partial \overline{S}}{\partial T} & \dfrac{\partial \overline{S}}{\partial \alpha} \\ \\ \dfrac{\partial \overline{X}}{\partial T} & \dfrac{\partial \overline{X}}{\partial \alpha} \end{pmatrix} \tag{9.10}$$

is symmetric and positive semidefinite; in particular, we have the ***Maxwell reciprocity relations***

$$\frac{\partial \overline{X}_i}{\partial \alpha_j} = \frac{\partial \overline{X}_j}{\partial \alpha_i}, \quad \frac{\partial \overline{X}_i}{\partial T} = \frac{\partial \overline{S}}{\partial \alpha_i}, \tag{9.11}$$

and the ***stability conditions***

$$\frac{\partial \overline{S}}{\partial T} \geq 0, \quad \frac{\partial \overline{X}_j}{\partial \alpha_j} \geq 0 \quad (j \in J). \tag{9.12}$$

Proof. By Theorem 8.3.2(i), the function ϕ defined by

$$\phi(\alpha_0, \alpha) := \log \int e^{-(\alpha_0 H - \alpha \cdot X)} = -W(\alpha_0 H - \alpha \cdot X)$$

is a convex function of α_0 and α. Put $\Omega = \hbar/\kappa$. Then, by Proposition 7.1.1,

$$\Delta(T, \alpha) = -\kappa T W(\beta(H - \alpha \cdot X)) = \kappa T \phi\Big(\frac{1}{\hbar T}, \frac{\alpha}{\hbar T}\Big) \tag{9.13}$$

is also convex. The condition $\Delta(T, \alpha) = 0$ is equivalent to

$$\int e^{-S/\hbar} = \int e^{-\beta(H - \alpha \cdot X)} = e^{\Delta/\kappa T} = 1,$$

the condition for a thermal state. This proves (i) and (ii).

(iii) The formulas for $\overline{S}$ and $\overline{X}$ follow by differentiation of (9.13) with respect to T and α, using (8.36). Equation (9.9) follows by taking values in (9.4), noting that T and α are real numbers.

(iv) By (iii), the matrix

$$\Sigma = \begin{pmatrix} \dfrac{\partial^2 \Delta}{\partial T^2} & \dfrac{\partial^2 \Delta}{\partial T \partial \alpha} \\[2ex] \dfrac{\partial^2 \Delta}{\partial \alpha \partial T} & \dfrac{\partial^2 \Delta}{\partial \alpha^2} \end{pmatrix}$$

is the Hessian matrix of the convex function Δ. Hence Σ is symmetric and positive semidefinite. (9.11) expresses the symmetry of Σ, and (9.12) holds since the diagonal entries of a positive semidefinite matrix are nonnegative. □

9.2.2 Remarks. (i) For $T < 0$, the same results hold, with the change that Δ is concave instead of convex, Σ is negative semidefinite, and the inequality signs in (9.12) are reversed. This is a rare situation; it can occur only in (nearly) massless systems embedded out of equilibrium within (much heavier) matter, such as spin systems (cf. Purcell & Pound [224]), radiation fields in a cavity (cf. Hsu & Barakat [128]), or vortices in 2-dimensional fluids (cf. Montgomery & Joyce [192], Eyinck & Spohn [83]). A massive thermal system couples significantly to kinetic energy. In this case, the total momentum p is an extensive quantity, related to the velocity v, the corresponding intensive variable, by $p = Mv$, where M is the extensive total mass of the system. From (9.8), we find that $\overline{p} = \Omega \partial \Delta / \partial v$, which implies that $\Delta = \Delta|_{v=0} + \frac{\overline{M}}{2\Omega} v^2$. Since the mass is positive, this expression is convex in v, not concave; hence $T > 0$. Thus, in a massive thermal system, the temperature must be positive.

(ii) In applications, the free scaling constant κ is usually chosen as

$$\kappa = \hbar/\Omega, \tag{9.14}$$

where Ω is a measure of **system size**, e.g., the total volume or total mass of the system. In actual calculations from statistical mechanics, the integral is usually a function of the

shape and size of the system. To make the result independent of it, one performs the so-called thermodynamic limit $\Omega \to \infty$; thus Ω must be chosen in such a way that this limit is nontrivial. Extensivity in single phase global equilibrium then justifies treating Ω as an arbitrary positive factor.

In phenomenological thermodynamics (cf. Section 7.1), one makes suitable, more or less heuristic assumptions on the form of the system function, while in **statistical mechanics**, one derives its form from (9.7) and specific choices for the quantities H and X within one of the settings described in Example 8.1.8. Given these choices, the main task is then the evaluation of the system function (9.6), from which the values of all quantities can be computed. (9.6) can often be approximately evaluated from the cumulant expansion (8.34) and/or a mean field approximation (8.43).

An arbitrary Gibbs state is generally not a thermal state. However, we can try to approximate it by an equilibrium state in which the extensive variables have the same values. The next result shows that the slack (the difference between the left hand side and the right hand side) in (9.15), which will turn out to be the microscopic form of the Euler inequality (7.2), is always nonnegative and vanishes precisely in equilibrium. Thus it can be used as a measure of how close the Gibbs state is to an equilibrium state.

9.2.3 Theorem. *Let $\langle\cdot\rangle$ be a Gibbs state with entropy S. Then, for arbitrary (T,α) satisfying $T > 0$ and the equation of state (9.7), the values $\overline{H} = \langle H\rangle$, $\overline{S} = \langle S\rangle$, and $\overline{X} = \langle X\rangle$ satisfy*

$$\overline{H} \geq T\overline{S} - \alpha \cdot \overline{X}. \tag{9.15}$$

Equality only holds if S is the entropy of a thermal state with intensive variables (T,α).

Proof. The equation of state implies that $S_c := T^{-1}(H - \alpha \cdot X)$ is the entropy of a thermal state. Now the assertion follows from Theorem 8.3.3, since $\langle S\rangle \leq \langle S_c\rangle = T^{-1}(\langle H\rangle - \alpha\cdot\langle X\rangle)$, with equality only if $S = S_c$. □

As the theorem shows, everything of macroscopic interest is deducible from an explicit formula for the system function. Hence one can use thermodynamics in many situations very successfully as a phenomenological theory without having to bother about microscopic details. It suffices that a phenomenological expression for $\Delta(T,\alpha)$ is available. In particular, the phenomenological axioms from Section 7.1 now follow by specializing the above to a **standard system**, characterized by the extensive quantities

$$H, X_0 = V, \quad X_j = N_j \ (j \neq 0), \tag{9.16}$$

where, as before, V denotes the (positive) **volume** of the system, and each N_j denotes the (nonnegative) number of molecules of a fixed chemical composition (we shall call these **particles of kind** j). However, H and the N_j are now quantities from $\mathbb{E}$, rather than thermal variables. We call

$$P := -\alpha_0 \tag{9.17}$$

the **pressure** and

$$\mu_j := \alpha_j \quad (j \neq 0) \tag{9.18}$$

the **chemical potential** of kind j; hence

$$\alpha \cdot X = -PV + \mu \cdot N.$$

Specializing the theorem, we find the phenomenological Euler equation

$$\overline{H} = T\overline{S} - PV + \mu \cdot \overline{N}. \tag{9.19}$$

Note that $\overline{V} = V$ since we took V as system size. For reversible changes, we have the first law of thermodynamics

$$d\overline{H} = Td\overline{S} - PdV + \mu \cdot d\overline{N} \tag{9.20}$$

and the Gibbs-Duhem equation

$$0 = \overline{S}dT - VdP + \overline{N} \cdot d\mu. \tag{9.21}$$

A comparison with Section 7.1 shows that dropping the bars from the values reproduces for $T > 0$, $P > 0$ and $\overline{S} \geq 0$ the axioms of phenomenological thermodynamics, except for the extensivity outside equilibrium (which has local equilibrium as its justification). The assumption $T > 0$ was justified in Remark 9.2.2(i), and $\overline{S} \geq 0$ will be justified in Section 9.5. But there seem to be no theoretical arguments which shows that the pressure of a standard system in the above sense must always be positive. (At $T < 0$, negative pressure is possible; see Example 9.2.5.) We'd appreciate getting information about this from readers of this book.

Apart from boundary effects, whose role diminishes as the system gets larger, the extensive quantities scale linearly with the volume. In the thermodynamic limit, corresponding to an idealized system infinitely extended in all directions, the boundary effects disappear and the linear scaling becomes exact, although this can be proved rigorously only in simple situations, e.g., for hard sphere model systems (Yang & Lee [297]) or spin systems (Griffiths [112]). A thorough treatment of the thermodynamic limit (e.g., Ruelle [243, 244], Thirring [267], or, in the framework of large deviation theory, Ellis [80]) in general needs considerably more algebraic and analytic machinery, e.g., the need to work in place of thermal states with more abstract KMS-states (which are limits of sequences of thermal states still satisfying a KMS condition (8.20)). Moreover, proving the existence of the limit requires detailed properties of the concrete microscopic description of the system.

For very small systems, typically atomic clusters or molecules, N is fixed and a **canonical ensemble** without the $\mu \cdot N$ term is more appropriate. For the thermodynamics of small systems (see, e.g., (Bustamente et al. [54], Gross [114], Kratky [158]) such as a single cluster of atoms, V is still taken as a fixed reference volume, but now changes in the physical volume (adsorption or dissociation at the surface) are not represented in the system, hence need not respect the thermodynamic laws. For large surfaces (e.g., adsorption studies in chromatography; see Karger et al. [146], Masel [189]), a thermal description is achievable by including additional variables (surface area and surface tension) to account for the boundary effects; but clearly, surface terms scale differently with system size than bulk terms.

Thus, whenever the thermal description is valid, computations can be done in a fixed reference volume which we take as system size Ω. (Formulas for an arbitrary volume V

are then derived by extensivity, scaling every extensive quantity with V/Ω.) The reference volume may be represented in the Euclidean $*$-algebra as a real number, so that in particular $\overline{V} = V$. Then (9.6) together with e.Deltascale implies that

$$\Delta(T, P, \mu) = V^{-1}\hbar T \log(e^{-\beta PV}) \int e^{-\beta(H-\mu\cdot N)},$$

hence

$$\Delta(T, P, \mu) = V^{-1}\hbar T(\log Z(T, V, \mu) - PV) = P(T, \mu) - P, \tag{9.22}$$

where

$$Z(T, V, \mu) := \int e^{-\beta(H-\mu\cdot N)} \tag{9.23}$$

is the so-called **grand canonical partition function** of the system and

$$P(T, \mu) := V^{-1}\hbar T \log Z(T, V, \mu), \tag{9.24}$$

while P without argument is the parameter in the left hand side of (9.22). With our convention of considering a fixed reference volume and treating the true volume by scaling extensive variables, this expression is independent of V, since it relates intensive variables unaffected by scaling. (A more detailed argument would have to show that the **thermodynamic limit** $P(T, \mu) := \lim_{V\to\infty} V^{-1}\hbar T \log Z(T, V, \mu)$ exists, and argue that thermodynamics is applied in practice only to systems where V is so large that the difference to the limit is negligible.

The equation of state (9.7) therefore takes the form

$$P = P(T, \mu). \tag{9.25}$$

Quantitative expressions for the equation of state can often be computed from (9.23)–(9.24) using the cumulant expansion (8.34) and/or a mean field approximation (8.43). Note that these relations imply that

$$e^{-\beta P(T,\mu)V} = \int e^{-\beta(H-\mu\cdot N)}.$$

Traditionally (see, e.g., Gibbs [102], Huang [130], Reichl [230]), the thermal state corresponding to (9.22)–(9.24) is called a **grand canonical ensemble**, and the following results are taken as the basis for microscopic calculations from statistical mechanics.

9.2.4 Theorem. *For a standard system in global equilibrium, values of an arbitrary quantity g can be calculated from* (9.23) *and*

$$\langle g \rangle = Z(T, \mu)^{-1} \int e^{-\beta(H-\mu\cdot N)} g. \tag{9.26}$$

The values of the extensive quantities are given in terms of the equation of state (9.24) *by*

$$\overline{S} = V\frac{\partial P}{\partial T}(T, \mu), \quad \overline{N}_j = V\frac{\partial P}{\partial \mu_j}(T, \mu) \tag{9.27}$$

and the phenomenological Euler equation (9.19).

Proof. Equation (9.24) implies that $Z(T,V,\mu) = e^{\beta PV}$, hence

$$\begin{aligned}\langle g\rangle &= \textstyle\int e^{-S/\hbar} g = \int e^{-\beta(H+PV-\mu\cdot N)} g \\ &= e^{-\beta PV} \textstyle\int e^{-\beta(H-\mu\cdot N)} g = Z(T,V,\mu)^{-1} \int e^{-\beta(H-\mu\cdot N)} g,\end{aligned}$$

giving (9.26). The formulas in (9.27) follow from (9.8) and (9.22). □

No thermodynamic limit was needed to derive the above results. Thus, everything holds – though with large limit resolutions in measurements – even for single small systems (Bustamente et al. [54], Gross [114], Kratky [158]).

9.2.5 Example. We consider the two level system from Example 8.2.4, using $\Omega = 1$ as system size. From (9.23) and (9.24), we find $Z(T,\mu) = 1 + e^{-E/\hbar T}$, hence

$$P(T,\mu) = \hbar T \log(1 + e^{-E/\hbar T}) = \hbar T \log(e^{E/\hbar T} + 1) - E.$$

From (9.26), we find

$$\overline{H} = \frac{Ee^{-E/\hbar T}}{1 + e^{-E/\hbar T}} = \frac{E}{e^{E/\hbar T} + 1}, \quad \hbar T = \frac{E}{\log(E/\overline{H} - 1)}.$$

(This implies that a two-level system has negative temperature and negative pressure if $\overline{H} > E/2$.) The **heat capacity** $C := d\overline{H}/dT$ takes the form

$$C = \frac{E^2}{\hbar T^2} \frac{e^{E/\hbar T}}{(e^{E/\hbar T} + 1)^2}.$$

It exhibits a pronounced maximum, the so-called **Schottky bump** (cf. Callen [55]), from which E can be determined. In view of (9.57) below, this allows the experimental estimation of the spectral gap of a quantum system. The phenomenon persists to some extent for multilevel systems; see Civitarese et al. [63].

9.3 The first law: Energy balance

We now discuss relations between changes of the values of extensive or intensive variables, as expressed by the first law of thermodynamics. To derive the first law in full generality, we use the concept of reversible transformations introduced in Section 7.1. Corresponding to such a transformation, there is a family of thermal states $\langle\cdot\rangle_\lambda$ defined by

$$\langle f\rangle_\lambda = \textstyle\int e^{-\beta(\lambda)(H-\alpha(\lambda)\cdot X)} f, \quad \beta(\lambda) = \dfrac{1}{\hbar T(\lambda)}.$$

Important: In case of local or microlocal equilibrium, where the thermal system carries a dynamics, it is important to note that reversible transformations are ficticious transformations which have nothing to do with how the system changes with time, or whether a

process is reversible in the dynamical sense that both the process and the reverse process can be realized dynamically. The time shift is generally *not* a reversible transformation.

We use differentials corresponding to reversible transformations; writing $f = S/\hbar$, we can delete the index f from the formulas in Section 8.2. In particular, we write the Kubo inner product (8.23) as

$$\langle g; h\rangle := \langle g; h\rangle_{S/\hbar}. \tag{9.28}$$

9.3.1 Proposition. *The value $\overline{g}(T,\alpha) := \langle g(T,\alpha)\rangle$ of every (possibly T- and α-dependent) quantity $g(T,\alpha)$ is a state variable satisfying the* ***differentiation formula***

$$d\langle g\rangle = \langle dg\rangle - \langle g - \overline{g}; dS\rangle/\hbar. \tag{9.29}$$

Proof. That $\overline{g}$ is a state variable is an immediate consequence of the zeroth law (9.1) since the entropy depends on T and α only. The differentiation formula follows from (8.35) and (9.28). □

9.3.2 Theorem. *For reversible changes, we have the* ***first law of thermodynamics***

$$d\overline{H} = Td\overline{S} + \alpha \cdot d\overline{X} \tag{9.30}$$

and the ***Gibbs-Duhem equation***

$$0 = \overline{S}dT + \overline{X} \cdot d\alpha. \tag{9.31}$$

Proof. Differentiating the equation of state (9.7), using the chain rule (7.10), and simplifying using (9.8) gives the Gibbs-Duhem equation (9.31). If we differentiate the phenomenological Euler equation (9.9), we obtain

$$d\overline{H} = Td\overline{S} + \overline{S}dT + \alpha \cdot d\overline{X} + \overline{X} \cdot d\alpha,$$

and using (9.31), this simplifies to the first law of thermodynamics. □

Because of the form of the energy terms in the first law (9.30), one often uses the analogy to mechanics and calls the intensive variables **generalized forces**, and differentials of extensive variables **generalized displacements**.

For the Gibbs-Duhem equation, we give a second proof which provides additional insight. Since H and X are fixed quantities for a given system, they do not change under reversible transformations; therefore

$$dH = 0, \quad dX = 0.$$

Differentiating the Euler equation (9.4), therefore gives the relation

$$0 = TdS + SdT + X \cdot d\alpha. \tag{9.32}$$

On the other hand, S depends explicitly on T and α, and by Corollary 8.1.11,

$$\langle dS\rangle = \int e^{-S/\hbar} dS = \hbar d\left(\int e^{-S/\hbar}\right) = \hbar d1 = 0, \tag{9.33}$$

taking values in (9.32) implies again the Gibbs-Duhem equation. By combining equation (9.32) with the Kubo product we get information about limit resolutions:

9.3.3 Theorem.
(i) Let g be a quantity depending continuously differentiable on the intensive variables T and α. Then

$$\langle g-\overline{g}; S-\overline{S}\rangle = \hbar T\Big(\frac{\partial \overline{g}}{\partial T} - \Big\langle \frac{\partial g}{\partial T}\Big\rangle\Big), \tag{9.34}$$

$$\langle g-\overline{g}; X_j-\overline{X}_j\rangle = \hbar T\Big(\frac{\partial \overline{g}}{\partial \alpha_j} - \Big\langle \frac{\partial g}{\partial \alpha_j}\Big\rangle\Big), \tag{9.35}$$

(ii) If the extensive variables H and X_j $(j\in J)$ are pairwise commuting then

$$\langle (S-\overline{S})^2\rangle = \hbar T\,\frac{\partial \overline{S}}{\partial T}, \tag{9.36}$$

$$\langle (X_j-\overline{X}_j)(S-\overline{S})\rangle = \hbar T\,\frac{\partial \overline{X}_j}{\partial T} \qquad (j\in J), \tag{9.37}$$

$$\langle (X_j-\overline{X}_j)(X_k-\overline{X}_k)\rangle = \hbar T\,\frac{\partial \overline{X}_j}{\partial \alpha_k} \qquad (j,k\in J), \tag{9.38}$$

$$\operatorname{res}(S) = \sqrt{\frac{\hbar T}{\overline{S}^2}\frac{\partial \overline{S}}{\partial T}}, \quad \operatorname{res}(X_j) = \sqrt{\frac{\hbar T}{\overline{X}_j^2}\frac{\partial \overline{X}_j}{\partial \alpha_j}}, \tag{9.39}$$

$$\operatorname{res}(H) = \sqrt{\frac{\hbar T}{\overline{H}^2}\Big(T\frac{\partial \overline{H}}{\partial T} + \alpha\cdot\frac{\partial \overline{H}}{\partial \alpha}\Big)}. \tag{9.40}$$

Proof. Multiplying the differentiation formula (9.29) by $\hbar T$ and using (9.32), we find, for arbitrary reversible transformations,

$$\hbar T(d\langle g\rangle - \langle dg\rangle) = \langle g-\overline{g}; S\rangle dT + \langle g-\overline{g}; X\rangle\cdot d\alpha.$$

Dividing by $d\lambda$ and choosing $\lambda = T$ and $\lambda = \alpha_j$, respectively, gives

$$\langle g-\overline{g}; S\rangle = \hbar T\Big(\frac{\partial \overline{g}}{\partial T} - \Big\langle \frac{\partial g}{\partial T}\Big\rangle\Big), \quad \langle g-\overline{g}; X_j\rangle = \hbar T\Big(\frac{\partial \overline{g}}{\partial \alpha_j} - \Big\langle \frac{\partial g}{\partial \alpha_j}\Big\rangle\Big).$$

(i) follows upon noting that $\langle g-\overline{g}; h-\overline{h}\rangle = \langle g-\overline{g}; h\rangle$ since by (8.26),

$$\langle g-\overline{g}; \overline{h}\rangle = \langle g-\overline{g}\rangle\overline{h} = (\langle g\rangle - \overline{g}) = 0.$$

If the extensive variables H and X_j $(j\in J)$ are pairwise commuting then we can use (8.27) to eliminate the Kubo inner product, and by choosing g as S and X_j, respectively, we find

(9.36)–(9.38). The limit resolutions (9.39) now follow from (8.45) and the observation that $\langle (g-\overline{g})^2\rangle = \langle (g-\overline{g})g\rangle - \langle g-\overline{g}\rangle\overline{g} = \langle (g-\overline{g})g\rangle = \langle g^2\rangle - \overline{g}^2$. The limit resolution (9.40) follows similarly from

$$\begin{aligned}\overline{H}^2\,\mathrm{res}(H)^2 &= \langle H-\overline{H}; H-\overline{H}\rangle = T\langle H-\overline{H}; S-\overline{S}\rangle + \alpha\cdot\langle H-\overline{H}; X-\overline{X}\rangle\\ &= \hbar T\Big(T\frac{\partial\overline{H}}{\partial T} + \alpha\cdot\frac{\partial\overline{H}}{\partial\alpha}\Big).\end{aligned}$$

□

Note that higher order central moments can be obtained in the same way, substituting more complicated expressions for f and using the formulas for the lower order moments to evaluate the right hand side of (9.34) and (9.35).

The extensive variables scale linearly with the system size Ω of the system. Hence, the limit resolution of the extensive quantities is $O(\sqrt{\hbar/\Omega})$ in regions of the state space where the extensive variables depend smoothly on the intensive variables. Since $\hbar$ is very small, they are negligible unless the system considered is very tiny. Thus, macroscopic thermal variables can generally be obtained with fairly high precision. The only exceptions are states close to **critical points** where the extensive variables need not be differentiable, and their derivatives may therefore become huge. In particular, in the thermodynamic limit $\Omega\to\infty$, uncertainties are absent except close to a critical point, where they lead to critical opacity.

9.3.4 Corollary. *For a standard thermal system,*

$$\mathrm{res}(S) = \sqrt{\frac{\hbar T}{\overline{S}^2}\frac{\partial\overline{S}}{\partial T}},\qquad \mathrm{res}(N_j) = \sqrt{\frac{\hbar T}{\overline{N}_j^2}\frac{\partial\overline{N}_j}{\partial\mu_j}}, \tag{9.41}$$

$$\mathrm{res}(H) = \sqrt{\frac{\hbar T}{\overline{H}^2}\Big(T\frac{\partial\overline{H}}{\partial T} + P\frac{\partial\overline{H}}{\partial P} + \mu\cdot\frac{\partial\overline{H}}{\partial\mu}\Big)}. \tag{9.42}$$

Proof. Apply (9.36), (9.38) and (9.42) to a standard system. □

Note that $\mathrm{res}(V) = 0$ since we regarded V as the system size, so that it is just a number.

The above results imply an approximate **thermodynamic uncertainty relation**

$$\Delta S\Delta T \geq \hbar T \tag{9.43}$$

for entropy S and the logarithm $\log T$ of temperature, analogous to the Heisenberg uncertainty relation (8.52) for position and momentum, in which the Boltzmann constant $\hbar$ plays a role analogous to Planck's constant $\hbar$. Indeed (Gilmore [103]), (9.43) can be derived by observing that (9.41) may be interpreted approximately as $(\Delta S)^2 \geq \hbar T\frac{\partial S}{\partial T}$; together with the first order Taylor approximation $\Delta S = \frac{\partial S}{\partial T}\Delta T$, we find that $\Delta S\Delta T = (\Delta S)^2\Big(\frac{\partial S}{\partial T}\Big)^{-1} \geq \hbar T$. A similar argument gives the approximate uncertainty relation

$$\Delta N_j\Delta\mu_j \geq \hbar T. \tag{9.44}$$

9.4 The second law: Extremal principles

The extremal principles of the second law of thermodynamics assert that in a nonthermal state, some energy expression depending on one of a number of standard boundary conditions is strictly larger than that of related thermal states. The associated thermodynamic potentials can be used in place of the system function to calculate all thermal variables given half of them. Thus, like the system function, thermodynamic potentials give a complete summary of the equilibrium properties of homogeneous materials. We only discuss the **Hamilton potential**

$$U(\overline{S}, \overline{X}) := \max_{T,\alpha} \{T\overline{S} + \alpha \cdot \overline{X} \mid \Delta(T, \alpha) = 0, T > 0\}$$

and the **Helmholtz potential**

$$A(T, \overline{X}) := \max_{\alpha} \{\alpha \cdot \overline{X} \mid \Delta(T, \alpha) = 0\};$$

other potentials can be handled in a similar way.

9.4.1 Theorem. ***(Second law of thermodynamics)***
(i) In an arbitrary state,

$$\overline{H} \geq U(\overline{S}, \overline{X}),$$

with equality iff the state is a thermal state of positive temperature. The remaining thermal variables are then given by

$$T = \frac{\partial U}{\partial \overline{S}}(\overline{S}, \overline{X}), \quad \alpha = \frac{\partial U}{\partial \overline{X}}(\overline{S}, \overline{X}), \tag{9.45}$$

$$U = \overline{H} = U(\overline{S}, \overline{X}). \tag{9.46}$$

In particular, a thermal state of positive temperature is uniquely determined by the values of $\overline{S}$ and $\overline{X}$.

(ii) Let $T > 0$. Then, in an arbitrary state,

$$\overline{H} - T\overline{S} \geq A(T, \overline{X}),$$

with equality iff the state is a thermal state of temperature T. The remaining thermal variables are then given by

$$\overline{S} = -\frac{\partial A}{\partial T}(T, \overline{X}), \quad \alpha = \frac{\partial A}{\partial \overline{X}}(T, \overline{X}), \tag{9.47}$$

$$\overline{H} = T\overline{S} + \alpha \cdot \overline{X} = A(T, \overline{X}) + T\overline{S}. \tag{9.48}$$

In particular, a thermal state of positive temperature is uniquely determined by the values of T and $\overline{X}$.

Proof. This is proved in the same way as Theorem 7.4.1; thus we give no details. □

The additivity of extensive quantities is again reflected in corresponding properties of the thermodynamic potentials:

9.4.2 Theorem.
(i) The function $U(\overline{S}, \overline{X})$ is a convex function of its arguments which is positive homogeneous of degree 1, i.e., for real $\lambda, \lambda^1, \lambda^2 \geq 0$,

$$U(\lambda\overline{S}, \lambda\overline{X}) = \lambda U(\overline{S}, \overline{X}), \tag{9.49}$$

$$U(\lambda^1\overline{S}^1 + \lambda^2\overline{S}^2, \lambda^1\overline{X}^1 + \lambda^2\overline{X}^2) \leq \lambda^1 U(S^1, X^1) + \lambda^2 U(S^2, X^2). \tag{9.50}$$

(ii) The function $A(T, \overline{X})$ is a convex function of X which is positive homogeneous of degree 1, i.e., for real $\lambda, \lambda^1, \lambda^2 \geq 0$,

$$A(T, \lambda\overline{X}) = \lambda A(T, \overline{X}), \tag{9.51}$$

$$A(T, \lambda^1\overline{X}^1 + \lambda^2\overline{X}^2) \leq \lambda^1 A(T, X^1) + \lambda^2 A(T, X^2). \tag{9.52}$$

Proof. This is proved in the same way as Theorem 7.4.2; thus we give no details. □

The extremal principles imply energy dissipation properties for time-dependent states. Since the present kinematical setting does not have a proper dynamical framework, it is only possible to outline the implications without going much into details.

9.4.3 Theorem.
(i) For any time-dependent system for which S and X remain constant and which converges to a thermal state with positive temperature, the Hamilton energy $\langle H \rangle$ attains its global minimum in the limit $t \to \infty$.

(ii) For any time-dependent system maintained at fixed temperature $T > 0$, for which X remains constant and which converges to a thermal state, the Helmholtz energy $\langle H - TS \rangle$ attains its global minimum in the limit $t \to \infty$.

Proof. This follows directly from Theorem 9.4.1. □

This result is the shadow of a more general, dynamical observation (that, of course, cannot be proved from kinematic assumptions alone but would require a dynamical theory). Indeed, it is a universally valid empirical fact that in all natural time-dependent processes, energy is lost or dissipated, i.e., becomes macroscopically unavailable, unless compensated by energy provided by the environment. Details go beyond the present framework, which adopts a strictly kinematic setting.

9.5 The third law: Quantization

The third law of thermodynamics asserts that the value of the entropy is always nonnegative. But it cannot be deduced from our axioms without making a further assumption, as a simple example demonstrates.

9.5.1 Example. The algebra $\mathbb{E} = \mathbb{C}^m$ with pointwise operations is a Euclidean $*$-algebra for any integral of the form

$$\int f = \frac{1}{N} \sum_{n=1}^{N} w_n f_n \quad (w_n > 0);$$

the axioms are trivial to verify. For this integral the state defined by

$$\langle f \rangle = \frac{1}{N} \sum_{n=1}^{N} f_n,$$

is a state with entropy S given by $S_n = \hbar \log w_n$. The value of the entropy

$$\overline{S} = \frac{1}{N} \sum_{n=1}^{m} S_n = \frac{\hbar}{N} \log \prod_{n=1}^{N} w_n,$$

is negative if we choose the w_n such that $\prod w_n < 1$.

Thus, we need an additional condition which guarantees the validity of the third law. Since the third law is also violated in classical statistical mechanics, which is a particular case of the present setting, we need a condition which forbids the classical interpretation of our axioms.

We take our inspiration from a simple information theoretic model of states discussed in Section 10.6 below, which has this property. (Indeed, the third law is a necessary requirement for the interpretation of the value of the entropy as a measure of internal complexity, as discussed there.) There, the integral is a sum over the components, and, since functions were defined componentwise,

$$\int F(f) = \sum_{n \in \mathcal{N}} F(f_n). \tag{9.53}$$

We say that a quantity f is **quantized** iff (9.53) holds with a suitable **spectrum** $\{f_n \mid n \in \mathcal{N}\}$ for all functions F for which $F(f)$ is strongly integrable; in this case, the f_n are called the **levels** of f. For example, in the quantum setting all trace class linear operators are quantized quantities, since these always has a discrete spectrum.

Quantization is the additional ingredient needed to derive the third law:

9.5.2 Theorem. ***(Third law of thermodynamics)***
If the entropy S is quantized then $\overline{S} \geq 0$. Equality holds iff the entropy has a single level only ($|\mathcal{N}| = 1$).

Proof. We have

$$1 = \int e^{-S/\hbar} = \sum_{n \in \mathcal{N}} e^{-S_n/\hbar}, \tag{9.54}$$

hence

$$\overline{S} = \int S e^{-S/\hbar} = \sum_{n\in\mathcal{N}} S_n e^{-S_n/\hbar}. \tag{9.55}$$

If $\mathcal{N} = \{n\}$ then (9.54) implies $e^{-S_n/\hbar} = 0$, hence $S_n = 0$, and (9.55) gives $\overline{S} = 0$. And if $|\mathcal{N}| > 1$ then (9.54) gives $e^{-S_n/\hbar} < 1$, hence $S_n > 0$ for all $n \in \mathcal{N}$, and (9.55) implies $\overline{S} > 0$. □

In quantum chemistry, energy H, volume V, and particle numbers $N_1, \dots, N_s$ form a quantized family of pairwise commuting Hermitian variables. Indeed, the Hamiltonian H has discrete energy levels if the system is confined to a finite volume, V is a number, hence has a single level only, and N_j counts particles hence has as levels the nonnegative integers. As a consequence, the entropy $S = T^{-1}(H + PV - \mu \cdot N)$ is quantized, too, so that the third law of thermodynamics is valid. The number of levels is infinite, so that the value of the entropy is positive.

A zero value of the entropy (**absolute zero**) is therefore an idealization which cannot be realized in practice. But Theorem 9.5.2 implies in this idealized situation that entropy and hence the joint spectrum of $(H,\ V,\ N_1, \dots,\ N_S)$ can have a single level only.

This is the situation discussed in ordinary quantum mechanics (pure energy states at fixed particle numbers). It is usually associated with the limit $T \to 0$, though at absolute temperature $T = 0$, i.e., infinite coldness β, the thermal formalism fails (but for low T asymptotic expansions are possible).

To see the behavior close to this limit, we consider for simplicity a canonical ensemble with Hamiltonian H (Example 8.2.4); thus the particle number is fixed. Since S is quantized, the spectrum of H is discrete, so that there is a finite or infinite sequence $E_0 < E_1 < E_2 < \dots$ of distinct energy levels. Denoting by P_n the (rank d_n) orthogonal projector to the d_n-dimensional eigenspace with energy E_n, we have the spectral decomposition

$$\phi(H) = \sum_{n\geq 0} \phi(E_n) P_n$$

for arbitrary functions ϕ defined on the spectrum. In particular,

$$e^{-\beta H} = \sum e^{-\beta E_n} P_n.$$

The partition function is

$$Z = \operatorname{tr} e^{-\beta H} = \sum e^{-\beta E_n} \operatorname{tr} P_n. = \sum e^{-\beta E_n} d_n.$$

As a consequence,

$$e^{-S/\hbar} = Z^{-1} e^{-\beta H} = \frac{\sum e^{-\beta E_n} P_n}{\sum e^{-\beta E_n} d_n} = \frac{\sum e^{-\beta(E_n - E_0)} P_n}{\sum e^{-\beta(E_n - E_0)} d_n},$$

hence values take the form

$$\langle f \rangle = \int e^{-S/\hbar} f = \int \Big(\frac{\sum e^{-\beta(E_n - E_0)} P_n}{\sum e^{-\beta(E_n - E_0)} d_n} \Big). \tag{9.56}$$

From this representation, we see that only the energy levels E_n with

$$E_n \leq E_0 + O(\hbar T)$$

contribute to a canonical ensemble of temperature T. If the temperature T is small enough, so that $\hbar T \ll E_2 - E_0$, the exponentials $e^{-\beta(E_n - E_0)}$ with $n \geq 2$ can be neglected, and we find

$$e^{-S/\hbar} \approx \frac{P_0 + e^{-\beta(E_1-E_0)}P_1}{d_0 + e^{-\beta(E_1-E_0)}d_1} = \frac{P_0}{d_0} + \frac{d_0 P_1 - d_1 P_0}{d_0(e^{\beta(E_1-E_0)}d_0 + d_1)}. \tag{9.57}$$

Thus, the system behaves essentially as the two level system discussed in Examples 8.2.4 and 9.2.5; the **spectral gap** $E_1 - E_0$ takes the role of E. In particular, if already $\hbar T \ll E_1 - E_0$, we find that

$$e^{-S/\hbar} = d_0^{-1}P_0 + O(e^{-\beta(E_1-E_0)}) \approx d_0^{-1}P_0$$

is essentially the projector to the subspace of minimal energy, scaled to ensure trace one.

In the **nondegenerate** case, where the lowest energy eigenvalue is simple, there is a corresponding normalized eigenvector ψ, unique up to a phase, satisfying the **Schrödinger equation**

$$H\psi = E_0\psi, \quad |\psi| = 1 \quad (E_0 \text{ minimal}). \tag{9.58}$$

In this case, the projector is $P_0 = \psi\psi^*$ and has rank $d_0 = 1$. Thus

$$e^{-S/\hbar} = \psi\psi^* + O(e^{-\beta(E_1-E_0)}).$$

has almost rank one, and the value takes the form

$$\langle g \rangle = \operatorname{tr} e^{-S/\hbar} g \approx \operatorname{tr} \psi\psi^* g = \psi^* g \psi. \tag{9.59}$$

In the terminology of quantum mechanics, E_0 is the **ground state energy**, the solution ψ of (9.58) is called the **ground state**, and

$$\langle g \rangle = \psi^* g \psi \tag{9.60}$$

is the expectation of the observable g in the ground state.

For a general **state vector** ψ normalized to satify $\psi^*\psi = 1$, the formula (9.60) defines the values in the **pure state** ψ. It is easily checked that (9.60) indeed defines a state in the sense of Definition 8.2.1. These are not Gibbs states, but their idealized limiting cases.

Our derivation therefore shows that – unless the ground state is degenerate – *a canonical ensemble at sufficiently low temperature is in an almost pure state described by the quantum mechanical ground state.*

Thus, the third law directly leads to the conventional form of quantum mechanics, which can therefore be understood as the low temperature limit of thermodynamics. It also indicates when a quantum mechanical description by a pure state is appropriate, namely always when the gap between the ground state energy and the next energy level is significantly larger than the temperature (measured in units where the Boltzmann constant is set to 1). This is the typical situation in most of quantum chemistry and justifies the use of the Born-Oppenheimer approximation in the absence of level crossing; cf. Smith [256], Yarkony [298]. Moreover, it gives the correct (mixed) form of the state in case of ground state degeneracy, and the form of the correction terms when the energy gap is not large enough for the ground state approximation to be valid.

Chapter 10

Models, statistics, and measurements

In this chapter, we discuss the relation between models and reality. This topic is difficult and to some extent controversial since it touches on unresolved foundational issues about the meaning of probability and the interpretation of quantum mechanics. By necessity, the ratio between the number of words and the number of formulas is higher than in other chapters.

We discuss in more detail the relation between different thermal models constructed on the basis of the same Euclidean $*$-algebra by selecting different lists of extensive quantities.

Moreover, a discussion of the meaning of uncertainty and probability gives the abstract setting introduced in the previous chapters both a deterministic and a statistical interpretation.

The interpretation of probability, statistical mechanics, and – today intrinsically interwoven – of quantum mechanics has a long history, resulting in a huge number of publications. Informative sources for the foundations of probability in general include Fine [87] and Hacking [116]. For statistical mechanics, see Ehrenfest [78], ter Haar [266], Penrose [214], Sklar [254], Grandy [295], and Wallace [282]. For the foundations of quantum mechanics, see Stapp [258], Ballentine [21], Home & Whitaker [126], Peres & Terno [218], Schlosshauer [247] and the reprint collection by Wheeler & Zurek [287].

10.1 Description levels

There is no fully objective way of defining how quantities and states are related to reality, since the observer modeling a particular situation may describe the same object from different perspectives and at different levels of faithfulness. Different observers may choose to study different materials or different experiments, or they may study the same material or the same experiment in different levels of detail, or draw the system boundary differently. For example, one observer may regard a measuring instrument as part of the system of

interest, while for another observer it only serves as a recording device.

All this affects the choice of the system of interest and its mathematical model in a subjective manner. In particular, silently changing the definition of what constitutes the system of interest is a major reason for apparent paradoxes discussed in the literature, and it requires care to disentangle the problems involved and to arrive at a clear view.

On the other hand, once the basic choices are made that unambiguously specify the system of interest, everything else can be described objectively.

In practice, relevant quantities and corresponding states are assigned to real life situations by well-informed judgment concerning the behavior of the equipment used. The validity of the assignment is experimentally tested by comparing experimental results with the chosen mathematical model. The model defines the meaning of the concepts: the theory defines what an object is.

For example, a substance is regarded as an ideal gas if it behaves to a satisfactory degree like the mathematical model of an ideal gas with certain values of temperature, pressure and volume. Similarly, a solid is regarded as a crystal if it behaves to a satisfactory degree like the mathematical model of a crystal for suitable numerical values of the model parameters.

In general, as put by the author of one of the most influential textbooks of thermodynamics: "Operationally, a system is in an equilibrium state if its properties are consistently described by thermodynamic theory." (Callen [55, p.15]) At first sight, this sounds like a circular definition. But this is not the case since the formal meaning of "consistently described by thermodynamic theory" is already known. The operational definition simply moves it from the domain of theory to the domain of reality by defining when a system deserves the designation "is in an equilibrium state". In particular, this definition allows one to determine experimentally whether or not a system is in equilibrium.

In general, we know or assume on the basis of past experience, claims of manufacturers, etc., that certain materials or machines reliably produce states that, to a satisfactory degree for the purpose of the experiment or application, depend only on variables that are accounted for in our theory and that are, to a satisfactory degree, either fixed or controllable. The nominal state of a system can be checked and, if necessary, corrected by **calibration**, using appropriate measurements that reveal the parameters characterizing the state.

We first emphasize the flexibility of the thermal setting. While the zeroth law may look very restrictive at first sight, by choosing a large enough family of extensive quantities the entropy of an *arbitrary* Gibbs state can be approximated arbitrarily well by a linear combination of these quantities. This does not solve the selection problem but gives a useful perspective:

The zeroth law appears simply as an embodiment of **Ockham's razor** "frustra fit per plura quod potest fieri per pauciora" (Ockham [210]), freely paraphrased in modern form: that we should opt for the most economic model explaining a phenomenon – by restricting attention to the relevant extensive quantities only. At each time t, there is – except in

degenerate cases – a *single* Gibbs state, with entropy $S(t)$, say, which best describes the system under consideration at the chosen level of modeling. Taking the description by the Gibbs state as fundamental, its value is the objective, true value of the entropy, relative only to the algebra of quantities chosen to model the system. A description of the state in terms of a thermal system is therefore adequate if (and, under an observability qualification to be discussed below, only if), for all relevant times t, the entropy $S(t)$ can be adequately approximated by a linear combination of the extensive quantities available at the chosen level of description.

In the preceding chapter, we assumed a fixed selection of extensive quantities defining the thermal model.

As indicated at the end of Section 7.1, observable differences from the conclusions derived from a thermal model known to be valid on some level imply that one or more conjugate pairs of thermal variables are missing in the model. So, how should the extensive quantities be selected?

The set of extensive variables depends on the application and on the desired accuracy of the model; it must be chosen in such a way that knowing the measured values of the extensive variables determines (to the accuracy specified) the complete behavior of the thermal system. The choice of extensive variables is (to the accuracy specified) completely determined by the level of accuracy with which the thermal description should fit the system's behavior. This forces everything else: The theory must describe the freedom available to characterize a particular thermal system with this set of extensive variables, and it must describe how the numerical values of interest can be computed for each state of each thermal system.

Clearly, physics cannot be done without approximation, and the choice of a resolution is unavoidable. (To remove even this trace of subjectivity, inherent in any approximation of anything, the entropy would have to be represented without any approximation, which would require to use the algebra of quantities of the still unknown theory of everything, and to demand that the extensive quantities exhaust this algebra.) Once the (subjective) choice of the resolution of modeling is fixed, this fixes the amount of approximation tolerable in the ansatz, and hence the necessary list of extensive quantities. This is the only subjective aspect of our setting. In contrast to the information theoretic approach where the choice of extensive quantities is considered to be the subjective matter of which observables an observer happens to have knowledge of.

In general, which quantities need to be considered depends on the resolution with which the system is to be modeled – the higher the resolution, the larger the family of extensive quantities. Thus – whether we describe bulk matter, surface effects, impurities, fatigue, decay, chemical reactions, or transition states, – the thermal setting remains the same since it is a universal approximation scheme, while the number of degrees of freedom increases with increasingly detailed models.

In phenomenological thermodynamics, the relevant extensive quantities are precisely those variables that are observed to make a difference in modeling the phenomenon of interest. Table 10.1 gives typical extensive variables (S and X_j), their intensive conjugate variables

Table 10.1: Typical conjugate pairs of thermal variables and their contribution to the Euler equation. The signs are fixed by tradition. (In the gravitational term, m is the vector with components m_j, the mass of a particle of kind j, g the acceleration of gravity, and h the height.)

extensive X_j	intensive α_j	contribution $\alpha_j X_j$
entropy S	temperature T	thermal, TS
particle number N_j	chemical potential μ_j	chemical, $\mu_j N_j$
conformation tensor C	relaxation force R	conformational $\sum R_{jk} C^{jk}$
strain ε^{jk}	stress σ_{jk}	elastic, $\sum \sigma_{jk} \varepsilon^{jk}$
volume V	pressure $-P$	mechanical, $-PV$
surface A_S	surface tension γ	mechanical, γA_S
length L	tension J	mechanical, JL
displacement q	force $-F$	mechanical, $-F \cdot q$
momentum p	velocity v	kinetic, $v \cdot p$
angular momentum J	angular velocity Ω	rotational, $\Omega \cdot J$
charge Q	electric potential Φ	electrical, ΦQ
polarization P	electric field strength E	electrical, $E \cdot P$
magnetization M	magnetic field strength B	magnetical, $B \cdot M$
electromagnetic field F	electromagnetic field strength $-F^s$	electromagnetic, $-\sum F^s_{\mu\nu} F^{\mu\nu}$
mass $M = m \cdot N$	gravitational potential gh	gravitational, ghM
energy-momentum U	metric g	gravitational, $\sum g_{\mu\nu} U^{\mu\nu}$

(T and α_j), and their contribution (TS and $\alpha_j X_j$) to the Euler equation (9.4)[1]. Some of the extensive variables and their intensive conjugates are vectors or (in elasticity theory, the theory of complex fluids, and in the relativistic case) tensors; cf. Balian [20] for the electromagnetic field and Beris & Edwards [33], Öttinger [209] for complex fluids.

To analyze the relation between two different thermal description levels, we compare a coarse system and a more detailed system quantitatively, taking for simplicity the temperature constant, so that the T-dependence can be suppressed in the formulas. When the Hamiltonian H and the $\mathbf{X}_j$ are fixed, the states are completely determined by α.

[1] The Euler equation looks like an energy balance. But since S is undefined, this formal balance has no contents apart from defining the entropy S in terms of the energy and other contributions. The energy balance is rather given by the first law discussed later, and is about *changes* in energy. Conservative work contributions are exact differentials. For example, the mechanical force $F = -dV(q)/dq$ translates into the term $-F \cdot dq = dV(q)$ of the first law, corresponding to the term $-F \cdot q$ in the Euler equation. The change of the kinetic energy $E_{\text{kin}} = mv^2/2$ contribution of linear motion with velocity v and momentum $p = mv$ is $dE_{\text{kin}} = d(mv^2/2) = mv \cdot dv = v \cdot dp$, which is exactly what one gets from the $v \cdot p$ contribution in the Euler equation. Since $v \cdot p = mv^2$ is larger than the kinetic energy, this shows that motion implies a contribution to the entropy of $(E_{\text{kin}} - v \cdot p)/T = -mv^2/2T$. A similar argument applies to the angular motion of a rigid body in its rest frame, providing the term involving angular velocity and angular momentum.

The variables and quantities of the fine system are written as before, but the variables and quantities associated with the coarser system get an additional index c. That the fine system is a refinement of the coarse system means that the extensive quantities of the coarse system are $X_c = CX$, with a fixed matrix C with linearly independent rows, whose components tell how the components of X_c are built from those of X. The entropy of the coarse system is then given by

$$S_c = T^{-1}(H - \alpha_c \cdot X_c) = T^{-1}(H - \alpha_c \cdot CX) = T^{-1}(H - \alpha \cdot X),$$

where

$$\alpha = C^T \alpha_c. \tag{10.1}$$

We see that the thermal states of the coarse model are just the states of the detailed model for which the intensive parameter vector α is of the form $\alpha = C^T \alpha_c$ for some α_c. Thus the coarse state space can simply be viewed as a lower-dimensional subspace of the detailed state space. Therefore, one expects the coarse description to be adequate precisely when the detailed state is close to the coarse state space, with an accuracy determined by the desired fidelity of the coarse model. Since the relative entropy (8.42),

$$\langle S_c - S \rangle = \langle T^{-1}(H - \alpha_c \cdot CX) - T^{-1}(H - \alpha \cdot X) \rangle = \langle T^{-1}(\alpha - C^T \alpha_c) \cdot X \rangle, \tag{10.2}$$

measures the amount of information in the detailed state which cannot be explained by the coarse state, we associate to an arbitrary detailed state α the coarse state α_c determined as a function of α by minimizing (10.2). If $\alpha^* = C^T \alpha_c \approx \alpha$ then

$$S_c = T^{-1}(H - \alpha^* \cdot X) \approx T^{-1}(H - \alpha \cdot X) = S,$$

and the coarse description is adequate. If $\alpha^* \not\approx \alpha$, there is no a priori reason to trust the coarse model, and we have to investigate to which extent its predictions will significantly differ from those of the detailed model. One expects the differences to be significant; however, in practice, there are difficulties if there are limits on our ability to prepare particular detailed states. The reason is that the entropy and chemical potentials can be prepared and measured only by comparison with sufficiently known states. For ideal gases, they are inherently ambiguous because of the gauge freedom discussed in Example 7.1.4, which implies that different models of the same situation may have nontrivial differences in Hamilton energy, entropy, and chemical potential. A similar ambiguity persists in more perplexing situations:

10.1.1 Example. (The Gibbs paradox)
Suppose that we have an ideal gas of two kinds $j = 1, 2$ of particles which are experimentally indistinguishable. Suppose that in the samples available for experiments, the two kinds are mixed in significantly varying proportions $N_1 : N_2 = q_1 : q_2$ which, by assumption, have no effect on the observable properties; in particular, their values are unknown but varying. The detailed model treats them as distinct, the coarse model as identical. Reverting to the barless notation of Section 7.1, we have

$$X = \begin{pmatrix} V \\ N_1 \\ N_2 \end{pmatrix}, \quad \alpha = \begin{pmatrix} -P \\ \mu_1 \\ \mu_2 \end{pmatrix},$$

and, assuming $C = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_1 & c_2 \end{pmatrix}$ for suitable $c_1, c_2 > 0$,

$$X_c = \begin{pmatrix} V \\ N_c \end{pmatrix} = \begin{pmatrix} V \\ c_1 N_1 + c_2 N_2 \end{pmatrix}, \quad \alpha_c = \begin{pmatrix} -P \\ \mu_c \end{pmatrix}.$$

From the known proportions, we find

$$N_j = x_j N_c, \quad x_j = \frac{q_j}{c_1 q_1 + c_2 q_2}.$$

The mixture behaves like an ideal gas of a single kind, hence

$$PV = \hbar T N_c, \quad H = h_c(T) N_c, \quad \mu_c = \hbar T \log \frac{\hbar T N_c}{V \pi_c}.$$

Now $N_c = (\hbar T)^{-1} PV = \sum N_j = \sum x_j N_c$ implies that $x_1 + x_2 = 1$. Because of indistinguishability, this must hold for any choice of $q_1, q_2 \geq 0$; for the two choices $q_1 = 0$ and $q_2 = 0$, we get $c_1 = c_2 = 1$, hence $N_c = \sum N_j$, and the x_j are mole fractions. Similarly, if we use for all kinds j of substances the same normalization for fixing the gauge freedom discussed in Example 7.1.4, the relation $h_c(T) N_c = H = \sum h_j(T) N_j = \sum h_j(T) x_j N_c$ implies for varying mole fractions that $h_j(T) = h_c(T)$ for $j = 1, 2$. From this, we get $\pi_j(T) = \pi_c(T)$ for $j = 1, 2$. Thus

$$H - H_c = \sum h_j(T) N_j - h_c(T) N_c = 0,$$

$$\mu_j - \mu_c = \hbar T \log \frac{\hbar T N_j}{V \pi_j} - \hbar T \log \frac{\hbar T N_c}{V \pi_c} = \hbar T \log x_j,$$

the Gibbs energy satisfies

$$G - G_c = \sum \mu_j N_j - \mu_c N_c = \sum (\mu_j - \mu_c) N_j = \hbar T N_c \sum x_j \log x_j,$$

and the entropy satisfies

$$\begin{aligned} S - S_c &= T^{-1}(H - PV + G) - T^{-1}(H_c - PV + G_c) \\ &= T^{-1}(G - G_c) = \hbar N_c \sum x_j \log x_j. \end{aligned}$$

The latter term is called the **entropy of mixing**. Its occurence is referred to as the **Gibbs paradox** (cf. Jaynes [140], Tseng & Caticha [271], Allahverdyan & Nieuwenhuizen [10], Uffink [273, Section 5.2]). It seems to say that there are two different entropies, depending on how we choose to model the situation. For fixed mole fractions, there is no real paradox since the fine and the coarse description differ only by a choice of the unobservable gauge parameters, and only gauge invariant quantities (such as entropy differences) have a physical meaning.

If the mole fractions may vary, the fine and the coarse description differ significantly. But the difference in the descriptions is observable only if we know processes which affect the different kinds differently.

Fixed chemical potentials can be prepared only through chemical contact with substances with known chemical potentials, and the latter must be computed from observed mole

fractions. Therefore, the chemical potentials can be calibrated only if we can prepare equilibrium states at fixed mole fraction. This requires that we are able to separate to some extent particles of different kinds.

Examples are a difference in mass, which allows a mechanical separation, a difference in molecular size or shape, which allows their separation by a semipermeable membrane, a difference in spin, which allows a magnetic separation, or a difference in scattering properties of the particles, which allows a chemical or radiation-based differentiation. In each of these cases, the particles become distinguishable; the coarse description is therefore inadequate and gives a wrong description for the entropy and the chemical potentials.

Generalizing from the example, we conclude that even when both a coarse model and a more detailed model are faithful to all experimental information possible at a given description level, there is no guarantee that they agree in the values of all thermal variables of the coarse model. In the language of control theory (see, e.g., Ljung [178]), agreement is guaranteed only when all parameters of the more detailed models are observable.

On the other hand, all observable state functions of the detailed system that depend only on the coarse state have the same value within the experimental accuracy, if both models are adequate descriptions of the situation. Thus, while the values of some variables need not be experimentally determinable, *the validity of a model is an objective property.*

Therefore, preferences for one or the other of two valid models can only be based on other criteria. The criterion usually employed in this case is Ockham's razor, although there may be differences of opinion on what counts as the most economic model. In particular, a fundamental description of macroscopic matter by means of quantum mechanics is hopelessly overspecified in terms of the number of degrees of freedom needed for comparison with experiment, most of which are in principle unobservable by equipment made of ordinary matter. But it is often the most economical model in terms of description length (though extracting the relevant information from it may be difficult). Thus, different people may well make different rational choices, or employ several models simultaneously.

As soon as a discrepancy of model predictions with experiment is reliably found, the model is inadequate and must be replaced by a more detailed or altogether different model. This is indeed what happened with the textbook example of the Gibbs paradox situation, ortho and para hydrogen, cf. Bonhoeffer & Harteck [45], Farkas [85]. Hydrogen seemed at first to be a single substance, but then thermodynamic data forced a refined description. Similarly, in spin echo experiments (see, e.g., Hahn [117, 118], Rothstein [241], Ridderbos & Redhead [234]), the specially prepared system appears to be in equilibrium but, according to Callen's empirical definition quoted on 220 it is not – the surprising future behavior (for someone not knowing the special preparation) shows that some correlation variables were neglected that are needed for a correct description.

Grad [110] speaks of "the adoption of a new entropy is forced by the discovery of new information". More precisely, the adoption of a new *model* (in which the entropy has different values) is forced, since the old model is simply wrong under the new conditions and remains valid only under some restrictions.

Observability issues aside, the coarser description usually has a more limited range of applicability; with the qualification discussed in the example, it is generally restricted to those systems whose detailed intensive variable vector α is close to the subspace of vectors of the form $C^T\alpha$ reproducible in the coarse model.

Finding the right family of thermal variables is therefore a matter of discovery, not of subjective choice. This is further discussed in Section 10.2.

10.2 Local, microlocal, and quantum equilibrium

As we have seen in Section 10.1, when descriptions on several levels are justified empirically, they differ significantly only in quantities that are negligible in the more detailed models and vanish in the coarser models, or by terms that are not observable in principle. We now apply the above considerations to various levels of equilibrium descriptions.

A global equilibrium description is adequate at some resolution if and only if only the nonequilibrium forces present in the finer description are small, and a more detailed local equilibrium description will (apart from variations of the Gibbs paradox, which should be cured on the more detailed level) agree with the global equilibrium description to the accuracy within which the differences in the corresponding approximations to the entropy, as measured by the relative entropy (8.42), are negligible. Of course, if the relative entropy of a thermal state relative to the true Gibbs state is large then the thermal state cannot be regarded as a faithful description of the true state of the system, and the thermal model is inadequate.

In statistical mechanics, where the microscopic dynamics is given, the relevant extensive quantities are those whose values vary slowly enough to be macroscopically observable at a given spatial or temporal resolution (cf. Balian [18]). Which ones must be included is a difficult mathematical problem that has been solved only in simple situations (such as monatomic gases) where a weak coupling limit applies. In more general situations, the selection is currently based on phenomenological consideration, without any formal mathematical support.

In equilibrium statistical mechanics, which describes time-independent, *global* equilibrium situations, the relevant extensive quantities are the additive conserved quantities of a microscopic system and additional parameters describing order parameters that emerge from broken symmetries or various defects not present in the ideal model. **Phase equilibrium** needs, in addition, copies of the extensive variables (e.g., partial volumes) for each phase, since the phases are spatially distributed, while the intensive variables are shared by all phases. **Chemical equilibrium** also accounts for exchange of atoms through a list of permitted chemical reactions whose length is again determined by the desired resolution.

In states not corresponding to global equilibrium – usually called **non-equilibrium states**, a thermal description is still possible assuming so-called **local equilibrium**. There, the natural extensive quantities are those whose values are locally additive and slowly varying in space and time and hence, reliably observable at the scales of interest. In the statistical

mechanics of local equilibrium, the thermal variables therefore become space- and time-dependent fields (Robertson [237]). On even shorter time scales, phase space behavior becomes relevant, and the appropriate description is in terms of **microlocal equilibrium** and position- and momentum-dependent phase space densities. Finally, on the microscopic level, a linear operator description in terms of **quantum equilibrium** is needed.

The present formalism is still applicable to local, microlocal, and quantum equilibrium (though most products now become inner products in suitable function spaces), but the relevant quantities are now time-dependent and additional dynamical issues (relating states at different times) arise; these are outside the scope of the present book.

In local equilibrium, one needs a hydrodynamic description by Navier-Stokes equations and their generalizations; see, e.g., Beris & Eswards [33], Oettinger [209], Edwards et al. [77]. In the local view, one gets the interpretation of extensive variables as locally conserved (or at least slowly varying) quantities (whence additivity) and of intensive variables as parameter fields, which cause non-equilibrium currents when they are not constant, driving the system towards global equilibrium. In microlocal equilibrium, one needs a kinetic description by the Boltzmann equation and its generalizations; see, e.g., Bornath et al. [48], Calzetta & Hu [56], Müller & Ruggeri [197].

Quantum equilibrium. Fully realistic microscopic dynamics must be based on quantum mechanics. In quantum equilibrium, the dynamics is given by quantum dynamical semigroups. We outline the ideas involved, in order to emphasize some issues that are usually swept under the carpet.

Even when described at the microscopic level, thermal systems of sizes handled in a laboratory are in contact with their environment, via containing walls, emitted or absorbed radiation, etc.. We therefore embed the system of interest into a bigger, completely isolated system and assume that the quantum state of the big system is described at a fixed time by a value map that assigns to a linear operator g in the big system the value $\langle g\rangle$ and satisfies the rules (R1)–(R4) for a state. The small system is defined by a Euclidean $*$-algebra $\mathbb{E}$ of linear operators densely defined on $\widehat{\mathbb{H}}$, composed of all meaningful expressions in field operators at arguments in the region of interest; the integral is given by the trace in the big system. Since the value map restricted to $g \in \mathbb{E}$ also satisfies the rules (R1)–(R4) for a state, the big system induces on the system of interest a state. By standard theorems (see, e.g., Thirring [267]), there is a unique **density operator** $\rho \in \mathbb{E}$ such that $\langle g\rangle = \int \rho g$ for all $g \in \mathbb{E}$ with finite value. Moreover, ρ is Hermitian and positive semidefinite. If 0 is not an eigenvalue of ρ then $\langle\cdot\rangle$ is a Gibbs state with entropy $S = -\hbar \log \rho$. Note that the entropy defined in this way depends on the choice of $\mathbb{E}$, hence on the set of quantities found to be relevant. (In contrast, if the big system that includes the environment is in an approximately pure state, as is often assumed, the value of the entropy of the big system is approximately zero.)

To put quantum equilibrium into the thermal setting, we simply choose a set of extensive variables spanning the algebra $\mathbb{E}$; then S can be written in the form (9.1). (A thermal description is not possible if 0 is an eigenvalue of ρ, an exceptional situation that can be

realized experimentally only for systems with extremely few quantum levels. This happens, e.g., when the state is pure, $\rho = \psi\psi^*$.)

Of course, ψ and hence the state $\langle\cdot\rangle$ depend on time. The time evolution is now quite different from the conservative dynamics usually assumed for the big system that includs the environment. The system of interest does *not* inherit a Hamiltonian dynamics from the isolated big system; instead, the dynamics of ρ is given by an integro-differential equation with a complicated memory term, defined by the so-called projector operator formalism described in detail in Grabert [109]; for summaries, see Rau & Müller [228] and Balian [18]. In particular, one can say nothing specific about the dynamics of $\overline{S}$. (In contrast, were the reduced system governed by a Hamiltonian dynamics, ρ would evolve by means of a unitary evolution; in particular, $\overline{S} = \langle S\rangle = -\bar{k}\operatorname{tr}\rho\log\rho$ would be time-independent.) A suitable starting point for a fundamental derivation, based on quantum field theory, are provided by the so-called exact renormalization group equations (see, e.g., Polonyi & Sailer [222], Berges [32]).

In typical treatments of reduced descriptions, one assumes that the memory decays sufficiently fast; this so-called **Markov assumption** can be justified in a weak coupling limit (Davies [71], Spohn [257]), corresponding to a system of interest that is only weakly interacting with the environment. But a typical thermal system, such as a glass of water on a desk is held in place by the container. Considered as a nearly independent system, the water would behave very differently, probably diffusing into space. Thus, it is questionable whether the Markov assumption is satisfied; a detailed investigation of the situation would be highly desirable. Apparently there are only few discussions of the problem how containers modify the dynamics of a large quantum system; see, e.g., Lebowitz & Frisch [173], Blatt [36] and Ridderbos [233]. One should expect a decoherence effect (Brune et al. [53]) of the environment on the system that, for large quantum systems, is extremely strong (Zurek [301]).

However, simply assuming the Markov assumption as the condition for regarding the system of interest to be **effectively isolated** allows one to deduce for the resulting **Markov approximation** a deterministic differential equation for the density operator. The dynamics then describes a linear quantum dynamical semigroup. For all known linear quantum dynamical semigroups (cf. Davies [71]) on a Hilbert space, the dynamics takes the form of a **Lindblad equation**

$$\dot{\rho} = \frac{i}{\hbar}(\rho H - H^*\rho) + P^*\rho \tag{10.3}$$

(Lindblad [176], Gorini et al. [107]), where the **effective Hamiltonian** H is a not necessarily Hermitian operator and P^* is the dual of a completely positive map P of the form

$$P(f) = Q^* J(f) Q \quad \text{for all } f \in \mathbb{E},$$

with some linear operator Q from $\mathbb{E}$ to a second $*$-algebra $\mathbb{E}'$ and some $*$-algebra homomorphism J from $\mathbb{E}$ to $\mathbb{E}'$. (Stinespring [261], Davies [71, Theorem 2.1]). The resulting dynamics is inherently dissipative; for time $t \to \infty$, $P^*\rho$ can be shown to tend to zero, which implies under a natural nondegeneracy assumption that the limiting state is a global equilibrium state.

No matter how large we make the system, it is necessary to take account of an unobserved environment, since all our observations are done in a limited region of space, which, however, interacts with the remainder of the universe. As a consequence, the time evolution of any system of signifcant size is irreversible. In particular, the prevalence here on earth of matter in approximate equilibrium could possibly be explained by the fact that the earth is extremely old.

We now consider relations within the hierarchy of the four levels. The quantum equilibrium entropy S_{qu}, the microlocal equilibrium entropy S_{ml}, the local equilibrium entropy S_{lc}, and the global equilibrium entropy S_{gl} denote the values of the entropy in a thermal description of the corresponding equilibrium levels. The four levels have an increasingly restricted set of extensive quantities, and the relative entropy argument of Theorem 8.3.3 can be applied at each level. Therefore

$$S_{\mathrm{qu}} \leq S_{\mathrm{ml}} \leq S_{\mathrm{lc}} \leq S_{\mathrm{gl}}. \tag{10.4}$$

In general, the four entropies might have completely different values. We discussfour essentially different possibilities,

(i) $S_{\mathrm{qu}} \approx S_{\mathrm{ml}} \approx S_{\mathrm{lc}} \approx S_{\mathrm{gl}}$,

(ii) $S_{\mathrm{qu}} \approx S_{\mathrm{ml}} \approx S_{\mathrm{lc}} \ll S_{\mathrm{gl}}$,

(iii) $S_{\mathrm{qu}} \approx S_{\mathrm{ml}} \ll S_{\mathrm{lc}} \leq S_{\mathrm{gl}}$,

(iv) $S_{\mathrm{qu}} \ll S_{\mathrm{ml}} \leq S_{\mathrm{lc}} \leq S_{\mathrm{gl}}$,

with different physical interpretations. As we have seen in Section 10.1, a thermal description is valid only if the entropy in this description approximates the true entropy sufficiently well. All other entropies, when significantly different, do not correspond to a correct description of the system; their disagreement simply means failure of the coarser description to match reality. Thus which of the cases (i)–(iv) occurs decides upon which descriptions are valid. (i) says that the state is in global equilibrium, and all four descriptions are valid. (ii) that the state is in local, but not in global equilibrium, and only the three remaining descriptions are valid. (iii) says that the state is in microlocal, but not in local equilibrium, and in particular not in global equilibrium. Only the quantum and the microlocal descriptions are valid. Finally, (iv) says that the state is not even in microlocal equilibrium, and only the quantum description is valid.

Assuming that the fundamental limitations in observability are correctly treated on the quantum level, the entropy is an objective quantity, independent of the level of accuracy with which we are able to describe the system. The precise value it gets in a model depends, however, on the model used and its accuracy. The observation (by Grad [110], Balian [18], and others) that entropy may depend significantly on the description level is explained by two facts that hold for variables in models of any kind, not just for the entropy, namely
(i) that if two models disagree in their observable predictions, at most one of them can be correct, and
(ii) that if a coarse model and a refined model agree in their observable predictions, the more detailed model has unobservable details.

Since unobservable details cannot be put to an experimental test, the more detailed model in case (ii) is questionable unless dictated by fundamental considerations, such as symmetry or formal simplicity.

10.3 Statistics and probability

Recall from Section 8.4 that a quantity g is considered to be significant if its resolution $\mathrm{res}(g)$ is much smaller than one, while it is considered as noise if it is much larger than one. If g is a quantity and $\widetilde{g}$ is a good approximation of its value then $\Delta g := g - \widetilde{g}$ is noise. Sufficiently significant quantities can be treated as deterministic; the analysis of noise is the subject of statistics.

Statistics is based on the idea of obtaining information about noisy quantities of a system by repeated **sampling** from a **population**[2] of independent systems with identical preparation, but differing in noisy details not controllable by the preparation. In the present context, such systems are described by the same Euclidean $*$-algebra $\mathbb{E}_0$, the same set of quantities to be sampled, and the same state $\langle\cdot\rangle_0$.

More precisely, the systems may be regarded as subsystems of a bigger system (e.g., the laboratory) whose set of quantities is given by a big Euclidean $*$-algebra $\mathbb{E}$. To model identically prepared subsystems we consider injective homomorphisms from $\mathbb{E}_0$ into $\mathbb{E}$ mapping each reference quantity $f \in \mathbb{E}_0$ to the quantity $f_l \in \mathbb{E}$ of the lth subsystem considered to be 'identical' with f. Of course, in terms of the big system, the f_l are not really identical; they refer to quantities distinguished by position and/or time. That the subsystems are **identically prepared** is instead modelled by the assumption

$$\langle f_l \rangle = \langle f_0 \rangle \quad \text{for all } f \in \mathbb{E}_0, \tag{10.5}$$

and that they are **independent** by the assumption

$$\langle f_k g_l \rangle = \langle f_k \rangle \langle g_l \rangle \quad \text{for all } f, g \in \mathbb{E}_0 \text{ and } k \neq l. \tag{10.6}$$

The following result is fundamental for statistical considerations:

10.3.1 Theorem. ***(Weak law of large numbers)***
For a family of quantities f_l $(l = 1, \ldots, N)$ satisfying (10.5) *and* (10.6)*, the* ***mean*** *quantity*

$$\widehat{f} := \frac{1}{N} \sum_{l=1}^{N} f_l$$

(which again is a quantity) satisfies

$$\langle \widehat{f} \rangle = \langle f_0 \rangle,$$
$$\sigma(\widehat{f}) = \sigma(f_0)/\sqrt{N}, \tag{10.7}$$

[2]Physicists usually speak of an **ensemble** in place of a population; but since in connection with the microcanonical, canonical, or grand canonical ensemble we use the term ensemble synonymous with state, we prefer the statistical term population to keep the discussion unambiguous.

Proof. Writing $\mu := \langle f\rangle_0$ and $\sigma := \sigma(f_0)$, we have

$$\langle \widehat{f}\,\rangle = \frac{1}{N}(\langle f_1\rangle + \ldots + \langle f_N\rangle) = \frac{1}{N}(\mu + \ldots + \mu) = \mu$$

and

$$\langle \widehat{f}^*\widehat{f}\,\rangle = \frac{1}{N^2}\Big\langle \Big(\sum_j f_j\Big)^*\Big(\sum_k f_k\Big)\Big\rangle = N^{-2}\sum_{j,k}\langle f_j^* f_k\rangle. \tag{10.8}$$

Now

$$\langle f_j^* f_j\rangle = \langle f_j\rangle^*\langle f_j\rangle + \sigma(f_j)^2 = |\mu|^2 + \sigma^2,$$

and by (10.6) for $j \neq k$,

$$\langle f_j^* f_k + f_k^* f_j\rangle = 2\,\mathrm{Re}\langle f_j^* f_k\rangle = 2\,\mathrm{Re}\langle f_j\rangle^*\langle f_k\rangle = 2\,\mathrm{Re}\,\mu^*\mu = 2|\mu|^2.$$

In the sum in (10.8), this leads to a contribution of $|\mu|^2 + \sigma^2$ for each of the N diagonal elements, and of $2|\mu|^2$ for each of the $\binom{N}{2}$ pairs of off-diagonal elements. Therefore

$$\langle \widehat{f}^*\widehat{f}\,\rangle = N^{-2}\Big(N(|\mu|^2 + \sigma^2) + \binom{N}{2}2|\mu|^2\Big) = N^{-1}\sigma^2 + |\mu|^2,$$

so that

$$\sigma(\widehat{f}\,)^2 = \langle \widehat{f}^*\widehat{f}\,\rangle - \langle \widehat{f}\,\rangle^*\langle \widehat{f}\,\rangle = N^{-1}\sigma^2,$$

and the assertions follow. □

As a significant body of work in probability theory shows, the conditions under which $\sigma(\widehat{f}\,) \to 0$ as $N \to \infty$ can be significantly relaxed; thus in practice, it is sufficient if (10.5) and (10.6) are approximately valid.

The significance of the weak law of large numbers lies in the fact that (10.7) becomes arbitrarily small as N becomes sufficiently large. Thus the uncertainty of quantities when averaged over a large population of identically prepared systems becomes arbitrarily small while the mean value reproduces the value of each quantity. Thus quantities averaged over a large population of identically prepared systems become highly significant when their value is nonzero, even when no single quantity is significant.

This explains the success of statistical mechanics to provide an effectively deterministic description of ideal gases, where all particles may be assumed to be independent and identically prepared. In real, nonideal gases, the independence assumption is only approximately valid because of possible interactions, and in liquids, the independence is completely lost. The power of the abstract theory discussed in the preceding chapters lies in the fact that it allows to replace simple statistical reasoning based on independence by more sophisticated algebraic techniques that give answers even in extremely complex interacting cases.

The weak law of large numbers also implies that, in a context where many repeated experiments are feasible, states can be given a **frequentist** interpretation, in which $\langle g\rangle$ is the **expectation** of g, empirically defined as an average over many realizations. In this case

(and only in this case), res(g) becomes the standard deviation of g, divided by the absolute value of the expectation; therefore, it measures the relative accuracy of the individual realizations.

On the other hand, in equilibrium thermodynamics, where a tiny number of macroscopic observations on a single system completely determine its state to engineering accuracy, such a frequentist interpretation is inappropriate. Indeed, as discussed by Sklar [254], a frequentist interpretation of statistical mechanics has significant foundational problems, already in the framework of classical physics.

Thus, the present framework captures correctly the experimental practice, and determines the conditions under which deterministic and statistical reasoning are justified:

Deterministic reasoning is sufficient for all quantities whose limit resolution is below the relative accuracy desired for a given description level.

Statistical reasoning is necessary precisely when the limit resolution of certain quantities is larger than the desired relative accuracy, and these quantities are sufficiently identical and independent to ensure that the limit resolution of their mean is below this accuracy.

In this way, we delegate statistics to its role as *the art of interpreting measurements*, as in classical physics. Indeed, to have a consistent interpretation, real experiments must be designed such that they allow one to determine approximately the properties of the state under study, hence the values of all quantities of interest. The uncertainties in the experiments imply approximations, which, if treated probabilistically, need an *additional* probabilistic layer accounting for measurement errors. Expectations from this secondary layer, which involve probabilistic statements about situations that are uncertain due to neglected but in principle observable details (cf. Peres [217]), happen to have the same formal properties as the values on the primary layer, though their physical origin and meaning is completely different.

Classical probability. Apart from the traditional axiomatic foundation of probability theory by Kolmogorov [156] in terms of measure theory there is a less well-known axiomatic treatment by Whittle [288] in terms of expectations, which is essentially the commutative case of the present setting. The exposition in Whittle [288] (or, in more abstract terms, already in Gelfand & Naimark [100]) shows that, if the X_j are pairwise commuting, it is possible to define for any Gibbs state in the present sense, random variables X_j in Kolmogorov's sense such that the expectation of all sufficiently regular functions $f(X)$ defined on the joint spectrum of (X) agrees with the value of f. It follows that in the pairwise commuting case, it is always possible to construct a probability interpretation for the quantities, completely independent of any assumed microscopic reality.

The details (which the reader unfamiliar with measure theory may simply skip) are as follows. We may associate with every vector X of quantities with commuting components a time-dependent, monotone linear functional $\langle\cdot\rangle_t$ defining the **expectation**

$$\langle f(X)\rangle_t := \int \rho(t) f(X)$$

at time t of arbitrary bounded continuous functions f of X. These functions define a commutative $*$-algebra $\mathbb{E}(X)$. The **spectrum** $\operatorname{Spec} X$ of X is the set of all $*$-homomorphisms (often called **characters**) from $\mathbb{E}(X)$ to $\mathbb{C}$, and has the structure of a Hausdorff space, with the **weak-$*$ topology** obtained by calling a subset S of $\operatorname{Spec} X$ closed if, for any pointwise convergent sequence (or net) contained in S, its limit is also in S. Now a monotone linear functional turns out to be equivalent to a multivariate probability measure $d\mu_t(X)$ (on the sigma algebra of Borel subsets of the spectrum Ω of X) defined by

$$\int d\mu_t(X) f(X) := \int \rho(t) f(X) = \langle f(X) \rangle_t.$$

Conversely, classical probability theory may be discussed in terms of the Euclidean $*$-algebra of **random variables**, i.e., Borel measurable complex-valued functions on a Hausdorff space Ω where bounded continuous functions are strongly integrable and the integral is given by $\int f := \int d\mu(X) f(X)$ for some distinguished measure μ.

If – as in quantum systems – the extensive quantities do not commute, a probabilistic interpretation in the Kolmogorov sense is no longer possible. In Section 10.5, we discuss what may take its place.

10.4 Classical measurements

A measuring instrument measures properties of a system of interest. However, the measured value is read off from the instrument, and hence is primarily a property of the measuring instrument and not one of the measured system. On the other hand, properties of the system are encoded in the state of the system and its dynamics. This state and what can be deduced from it are the only objective properties of the system.

In order that a measurement on a system deserves its name there must be a quantitative relation between the state of the system and the measured values. This relation may be deterministic or stochastic, depending on what is measured.

Measurements are therefore possible only if the microscopic laws imply relations between properties of the measured system and the values read off from the measuring instrument. These relations may be either deduced from a theoretical analysis, or they may be guessed from experimental evidence. In general, the theoretical analysis leads to difficult many-particle problems that can be solved only in a stochastic approximation by idealized situations; from such idealizations one then transfers insight to make educated guesses in cases where an analysis is too difficult.

The behavior required in the following discussion for a classical or a statistical instrument guarantees **reproducibility** of measurements, a basic requirement of natural sciences, in the sense that systems prepared in the same state will behave alike when measured. Here 'alike' is interpreteted for classical instruments in the deterministic sense of 'approximately equal within the specified accuracy', and for statistical instruments in the sense of 'reproducing in the long run approximately the same probabilities and mean values'.

When measuring classical or quantum systems that are **macroscopic**, i.e., large enough to be described sufficiently well by the methods of statistical mechanics, one measures more or less accurately extensive or intensive variables of the system and one obtains essentially deterministic results. A **classical instrument** is a measuring instrument that measures such deterministic values within some known margin of accuracy. Note that this gives an operational meaning to the term *classical*, although every classical instrument is, of course, a quantum mechanical many-particle system when modelled in full detail. Whether a particular instrument behaves classically can in principle be found out by an analysis of the measurement process considered as a many-particle system, although the calculations can be done in practice only under simplifying assumptions. For some concrete models, see, e.g., Allahverdyan et al. [9]. Thus there is no split between the classical and the quantum world but a gradual change from quantum to classical as the system gets larger and the limit resolution improves.

It is interesting to discover the nature of thermodynamic observables[3]. We encountered intensive variables, which are parameters characterizing the state of the system, extensive variables, values that are functions of the intensive variables and of the parameters (if there are any) in the Hamiltonian, and limit resolutions, which, as functions of values, are also functions of the intensive variables. Thus all thermodynamic observables of practical interest are functions of the parameters defining the thermal state or the Hamiltonian of the system. Which parameters these are depends of course on the assumed model.

For an arbitrary model of an arbitrary system we perform a natural step of extrapolation, substantiated later (in Section 19.1) by the Dirac-Frenkel variational principle, and take the parameters characterizing a family of Hamiltonians and a family of states that describe the possible states of a system. as the basic variables. We call these parameters the **model parameters**; the values of the model parameters completely characterize a particular system described by the model. An **observable** of the model is then a function of these basic variables.

Thus we may say that a classical instrument is characterized by the fact that upon measurement the measurement result approximates with a certain accuracy the value of a function F of the model parameters. As customary, one writes the result of a measurement as an **uncertain number** $F_0 \pm \Delta F$ consisting of a main value F_0 and a deviation ΔF, with the meaning that the error $|F_0 - F|$ is at most a small multiple of ΔF. Because of possible systematic errors, it is generally not possible to interpret F_0 as mean value and ΔF as standard deviation. Such an interpretation is valid only if the instrument is calibrated to satisfy the implied statistical relation.

In particular, since $\langle f \rangle$ is a function of the model parameters, a measurement may yield the value $\langle f \rangle$ of a quantity f, and is then said to be a classical instrument for **measuring** f. As an important special case, all readings from a photographic image or from the scale of a measuring instrument, done by an observer, are of this nature when considered as measurements of the instrument by the observer. Indeed, what is measured by the eye is the particle density of blackened silver on a photographic plate or of iron of the tip of

[3]We use the term observable with its common-sense meaning. In quantum mechanics, the term has also a technical meaning that we do not use, denoting there a self-adjoint linear operator on a Hilbert space.

the pointer on the scale, and these are extensive variables in a continuum mechanical local equilibrium description of the instrument.

The measurement of a tiny, **microscopic** system, often consisting of only a single particle, is of a completely different nature. Now the limit resolutions do not benefit from the law of large numbers, and the relevant quantities often are no longer significant. Then the necessary quantitative relations between properties of the measured system and the values read off from the measuring instrument are only visible as stochastic correlations. In a single measurement of a microscopic system, one can only glean very little information about the state of a system; conversely, from the state of the system one can predict only probabilities for the results of a single measurement. The results of single measurements are no longer reproducably observable numbers; reproducably observable – and hence the carrier of scientific information – are only probabilities and statistical mean values.

To obtain comprehensive information about the state of a single microscopic system is therefore impossible. To collect enough information about the prepared state and hence the state of each system measured, one needs either time-resolved measurements on a single system (available, e.g., for atoms in ion traps or for electrons in quantum dots), or a population of identically prepared systems.

Extrapolating from the macroscopic case, it is natural to consider again the parameters characterizing a family of states that describe the possible states of a system as the basic numbers whose functions define observables in the present, nontechnical sense. This is now a less well-founded assumption based only on the lack of a definite boundary between the macroscopic and the microscopic regime, and an application of Ockham's razor to minimize the needed assumptions.

Measurements in the form of clicks, flashes or events (particle tracks) in scattering experiments may be described in terms of a **statistical instrument** characterized by a discrete family of possible measurement results $a_1, a_2, \ldots$ that may be real or complex numbers, vectors, or fields, and nonnegative Hermitan quantities $P_1, P_2, \ldots$ satisfying

$$P_1 + P_2 + \ldots = 1 \tag{10.9}$$

such that the instrument gives the result a_k with probability

$$p_k = \langle P_k \rangle \tag{10.10}$$

if the measured system is in the state $\langle \cdot \rangle$. The nonnegativity of the P_k implies that all probabilities are nonnegative, and (10.9) guarantees that the probabilities always add up to 1.

An instructive example is the **photoelectric effect**, the measurement of a classical free electromagnetic field by means of a photomultiplier. A detailed discussion is given in Chapter 9 of Mandel & Wolf [181]; here we only give an informal summary of their account.

Classical input to a quantum system is conventionally represented in the Hamiltonian of the quantum system by an interaction term containing the classical source as an external field or potential. In the semiclassical analysis of the photoelectric effect, the detector is modelled as a many-electron quantum system, while the incident light triggering the detector is modelled as an external electromagnetic field. The result of the analysis is that if the classical field consists of electromagnetic waves (light) with a frequency exceeding some threshold then the detector emits a random stream of photoelectrons with a rate that, for not too strong light, is proportional to the intensity of the incident light. The predictions are quantitatively correct for normal light.

The response of the detector to the light is statistical, and only the rate (a short time mean) with which the electrons are emitted bears a quantitative relation with the intensity. Thus the emitted photoelectrons form a statistical measurement of the intensity of the incident light.

The results on this analysis are somewhat surprising: The discrete nature of the electron emissions imply that a photodetector responds to classical light as if it were composed of randomly arriving photons (the explanation of the photoeffect for which Einstein received the Nobel prize), although the semiclassical model used to derive the quantitatively correct predictions does not involve photons at all!

This shows the importance of differentiating between prepared states of the system (here of classical light) and measured events in the instrument (here the amplified emitted electrons). The measurement results are primarily a property of the instrument, and their interpretation as a property of the system needs theoretical analysis to be conclusive.

10.5 Quantum probability

Although quantum mechanics generally counts as an intrinsically statistical theory, it is important to realize that it not only makes assertions about probabilities but also makes many deterministic predictions verifiable by experiment.

These deterministic predictions fall into two classes:

(i) Predictions of numerical values believed to have a precise value in nature:

- The most impressive proof of the correctness of quantum field theory in microphysics is the **magnetic moment** of the electron, predicted by quantum electrodynamics (QED) to the phenomenal accuracy of 12 significant digit agreement with the experimental value. It is a universal constant, determined solely by the two parameters in QED, the electron mass and the fine structure constant.
- QED also predicts correctly emission and absorption spectra of atoms and molecules, both the spectral positions and the corresponding line widths.
- Quantum hadrodynamics allows the prediction of the masses of all isotopes of the chemical elements in terms of models with only a limited number of parameters.

(ii) Predictions of qualitative properties, or of numerical values believed to be not exactly determined but which are accurate with a high, computable limit resolution.

- QED predicts correctly the color of gold, the liquidity of mercury at room temperature, and the hardness of diamond.
- Quantum mechanics enables the computation of thermodynamic state equations for a huge number of materials. Equations of states are used in engineering in a deterministic manner.
- From quantum mechanics one may also compute transport coefficients for deterministic kinetic equations used in a variety of applications.

Thus quantum mechanics makes both deterministic and stochastic assertions, depending on which system it is applied to and on the state or the variables to be determined. Statistical mechanics, as discussed in Chapters 8 and 9, is mainly concerned with deterministic prediction of class (ii) in the above classification.

Interestingly, our definition of classical instruments also covers joint position-momentum measurements of **coherent states**, the quantum states discussed in Section 20.7. They are parameterized by position and momentum, and describe single quantum particles with essentially classical trajectories, such as they can be seen as particle tracks on photographic plates or in bubble chambers. The deterministic nature of the recorded tracks is due to the interaction of such a particle with the many-particle system formed by the recording device.

Predictions of class (i) are partly related to spectral properties of the Hamiltonian of a quantum system, which we shall discuss in Chapter 23, and partly to properties deduced from form factors, which are deterministic byproducts of scattering calculations. In both cases, classical measurements account adequately for the experimental record.

Particle scattering itself, however, is a typical stochastic phenomenon. The same holds for radioactive decay, when modelled on the level of individual particles; it needs a stochastic description as a branching process, similar to classical birth and death processes in biological population dynamics. In the remainder of this section, we consider the fundamental aspects of this stochastic part of quantum mechanics.

A **statistical instrument** in the quantum case is mathematically equivalent to what is called in the literature a **positive operator-valued measure**, short **POVM**, defined as a family $P_1, P_2, \ldots$ of Hermitian, positive semidefinite operators satsifying (10.9) (or a continuous generalization of this). They originated around 1975 in work by **Helstrom** [125] on quantum detection and estimation theory and are discussed in some detail in Peres [217]. They describe the most general quantum measurement of interest in quantum information theory. Which operators P_k correctly describe a statistical instrument can in principle be found out by suitable **calibration measurements**. Indeed, if we feed the instrument with enough systems prepared in known states $\langle\cdot\rangle_j$, we can measure approximate probabilities $p_{jk} \approx \langle P_k\rangle_j$. By choosing the states diverse enough, one may approximately

reconstruct P_k from this information by a process called **quantum tomography**. In quantum information theory, the Hilbert spaces are finite-dimensional, hence the quantities form some algebra $\mathbb{E} = \mathbb{C}^{N\times N}$; then N^2 values $\langle P_k\rangle_j$ for linearly independent states suffice for this reconstruction. The optimal reconstruction using a minimal number of individual measurements is the subject of **quantum estimation theory**, still an active frontier of research.

Before 1975, quantum measurements used to be described in terms of **ideal** statistical measurements, the special case of POVMs where the P_k form a family of **orthogonal projectors**, i.e., linear operators satisfying

$$P_k^2 = P_k = P_k^*, \quad P_jP_k = 0 \quad \text{for } j \neq k,$$

on the eigenspaces of a self-adjoint operator A (or the components of a vector A of commuting, self-adjoint operators) with discrete spectrum given by $a_1, a_2, \ldots$. In this case, the statistical instrument is said to perform an **ideal measurement** of A, and the rule (10.10) defining the probabilities is called **Born's rule**. The rule is named after Max Born [46], who derived it in 1926 in the special case of pure states (defined in (9.60)) and was rewarded in 1954 with the Nobel prize for this at that time crucial insight into the nature of quantum mechanics.

Ideal measurements of A have quite strong properties since under the stated assumptions, the instrument-based statistical average

$$\overline{f(A)} = p_1 f(a_1) + p_2 f(a_2) + \ldots$$

agrees for all functions f defined on the spectrum of A with the model-based value $\langle f(A)\rangle$. On the other hand, these strong properties are bought at the price of idealization, since they result in effects incompatible with real measurements. For example, according to Born's rule, the ideal measurement of the energy of a system whose Hamiltonian H is discrete always yields an exact eigenvalue of H, the only statistical component is the question which of the eigenvalues is obtained. This is impossible in a real measurement; the precise measurement of the Lamb shift, a difference of eigenvalues of the Hamiltonian of the hydrogen atom, was even worth a Nobel prize (1955 for Willis Lamb).

In general, the correspondence between values and eigenvalues is only approximate, and the quality of the approximation improves with improved resolution. The correspondence is perfect only at resolution zero, i.e., for completely sharp measurements. To discuss this in detail, we need some results from functional analysis. The **spectrum** $\operatorname{Spec} f$ of a linear operator on a Euclidean space $\mathbb{H}$ is the set of all $\lambda \in \mathbb{C}$ for which no linear operator $R(\lambda)$ from the completion $\overline{\mathbb{H}}$ of $\mathbb{H}$ to $\mathbb{H}$ exists such that $(\lambda - f)R(\lambda)$ is the identity. $\operatorname{Spec} f$ is always a closed set. A linear operator $f \in \operatorname{Lin}\mathbb{H}$ is called **essentially self-adjoint** if it is Hermitian and its spectrum is real (i.e., a subset of $\mathbb{R}$). For N-level systems, where $\mathbb{H}$ is finite-dimensional, the spectrum coincides with the set of eigenvalues, and every Hermitian operator is essentially self-adjoint. In infinite dimensions, The spectrum contains the eigenvalues, but not every number in the spectrum must be an eigenvalue; and whether a Hermitian operator is essentially self-adjoint is a question of correct boundary conditions.

10.5.1 Theorem. *Let f be essentially self-adjoint, with value $\overline{f} := \langle f \rangle$ and standard deviation $\sigma(f)$ in a given state. Then the spectrum of f contains some real number λ with*

$$|\lambda - \overline{f}| \leq \sigma(f). \tag{10.11}$$

Moreover, if $\overline{f} \neq 0$ then the spectrum of f contains some real number λ with

$$\frac{\lambda - \overline{f}|}{|\overline{f}|} \leq \operatorname{res}(f). \tag{10.12}$$

Proof. The linear operator $g = (f - \overline{f})^2 - \sigma(f)^2$ is a quadratic function of f, hence its spectrum consists of all $\lambda' := (\lambda - \overline{f})^2 - \sigma(f)^2$ with $\lambda \in \operatorname{Spec} f$; in particular, it is real. Put $\lambda_0 := \inf \operatorname{Spec} g > 0$. Then $g - \lambda_0$ is a Hermitian operator with a real, nonnegative spectrum, hence positive semidefinite. (In infinite dimensions, this requires the use of the spectral theorem.) Thus $g - \varepsilon \geq 0$ and $0 \leq \langle g - \lambda_0 \rangle = \langle (f - \overline{f})^2 \rangle - \sigma(f)^2 - \lambda_0 = -\lambda_0$. Therefore $\lambda_0 \leq 0$. Since $\operatorname{Spec} g$ is closed, λ_0 is in the spectrum, hence has the form $(\lambda - \overline{f})^2 - \sigma(f)^2$ with $\lambda \in \operatorname{Spec} f$. This λ satisfies (10.11), and, if $\overline{f} \neq 0$, also (10.12). □

In particular, if one can make a sharp measurement (with $\sigma(f) = 0$) then the value $\langle f \rangle$ belongs to the spectrum. In practice, this is the case only for quantities f whose spectrum (set of sharp values) consists of small integers.

Binary tests. There is, however, an important special case of Born's rule that frequently applies essentially exactly. An **ideal binary statistical measurement**, e.g., the click of a detector, is described by a single orthogonal projector P; the POVM is then given by $P_1 = P$ for the measurement result $a_1 = 1$ (click) and by $P_2 = 1 - P$ for the measurement result $a_2 = 0$ (no click). In particular, a **test for a state** φ with $\varphi^* \varphi = 1$ is an ideal binary statistical measurement with orthogonal projector $P = \varphi\varphi^*$; the reader should check that indeed $P^2 = P = P^*$. By the above, such a test turns out positive with probability $p = \langle \varphi\varphi^* \rangle$. In particular, if the system is in a pure state ψ then (9.60) implies that

$$p = \langle \varphi\varphi^* \rangle = \psi^* \varphi\varphi^* \psi = |\varphi^* \psi|^2.$$

This is the well-known **squared probability amplitude** formula, the original form of Born's rule. As a consequence, the test for φ always turns out positively if the measured system is in the pure state φ. However, it also turns out positively with a positive probability if the measured system is in a pure state different from φ, as long as it is not orthogonal to it.

By a suitable sequence of binary tests, it is possible in principle to determine with arbitrary accuracy the state in which a stationary source of particles prepares the particles. Indeed, this can be done again with quantum tomography. In case of N-level systems represented by $\mathbb{E} = \mathbb{C}^{N \times N}$, a general state is characterized by its **density matrix** ρ, a complex Hermitian $N \times N$-matrix with trace one, together with the trace formula

$$\langle f \rangle = \operatorname{tr} \rho f.$$

This implies that a set of $N^2 - 1$ tests for specific states, repeated often enough, suffices for the state determination. Indeed, it is easy to see that repeated tests for the states e^j, the unit vectors with just one entry one and other entries zero, tests the diagonal elements of the density matrix, and since the trace is one, one of these diagonal elements can be computed from the knowledge of all others. Tests for $e^j + e^k$ and $e^j + ie^k$ for all $j < k$ then allow the determination of the (j, k) and (k, j) entries. Thus frequent repetition of a total of $N - 1 + 2\binom{N}{2} = N^2 - 1$ particular tests determines the full state. The optimal reconstruction to a given accuracy, using a minimal number of individual measurements, is again a nontrivial problem of quantum estimation theory.

10.6 Entropy and information theory

The concept of entropy also plays an important role in **information theory**. To connect the information theoretical notion of entropy with the present setting, we present in this section an informal example of a simple stochastic model in which the entropy has a natural information theoretical interpretation. We then discuss what this may teach us about a non-stochastic macroscopic view of the situation.

We assume that we have a simple stationary device that, in regular intervals, delivers a reading n from a countable set $\mathcal{N}$ of possible readings. For example, the device might count the number of events of a certain kind in fixed periods of time; then $\mathcal{N} = \{0, 1, 2, \ldots\}$.

We suppose that, by observing the device in action for some time, we are led to some conjecture about the (expected) relative frequencies p_n of readings $n \in \mathcal{N}$; since the device is stationary, these relative frequencies are independent of time. If $\mathcal{N}$ is finite and not too large, we might take averages and wait until these stabilize to a satisfactory degree; if $\mathcal{N}$ is large or infinite, most $n \in \mathcal{N}$ will not have been observed, and our conjecture must depend on educated guesses. (The appropriateness of the conjecture, the relation to the knowledge of the guesser, and how to improve a conjecture when new information arrives are the subject of **Bayesian statistics**; cf. Section 10.7.)

Clearly, in order to have a consistent interpretation of the p_n as relative frequencies, we need to assume that *each* reading is possible:

$$p_n > 0 \text{ for all } n \in \mathcal{N}, \tag{10.13}$$

and *some* reading occurs with certainty:

$$\sum_{n \in \mathcal{N}} p_n = 1. \tag{10.14}$$

For reasons of economy, we shall not allow $p_n = 0$ in (10.13), which would correspond to readings that are either impossible, or occur too rarely to have a scientific meaning. Clearly, this is no loss of generality.

Knowing relative frequencies only means that (when $\mathcal{N} > 1$) we only have incomplete information about future readings of the device. We want to calculate the information

deficit by counting the expected number of questions needed to identify a particular reading unknown to us, but known to someone else who may answer our questions with yes or no.

Consider arbitrary strategies s for asking questions, and denote by s_n the number of questions needed to determine the reading n with strategy s. Since there are two possible answers for each question, we can distinguish with q questions at most 2^q different cases. However, since reading n is assumed to be determined after s_n questions, the answers to the later questions do not matter, and reading n is obtained in 2^{q-s_n} of the 2^q cases when $s_n \le q$. Thus, no matter which strategy is used,

$$\sum_{s_n \le q} 2^{q-s_n} \le 2^q.$$

If we divide by 2^q and then make q arbitrarily large we find that

$$\sum_{n \in \mathcal{N}} 2^{-s_n} \le 1. \tag{10.15}$$

Since we do not know in advance the reading, we cannot determine the precise number of questions needed in a particular unknown case. However, knowledge of the relative frequencies allows us to compute the average number of questions needed, namely

$$\overline{s} = \sum_{n \in \mathcal{N}} p_n s_n. \tag{10.16}$$

To simplify notation, we introduce the abbreviation

$$\textstyle\int f := \sum_{n \in \mathcal{N}} f_n \tag{10.17}$$

for every quantity f indexed by the elements from $\mathcal{N}$, and we use the convention that inequalities, operations and functions of such quantities are understood componentwise. Then we can rewrite (10.13)–(10.16) as

$$p > 0, \quad \textstyle\int p = 1 \ , \tag{10.18}$$

$$\overline{s} = \textstyle\int ps, \quad \int 2^{-s} \le 1 \ , \tag{10.19}$$

and

$$\overline{f} = \langle f \rangle := \textstyle\int pf \tag{10.20}$$

is the average of an arbitrary quantity f indexed by $\mathcal{N}$.

It is not difficult to construct a strategy s realizing given integral values s_n ($n \in \mathcal{N}$) whenever (10.15) holds. We now idealize the situation a little by allowing the s_n to be arbitrary nonnegative real numbers instead of integers only. This is justified when the size of $\mathcal{N}$ is large or infinite since then most s_n will be large numbers that can be approximated by integers with a tiny relative error.

Thus we redefine a **strategy** to be a quantity $s \ge 0$ satisfying $\int 2^{-s} \le 1$. We now ask for a strategy s (in the new, generalized sense) that makes the number $\overline{s}$ as small as possible.

10.6.1 Theorem. *The* ***entropy*** S, *defined as the quantity*

$$S := -\hbar \log p, \quad \text{where } \hbar = \frac{1}{\log 2}, \tag{10.21}$$

satisfies $\overline{S} \le \overline{s}$, *with equality if and only if* $s = S$. *(One also needs* $\int 2^{-s} = 1$, *but this holds for* $s = S$.*)*

Proof. (10.21) implies $\log p = -S \log 2$, hence $p = 2^{-S}$. Therefore

$$2^{-s} = p2^{S-s} = pe^{(S-s)\log 2} \ge p(1 + (S-s)\log 2),$$

with equality iff $S = s$. Thus

$$p(S-s) \le \frac{1}{\log 2}(2^{-s} - p) = \hbar(2^{-s} - p)$$

and

$$\begin{aligned} \overline{S} - \overline{s} &= \textstyle\int p(S-s) \le \int \hbar(2^{-s} - p) \\ &= \hbar \textstyle\int 2^{-s} - \hbar \int p \le \hbar - \hbar = 0. \end{aligned}$$

Hence $\overline{s} \ge \overline{S}$, and equality holds iff $s = S$. □

Since (10.21) implies the relation

$$p = e^{-S/\hbar},$$

we have $\langle f \rangle = \int pf = \int e^{-S/\hbar} f$. Thus, the expectation mapping is a Gibbs state with entropy S, explaining the name. Note that $s = S$ defines an admissible strategy since

$$\sum_{n \in \mathcal{N}} 2^{-S_n} = \int 2^{-S} = \int p = 1,$$

hence $2^{-S_n} \le 1$, $S_n \ge 0$ for all $n \in \mathcal{N}$. Thus, the entropy S is **the unique optimal decision strategy.** The **expected entropy**, i.e., the mean number

$$\overline{S} = \langle S \rangle = \int pS = -\hbar \int p \log p \tag{10.22}$$

of questions needed in an optimal decision strategy, is nonnegative,

$$\overline{S} \ge 0. \tag{10.23}$$

$\overline{S}$ measures the **information deficit** of the device with respect to our conjecture about relative frequencies. Traditionally, the expected entropy is simply called the *entropy*, while we reserve this word for the random variable (10.21). Also commonly used is the name *information* for $\overline{S}$, which invites linguistic paradoxes since ordinary language associates with information a connotation of relevance or quality that is absent here. The classical book on information theory by Brillouin [51] emphasizes this very carefully, by distinguishing absolute information from its human value or meaning. Katz [147] uses the phrase *missing information*.

The information deficit says nothing at all about the quality of the information contained in the summary p of our past observations. An inappropriate p can have arbitrarily small information deficit and still give a false account of reality. For example, if for some small $\varepsilon > 0$,

$$p_n = \varepsilon^{n-1}(1-\varepsilon) \quad \text{for } n = 1, 2, \ldots, \tag{10.24}$$

expressing that the reading is expected to be nearly always 1 ($p_1 = 1 - \varepsilon$) and hardly ever large, then

$$\overline{S} = \hbar\Big(\log(1-\varepsilon) + \frac{\varepsilon}{1-\varepsilon}\log\varepsilon\Big) \to 0 \text{ as } \varepsilon \to 0.$$

Thus the information deficit can be made very small by the choice (10.24) with small ε, independent of whether this choice corresponds to the known facts. The real information value of p depends instead on the care with which the past observations were interpreted, which is a matter of data analysis and not of our model of the device. If the data analysis is done poorly, the resulting expectations will simply not be matched by reality. This shows that the entropy reflects objective properties of the stochastic process, and – contrary to claims in the literature – has nothing to do with our knowledge of the system, a subjective, ill-defined notion.

Relations to thermodynamics. Now suppose that the above setting happens at a very fast, unobservable time scale, so that we can actually observe only short time averages (10.20) of quantities of interest. Then $\overline{f} = \langle f \rangle$ simply has the interpretation of the time-independent observed value of the quantity f. The information deficit simply becomes the observed value of the entropy S. Since the information deficit counts the number of optimal decisions needed to completely specify a (microscopic) situation of which we know only (macroscopic) observed values, the observed value of the entropy quantifies the **intrinsic** (microscopic) **complexity** present in the system.

However, the unobservable high frequency fluctuations of the device do not completely disappear from the picture. They show up in the fact that generally $\overline{g^2} \neq \overline{g}^2$, leading to a nonzero limit resolution (8.45) of Hermitian quantities. This is precisely the situation characteristic of the traditional treatment of thermodynamics within classical equilibrium statistical mechanics, if we assume that the system is **ergodic**, i.e., that population averages equal time averages. Then, all observed values are time-independent, described by equilibrium thermal variables. But the underlying high-frequency motions of the atoms making up a macroscopic substance are revealed by nonzero limit resolutions. However, the assumption that all systems for which thermodynamics works are ergodic is problematic; see, e.g., the discussion in Sklar [254].

Note that even a deterministic but chaotic high frequency dynamics, viewed at longer time scales, looks stochastic, and exactly the same remarks about the unobservable complexity and the observable consequences of fluctuations apply. Even if fluctuations are observable directly, these observations are intrinsically limited by the necessary crudity of any actual measurement protocol. For the best possible measurements (and only for these), the resolution of f in the experiment is given by the limit resolution $\operatorname{res}(f)$, the size of the unavoidable fluctuations.

Due to the quantum structure of high frequency phenomena on an atomic or subatomic scale, it seems problematic to interpret thermodynamic limit resolutions in terms of a simple short time average of some underlying microscopic reality. Thus an information theoretic interpretation of the physical entropy seems questionable.

10.7 Subjective probability

The formalism of statistical mechanics is closely related to that used in statistics for random phenomena expressible in terms of exponential families; cf. Remark 9.1.2(viii). Exponential families play an important role in Bayesian statistics. Therefore a Bayesian, subjective probability interpretation to statistical mechanics is possible in terms of the knowledge of an observer, using an information theoretic approach. See, e.g., Balian [19] for a recent exposition in terms of physics, and Barndorff-Nielsen [25, 26] for a formal mathematical treatment. In such a treatment, the present integral plays the role of a **noninformative prior**, i.e., of the state considered to be least informative. This noninformative prior is often improper, i.e., not a probability distribution, since $\int 1$ need not be defined.

Motivated by the subjective, information theoretic approach to probability, Jaynes [137, 138] used the maximum entropy principle to derive the thermodynamic formalism. The **maximum entropy principle** asserts that one should model a system with the statistical distribution that maximizes the expected entropy subject to the known information about certain expectation values. This principle is sometimes considered as a rational, unprejudiced way of accounting for available information in incompletely known statistical models. Based on Theorem 8.3.3, it is not difficult to show that when the known information is given by the expectations of the quantities $X_1, \ldots, X_n$, the optimal state in the sense of the maximum entropy principle is a Gibbs state whose entropy is a linear combination of 1 and the X_k.

However, the maximum entropy principle is an unreliable general purpose tool, and gives an appropriate distribution only under quite specific circumstances.

10.7.1 Example. If we have information in the form of a large but finite sample of realizations $x(\omega_k)$ of a random variable x in N independent experiments ω_k $(k = 1, \ldots, n)$, we can obtain approximate information about all moments $\langle x^n \rangle$ $\langle x^n \rangle \approx N^{-1} \sum x(\omega_k)^n / N$ $(n = 0, 1, 2, \ldots)$ by taking the appropriate sample means,

$$\langle x^n \rangle \approx \sum w_k x(\omega_k)^n / \sum w_k \quad (n = 0, 1, 2, \ldots),$$

where the w_k are appropriate positive weights (typically chosen such that the experimental errors in $w_k x(\omega_k)$ is approximately constant. It is not difficult to see that the maximum entropy principle would infer that the distribution of x is discrete, namely that of the sample distribution.

If we take as uninformative prior for a real-valued random variable x the Lebesgue measure, $\int f(x) := \int f(x) dx$, and only know that the mean of x is 1, say, the maximum entropy

principle does not produce a sensible probability distribution. If we add the knowledge of the second moment $\langle x^2 \rangle = 1$, say, we get a Gaussian distribution with mean 1 and standard deviation $1/\sqrt{2}$. Adding the further knowledge of $\langle x^3 \rangle$, the maximum entropy principle fails again to produce a sensible distribution. If, on the other hand, after knowing that $\langle x \rangle = 1$ we learn that the random variable is in fact nonnegative and integer-valued, this cannot be accounted for by the principle, and the probability of obtaining a negative value remains large. But if we take as prior the discrete measure on nonnegative integers defined by $\int f(x) := \sum_{x=0}^{\infty} f(x)/x!$, the supposedly noninformative prior has become much more informative, the knowledge of the mean produces via the maximum entropy principle a Poisson distribution.

If we know that a random variable x is nonnegative and has $\langle x^2 \rangle = 1$; the Lebesgue measure on $\mathbb{R}_+$ as noninformative prior gives for x a distribution with density $\sqrt{2/\pi} e^{-x^2/2}$. But we can consider instead our knowledge about $y = x^2$, which is nonnegative and has $\langle y \rangle = 1$; the same noninformative prior now gives for y a distribution with density e^{-y}. The distribution of $x = \sqrt{y}$ resulting from this has density $2xe^{-x^2/2}$. Thus the result depends on whether we regard x or y as the relevant variable.

We see that the choice of expectations to be used as constraints reflects prior assumptions about which expectations are likely to be relevant. Moreover, the prior, far from being uninformative, reflects the prejudice assumed in the complete absence of knowledge. The prior that must be assumed to describe the state of complete ignorance significantly affects the results of the maximum entropy principle, and hence makes the application of the principle ambiguous.

The application of the maximum entropy principle becomes reliable only if the information is available in form of the expectation values of a sufficient statistics of the true model; see, e.g., Barndorff-Nielsen [25]. Which statistical model may be considered sufficient depends on the true situation and is difficult to assess in advance.

In particular, a Bayesian interpretation of statistical mechanics in the manner of Jaynes is appropriate if and only if

- correct, complete and sufficiently accurate information about the expectation of all relevant quantities is assumed to be known, and
- the noninformative prior is fixed by the constructions of Example 8.1.8, namely as the correctly weighted Liouville measure in classical physics and as the microcanonical ensemble (the trace) in quantum physics.

Only this guarantees that the knowledge assumed and hence the results obtained are completely impersonal and objective, as required for scientfic results, and agree with standard thermodynamics, as required for agreement with nature. However, this kind of knowledge is clearly completely hypothetical and has nothing to do with the real, partial and imprecise knowledge of real observers.

Part III

Lie algebras and Poisson algebras

Chapter 11

Lie algebras

Part III introduces the basics about Lie algebras and Lie groups, with an emphasis on the concepts most relevant to the conceptual side of physics.

This chapter introduces Lie algebras together with the slightly richer structure of a Lie $*$-algebra usually encountered in the mechanical applications. We introduce tools for verifying the Jacobi identity, and establish the latter both for the Poisson bracket of a classical harmonic oscillator and, for quantum systems, for the commutator of linear operators.

Further Lie algebras arise as algebras of matrices closed under commutation, as algebras of derivations in associative algebras, as centralizers or quotient algebras, and by complexification. An overview over semisimple Lie algebras and their classification concludes the chapter.

In finite dimensions, the relation is almost one-to-one, the "almost" being due to the fact that the so-called universal covering group of a finite-dimensional Lie algebra (defined in Section 13.4) may have a nontrivial discrete normal subgroup.

Many finite-dimensional Lie groups arise as groups of square invertible matrices, and we discuss the most important families, in particular the unitary and the orthogonal groups. We introduce group representations, which relate groups of matrices (or linear operators) to abstract Lie groups, and will turn out to be most important for understanding the spectrum of quantum systems.

Of particular importance for systems of oscillators are the Heisenberg groups, the universal covering groups of the Heisenberg algebras. Their product law is given by the famous Weyl relations, which are an exactly representable case of the Baker–Campbell–Hausdorff formula valid for many other Lie groups, in particular for arbitrary finite-dimensional ones. We also discuss the Poincaré group. This is the symmetry group of space-time, and forms the basis for relativity theory.

11.1 Basic definitions

We start with the definition of a Lie algebra over a field $\mathbb{K}$, usually implicitly given by the context. In our course, $\mathbb{K}$ is either the field $\mathbb{C}$ of complex numbers, occasionally the field $\mathbb{R}$ of real numbers. Lie algebras over other fields, such as the rationals $\mathbb{Q}$ or finite fields $\mathbb{Z}_p$ for p prime, also have interesting applications in mathematics, physics and engineering, but these are outside the scope of this book. To denote the Lie product, we use the symbol $\angle$ introduced at the end of Section 1.3. (This replaces other, bracket-based notations common in the literature.)

11.1.1 Definition.
(i) A **Lie product** on a vector space $\mathbb{L}$ over $\mathbb{K}$ is a bilinear operation on $\mathbb{L}$ satisfying

(L1) $f\angle f = 0$,

(L2) $f\angle(g\angle h) + g\angle(h\angle f) + h\angle(f\angle g) = 0$ for all $f, g, h \in \mathbb{L}$.

Equation (L2) is called the **Jacobi identity**.

(ii) For subsets A, B of $\mathbb{L}$, we write

$$A\angle B := \{f\angle g \mid f \in A, g \in B\},$$

and for $f, g \in \mathbb{L}$,

$$A\angle g := A\angle\{g\}, \quad f\angle B := \{f\}\angle B.$$

(iii) A **Lie algebra** over $\mathbb{K}$ is a vector space $\mathbb{L}$ over $\mathbb{K}$ with a distinguished Lie product. Elements $f \in \mathbb{L}$ with $f\angle\mathbb{L} = 0$ are called **(Lie) central**; the set $Z(\mathbb{L})$ of all these elements is called the **center** of $\mathbb{L}$. A **real (complex)** Lie algebra is a Lie algebra over $\mathbb{K} = \mathbb{R}$ (resp. $\mathbb{K} = \mathbb{C}$). Unless confusion is possible, we use the same symbol $\angle$ for the Lie product in different Lie algebras.

Clearly, if $f\angle g$ defines a Lie product of f and g, so does $f\angle_\iota g := \iota(f\angle g)$ for all $\iota \in \mathbb{K}$. Thus the same vector space may be a Lie algebra in different ways.

In physics, finite-dimensional Lie algebras are often defined in terms of basis elements X_k called **generators** and **structure constants** c_{jkl}, such that

$$X_j\angle X_k = \sum_l c_{jkl} X_l\,. \tag{11.1}$$

By taking linear combinations and using the bilinearity of the Lie product, the structure constants determine the Lie product completely. Conversely, since the generators form a basis, the structure constants are determined uniquely by the basis. They depend, however, on the basis chosen. Frequently, there are distinguished bases with a physical interpretation in which the structure constants are particularly simple, and most of them vanish. If a basis and the structure constants are given, many Lie algebra computations can be done automatically; important software packages include LIE (van Leeuwen et al. [278]) and LTP (Torres-Torriti [269]). In this book, we usually prefer a basis-free approach,

resorting to basis-dependent formulas only to make connections with traditional physics notation.

As a consequence of (L1) (and in fact equivalent to it), we have the following antisymmetry property:

$$f\angle g = -g\angle f\,.$$

This follows from observing that $f\angle 0 = 0\angle f = 0$ and

$$\begin{aligned} 0 &= (f+g)\angle(f+g) = f\angle f + f\angle g + g\angle f + g\angle g \\ &= f\angle g + g\angle f\,. \end{aligned}$$

Using the antisymmetry property of the Lie product one can write the Jacobi identity in two other important forms, each equivalent with the Jacobi identity:

$$f\angle(g\angle h) = (f\angle g)\angle h + g\angle(f\angle h)\,, \tag{11.2}$$

$$(f\angle g)\angle h = (f\angle h)\angle g + f\angle(g\angle h)\,. \tag{11.3}$$

These formulas say that one can apply the Lie product to a compound expression in a manner familiar from the product rule for differentiation.

An important but somewhat trivial class of Lie algebras are the **abelian** Lie algebras, where $f\angle g = 0$ for all $f, g \in \mathbb{L}$. It is trivial to check that (L1) and (L2) are satisfied. Clearly, every vector space can be turned into an abelian Lie algebra by defining $f\angle g = 0$ for all vectors f and g. In particular, the field $\mathbb{K}$ itself and the center of any Lie algebra are abelian Lie algebras.

A subspace $\mathbb{L}'$ of a Lie algebra $\mathbb{L}$ is a **Lie subalgebra** if it is closed under the Lie product, i.e., if $f\angle g \in \mathbb{L}'$ for all $f, g \in \mathbb{L}'$. In this case, the restriction of the Lie product $\angle$ of $\mathbb{L}$ to $\mathbb{L}'$ turns $\mathbb{L}'$ into a Lie algebra. That is, a Lie subalgebra is a subspace that is a Lie algebra with the same Lie product. (For example, the subspace $\mathbb{K}f$ spanned by an arbitrary element f of a Lie algebra is an abelian Lie subalgebra.) A Lie subalgebra is **nontrivial** if it is not the whole Lie algebra and contains a nonzero element.

The property $(L1)$ is usually easy to check. It is harder to check the Jacobi identity $(L2)$ for a proposed Lie product; direct calculations can be quite messy when many terms have to be calculated before one finds that they all cancel. Since we will encounter many Lie products that must be verified to satisfy the Jacobi identity, we first develop some technical machinery to make life easier, or at least more structured. For a given binary bilinear operation $\circ$ on $\mathbb{L}$, we define the **associator** of $f, g, h \in \mathbb{L}$ as

$$[f, g, h] := (f \circ g) \circ h - f \circ (g \circ h)\,. \tag{11.4}$$

11.1.2 Proposition. *If the associator of a bilinear operator $\circ$ on $\mathbb{L}$ satisfies*

$$[f, g, h] + [g, h, f] + [h, f, g] - [f, h, g] - [h, g, f] - [g, f, h] = 0\,, \tag{11.5}$$

then

$$f\angle g := f \circ g - g \circ f$$

defines a Lie product on $\mathbb{L}$.

Proof. Define

$$J(f,g,h) := f\angle(g\angle h) + g\angle(h\angle f) + h\angle(f\angle g)\,,$$

and define

$$S(f,g,h) := [f,g,h] + [g,h,f] + [h,f,g] - [f,h,g] - [h,g,f] - [g,f,h]\,.$$

Writing out $S(f,g,h)$ and $J(f,g,h)$ with $f\angle g := f\circ g - g\circ f$, one sees $J(f,g,h) = -S(f,g,h)$ and hence if $S(f,g,h) = 0$ for all f, g and h, then the Jacobi identity is satisfied for all f, g and h. The antisymmetry property $f\angle f = 0$ is trivial. □

11.1.3 Theorem. *The binary operation $\angle$ defined on the vector space $C^\infty(\mathbb{R}\times\mathbb{R})$ by*

$$f\angle g := f_p g_q - g_p f_q\,,$$

where $f_p = \partial f/\partial p$ and $f_q = \partial f/\partial q$, is a Lie product.

Proof. We calculate the associator for the bilinear operator $f\circ g = f_p g_q$. We have

$$\begin{aligned}
[f,g,h] &= (f\circ g)_p h_q - f_p(g\circ h)_q \\
&= (f_p g_q)_p h_q - f_p(g_p h_q)_q \\
&= f_{pp} g_q h_q + f_p g_{qp} h_q - f_p g_{pq} h_q - f_p g_p h_{qq} \\
&= f_{pp} g_q h_q - f_p g_p h_{qq}
\end{aligned}$$

Writing the cyclic permutations we get

$$\begin{aligned}
[f,g,h] + [g,h,f] + [h,f,g] &= f_{pp} g_q h_q + g_{pp} h_q f_q + h_{pp} f_q g_q \\
&\quad - f_p g_p h_{qq} - g_p h_p f_{qq} - h_p f_p g_{qq}\,,
\end{aligned}$$

which is symmetric in f, g; hence the identity (11.5) is satisfied. Proposition 11.1.2 therefore implies that $\angle$ is a Lie product.

The reader is invited to prove this result also by a direct calculation. □

We end this section by introducing some concepts needed at various later points but collected here for convenience. If $\mathbb{L}$ and $\mathbb{L}'$ are Lie algebras we call a linear map $\phi : \mathbb{L} \to \mathbb{L}'$ a **homomorphism** (of Lie algebras) if

$$\phi(f\angle g) = \phi(f)\angle\phi(g)$$

for all $f, g \in \mathbb{L}$. Note that the left-hand side involves the Lie product in $\mathbb{L}$, whereas the right-hand side involves the Lie product in $\mathbb{L}'$. An injective homomorphism is called an **embedding** of $\mathbb{L}$ into $\mathbb{L}'$. We call two Lie algebras $\mathbb{L}$ and $\mathbb{L}'$ **isomorphic** if there is a homomorphism $\phi : \mathbb{L} \to \mathbb{L}'$ and a homomorphism $\psi : \mathbb{L}' \to \mathbb{L}$ such that $\psi\circ\phi$ is the identity on $\mathbb{L}$ and $\phi\circ\psi$ is the identity on $\mathbb{L}'$. Then ϕ is called an **isomorphism**, and ψ is the inverse isomorphism.

Given a Lie algebra $\mathbb{L}$ and a subalgebra $\mathbb{L}'$, the **centralizer** $C_{\mathbb{L}'}(S)$ in $\mathbb{L}'$ of a subset $S \subset \mathbb{L}$ is defined by

$$C_{\mathbb{L}'}(S) = \{f \in \mathbb{L}' \mid f\angle g = 0 \quad \text{for all } g \in S\} \ .$$

In words, $C_{\mathbb{L}'}(S)$ consists of all the elements in $\mathbb{L}'$ that Lie commute with all elements in S. One may use the Jacobi identity to see that $C_{\mathbb{L}'}(S)$ is a Lie subalgebra of $\mathbb{L}'$.

An **ideal** of $\mathbb{L}$ is a subspace $I \subseteq \mathbb{L}$ such that $f\angle g \in I$ for all $f \in \mathbb{L}$ and for all $g \in I$. In other notation $\mathbb{L}\angle I = I\angle\mathbb{L} \subseteq I$. Note that 0 and $\mathbb{L}$ itself are always ideals; they are called the trivial ideals. Also, the center of a Lie algebra is always an ideal. A less trivial ideal is the **derived Lie algebra** $\mathbb{L}^{(1)}$ of $\mathbb{L}$ consisting of all elements that can be written as a finite sum of elements of $\mathbb{L}\angle\mathbb{L}$. If $I \subseteq \mathbb{L}$ is an ideal in $\mathbb{L}$ one may form the quotient Lie algebra $\mathbb{L}/I$, whose elements are the equivalence classes $[f]$ of all $g \in \mathbb{L}$ such that $f - g \in I$, with addition, scalar multiplication, and Lie product given by

$$\alpha[g] := [\alpha g] \,, \quad [f] + [g] := [f + g] \,, \quad [f]\angle[g] := [f\angle g] \,.$$

It is well-known that the vector space operations are well-defined. The Lie product is well-defined since $f' \in [f]$ implies $f' - f \in I$, hence $(f - f')\angle g \in I$ and $[f']\angle[g] = [f'\angle g] = [f\angle g + (f' - f)\angle g] = [f\angle g]$.

If $\mathbb{L}$ and $\mathbb{L}'$ are Lie algebras, their **direct sum** $\mathbb{L} \oplus \mathbb{L}'$ is the direct sum of the vector spaces equipped with the Lie product defined by

$$(x + x')\angle(y + y') = x\angle y + x'\angle y'$$

for all $x, y \in \mathbb{L}$ and all $x', y' \in \mathbb{L}'$. It is easily verified that the axioms are satisfied.

11.2 Lie algebras from derivations

Equation (11.2),

$$f\angle(g\angle h) = (f\angle g)\angle h + g\angle(f\angle h) \,.$$

resembles the product rule for (partial) differentiation;

$$\frac{\partial}{\partial x}(gh) = \frac{\partial g}{\partial x}h + g\frac{\partial h}{\partial x} \,.$$

To make the similarity more apparent we introduce for every element $f \in \mathbb{L}$ a linear operator $\mathrm{ad}_f : \mathbb{L} \to \mathrm{Lin}\,\mathbb{L}$, the **derivative in direction** f, given by

$$\mathrm{ad}_f g := f\angle g \,.$$

The notation reflects the fact that the operator $\mathrm{ad} : \mathbb{L} \to \mathrm{Lin}\,\mathbb{L}$ defined by

$$\mathrm{ad} f := \mathrm{ad}_f$$

is the **adjoint representation** of $\mathbb{L}$; see Sections 13.3 and 13.5.

Note that an element $f \in \mathbb{L}$ is in the center $Z(\mathbb{L}) = C_{\mathbb{L}}(\mathbb{L})$ of $\mathbb{L}$ if and only if the linear operator ad_f is zero.

11.2.1 Example. For f in the Lie algebra $C^\infty(\mathbb{R}\times\mathbb{R})$ constructed in Theorem 11.1.3, we have

$$\mathrm{ad}_f g = f\angle g = f_p g_q - f_q g_p = \left(f_p\frac{\partial}{\partial q} - f_q\frac{\partial}{\partial p}\right) g\,. \tag{11.6}$$

The vector field X_f on $\mathbb{R}\times\mathbb{R}$ defined by the coefficients of ad_f is called the **Hamiltonian vector field** defined by f; cf. Chapter 12. In particular, the Hamiltonian derivative operators with respect to p and q take the explicit form

$$X_p = \frac{\partial}{\partial q}\,, \quad X_q = -\frac{\partial}{\partial p}\,,$$

and we have

$$\mathrm{ad}_f = f_p X_p + f_q X_q.$$

With the convention that operators bind stronger than the Lie product, the Jacobi identity can be written in the form

$$\mathrm{ad}_f(g\angle h) = \mathrm{ad}_f g\angle h + g\angle \mathrm{ad}_f h\,.$$

The Jacobi identity is thus equivalent to saying that the operator ad_f defines for every f a derivation of the Lie algebra.

11.2.2 Definition.
(i) A **derivation** of a vector space $\mathbb{A}$ with a bilinear product $\circ$ is a linear map $\delta : \mathbb{A}\to\mathbb{A}$ satisfying the product rule (or **Leibniz identity**)

$$\delta(f\circ g) = \delta f\circ g + f\circ\delta g\,,$$

for all $f, g\in\mathbb{A}$. We denote by $\mathrm{Der}\,\mathbb{A}$ the set of all derivations of $\mathbb{A}$. (In the cases of interest, $\mathbb{A}$ is an associative algebra with the associative product as $\circ$, or a Lie algebra with the Lie product as $\circ$.

(ii) If $\mathbb{E}$ is an associative algebra $\mathbb{E}$, a **(left) $\mathbb{E}$-module** is an additive abelian group $\mathbb{V}$ together with a multiplication mapping which assigns to $f\in\mathbb{E}$ and $x\in\mathbb{V}$ a product $fx\in\mathbb{V}$ such that

$$f(x+y) = fx + fy, \quad (f+g)x = fx + gx, \quad f(gx) = (fg)x$$

for all $f, g\in\mathbb{E}$ and all $x, y\in\mathbb{V}$.

11.2.3 Proposition. *The commutator of two derivations is a derivation. In particular,* $\mathrm{Der}\,\mathbb{A}$ *is a Lie subalgebra of* $\mathrm{Lin}\,\mathbb{A}$ *with Lie product*

$$\delta\angle\delta' := [\delta, \delta'].$$

Moreover, if $\mathbb{A}$ *is commutative and associative then the* ***product*** $f\delta$ *of* $\delta\in\mathrm{Der}\,\mathbb{E}$ *and* $f\in\mathbb{E}$ *defined by*

$$(f\delta)g := f(\delta g)$$

is a derivation, and turns $\mathrm{Der}\,\mathbb{E}$ *into an* $\mathbb{E}$*-module.*

Proof. Since Der $\mathbb{E}$ is a linear vector space, and since the antisymmetry property and the Jacobi identity are already satisfied in $\operatorname{Lin}\mathbb{E}$, we only need to check that the Lie product of two derivations is again a derivation. We have:

$$\begin{aligned}(\delta\angle\delta')(fg) &= (\delta\delta')(fg) - (\delta'\delta)(fg)\\ &= \delta((\delta' f)g + f(\delta' g)) - \delta'((\delta f)g + f(\delta g))\\ &= (\delta\delta' f)g + f\delta\delta' g - (\delta'\delta f)g - f\delta\delta' g\\ &= (\delta\angle\delta' f)g + f(\delta\angle\delta' g)\end{aligned}$$

This proves the first part. The second part is straightforward. □

11.2.4 Proposition. *The* ***centralizer*** *of a subset S of* $\operatorname{Lin}\mathbb{E}$*, defined as*

$$C(S) := \{\delta \in \operatorname{Der}\mathbb{E} \mid A\angle\delta = 0 \quad \textit{for all } A \in S\}\,,$$

is a Lie subalgebra of Der $\mathbb{E}$*.*

Proof. As before, we only need to prove that the Lie product closes within $C(S)$. If $\delta, \delta' \in C(S)$, the Jacobi identity in the form (11.2) implies

$$A\angle(\delta\angle\delta') = (A\angle\delta)\angle\delta' + \delta\angle(A\angle\delta') = 0\,.$$

□

11.3 Linear groups and their Lie algebras

In quantum mechanics, linear operators play a central role; they appear in two essentially different ways: Operators describing time evolution and canonical transformations are linear operators U on a Hilbert space, that are **unitary** in the sense that $U^*U = UU^* = 1$, and hence bounded[1]. The unitary operators form a group, which in many cases of interest is a so-called Lie group.

On the other hand, many important quantities in quantum mechanics are described in terms of unbounded linear operators that are defined not on the whole Hilbert space but only on a dense subspace. Usually, the linear operators of interest have a common dense domain $\mathbb{H}$ on which they are defined and which they map into itself. $\mathbb{H}$ inherits from the Hilbert space the Hermitian inner product, hence is a complex **Euclidean space**, and the Hilbert space can be reconstructed from $\mathbb{H}$ as the **completion** $\overline{\mathbb{H}}$ of $\mathbb{H}$ by equivalence classes of Cauchy sequences, in the way familiar from the construction of the real numbers from rationals. We therefore consider the algebra $\operatorname{Lin}\mathbb{H}$ of continuous linear operators on a Euclidean space $\mathbb{H}$, with composition as associative product.

[1]The bounded operators on a Hilbert space a so-called C^*-algebra; see for example Rickart [232], Baggett [17], or Werner [285]. But we do not use this fact.

In this section, we define the basic concepts relevant for a study of groups and Lie algebras inside algebras of operators. Since for these concepts neither the operator structure nor the coefficient field matters in most cases - as long as the characteristic is not two -, we provide a slightly more general framework. In the next section, we apply the general framework to the algebra $\mathbb{C}^{n\times n} = \operatorname{Lin}\mathbb{C}^n$ of complex $n \times n$-matrices, considered in the standard way as linear operators on the space $\mathbb{C}^n$ of column vectors with n complex entries. Many of the Lie groups and Lie algebras arising in the applications are naturally defined as subgroups or subspaces of this algebra.

An **(associative) algebra** over a field $\mathbb{K}$ is a vector space $\mathbb{E}$ over $\mathbb{K}$ with a bilinear, associative multiplication. For example, every $*$-algebra is an associative algebra over $\mathbb{C}$. As traditional, the product of an associative algebra (and in particular that of $\operatorname{Lin}\mathbb{H}$ and $\mathbb{K}^{n\times n}$) is written by juxtaposition. An associative algebra $\mathbb{E}$ is called **commutative** if $fg = gf$ for all $f, g \in \mathbb{E}$, and **noncommutative** otherwise. In many cases we assume that such an algebra has a unit element 1 with respect to multiplication; after the identification of the multiples of 1 with the elements of $\mathbb{K}$, this is equivalent to assuming that $\mathbb{K} \subseteq \mathbb{E}$. If $\mathbb{E}$ and $\mathbb{E}'$ are associative algebras over $\mathbb{K}$ with 1, then a $\mathbb{K}$-linear map $\phi : \mathbb{E} \to \mathbb{E}'$ is an algebra homomorphism if $\phi(fg) = \phi(f)\phi(g)$ and $\phi(1) = 1$. Often we omit the reference to the ground field $\mathbb{K}$ and assume a ground field has been chosen.

We now show that every associative algebra has many Lie products, and thus can be made in many ways into a Lie algebra. For commutative algebras, the construction is uninteresting since it only leads to abelian Lie algebras.

11.3.1 Theorem. *Let $\mathbb{E}$ be an associative algebra. Then, for every $J \in \mathbb{E}$, the binary operation $\measuredangle_J$ defined on $\mathbb{E}$ by*

$$f \measuredangle_J g := fJg - gJf$$

is a Lie product. In particular ($J = 1$), the binary operation $\angle$ defined on $\mathbb{E}$ by

$$f \angle g := [f, g]$$

where

$$[f, g] := fg - gf$$

*denotes the **commutator** of f and g, is a Lie product.*

Proof. We compute the associator (11.4) for the bilinear operation $f \circ g := fJg$:

$$[f, g, h] = (f \circ g)Jh - fJ(g \circ h) = fJgJh - fJgJh = 0\,,$$

by associativity. Hence the associator of $\circ$ satisfies (11.5), and we conclude that $\measuredangle_J$ is a Lie product. □

Note that $Jf \angle Jg = J(f \measuredangle_J g)$. Hence the corresponding Lie algebras are isomorphic when J is invertible.

If $\mathbb{E}$ and $\mathbb{E}'$ are two associative algebras with unity, we may turn them into Lie algebras by putting $f\angle g = [f,g]$ in both $\mathbb{E}$ and $\mathbb{E}'$. We denote by $\mathbb{L}$ and $\mathbb{L}'$ the Lie algebra associated to $\mathbb{E}$ and $\mathbb{E}'$, respectively. If ϕ is an algebra homomorphism from $\mathbb{E}$ to $\mathbb{E}'$ then ϕ induces a Lie algebra homomorphism between the Lie algebras $\mathbb{L}$ and $\mathbb{L}'$. Indeed $\phi(f\angle g) = \phi(fg - gf) = \phi(f)\phi(g) - \phi(g)\phi(f) = \phi(f)\angle\phi(g)$.

Theorem (11.3.1) applies in particular to $\mathbb{E} = \mathbb{K}^{n\times n}$. The Lie algebra $\mathbb{K}^{n\times n}$ with Lie product $f\angle g := [f,g]$ is called the **general linear algebra** $gl(n,\mathbb{K})$ over $\mathbb{K}$. If $\mathbb{K} = \mathbb{C}$, we simply write $gl(n) = gl(n,\mathbb{C})$; similar abbreviations apply without notice for the names of other Lie algebras introduced later.

11.3.2 Definition.
(i) A **Hausdorff $*$-algebra** is a $*$-algebra $\mathbb{E}$ with a Hausdorff topology in which addition, multiplication, and conjugation are continuous. An element $f \in \mathbb{E}$ is called **complete** if the initial-value problem

$$\frac{d}{dt}U(t) = fU(t), \quad U(0) = 1 \tag{11.7}$$

has a unique solution $U : \mathbb{R} \to \mathbb{E}$. Then the mapping U is called a **one-parameter group** with **infinitesimal generator** f, and we write $e^{tf} := U(t)$; this notation is unambiguous since it is easily checked that $e^{t(sf)} = e^{(ts)f}$ for $s,t \in \mathbb{R}$. An element $f \in \mathbb{E}$ is called **self-adjoint** if $f^* = f$ and the product if with the imaginary unit is complete. We call an element $g \in \mathbb{E}$ **exponential** if it is of the form $g = e^f$ for some complete $f \in \mathbb{E}$. We call a Hausdorff $*$-algebra $\mathbb{E}$ an **exponential algebra** if the set of exponential elements in $\mathbb{E}$ is a neighborhood of 1.

(ii) A **linear group** is a set $\mathbb{G}$ of invertible elements of some associative algebra $\mathbb{E}$ such that $1 \in \mathbb{G}$ and

$$g, g' \in \mathbb{G} \quad \Rightarrow \quad g^{-1}, gg' \in \mathbb{G}.$$

If $\mathbb{E}$ is given with a topology in which its operations are continuous, we consider $\mathbb{G}$ as a topological group with the topology induced by calling a subset of $\mathbb{G}$ open or closed if it is the intersection of an open or closed set of $\mathbb{E}$ with $\mathbb{G}$.

(iii) A **linear Lie group** is a closed subgroup of the group $\mathbb{E}^\times$ of all invertible elements of an exponential algebra $\mathbb{E}$. A **Lie group** is a group $\widetilde{\mathbb{G}}$ with a Hausdorff topology that is **isomorphic** to some linear Lie group $\mathbb{G}$, i.e., for which there is a continuous, invertible mapping $\phi : \widetilde{\mathbb{G}} \to \mathbb{G}$ such that ϕ and ϕ^{-1} are continuous and $\phi(1) = 1$, $\phi(gg') = \phi(g)\phi(g')$ for all $g, g' \in \widetilde{\mathbb{G}}$.

For all exponential algebras $\mathbb{E}$, the group $\mathbb{E}^\times$ is a linear Lie group. Note that the law $e^f e^{f'} = e^{f+f'}$ holds if f and f' commute but not in general. In particular,

$$e^f e^{-f} = e^0 = 1.$$

If $\mathbb{E}$ is a **Banach algebra**, i.e., if the topology of $\mathbb{E}$ is induced by a norm $\|\cdot\|$ satisfying $\|fg\| \le \|f\|\,\|g\|$, it is not very difficult to show that every $f \in \mathbb{E}$ is complete, and we have

for all $f \in \mathbb{E}$ the absolute convergent series expansion

$$e^f = \sum_{k=0}^{\infty} \frac{f^k}{k!},$$

and that $f = \log g$, where

$$\log g := -\sum_{k=1}^{\infty} \frac{(1-g)^k}{k} \quad \text{for } \|1-g\| < 1,$$

provides an f such that $g = e^f$. Therefore every Banach algebra is exponential. Note that the **exponential mapping**, which maps a matrix $f \in \mathbb{E}$ to $e^f \in \mathbb{E}^\times$, is usually not surjective.

The above applies to the case $\mathbb{E} = \mathbb{C}^{n\times n}$ with the maximum norm, which is a Banach algebra, which covers all finite-dimensional Lie groups. In infinite dimensions, however, many interesting linear Lie groups are not definable over Banach algebras (see, e.g., Neeb [200]).

11.4 Classical Lie groups and their Lie algebras

This section is not yet in a good form.

A **matrix group** is a linear group in an algebra $\mathbb{K}^{n\times n}$. In this section, we define the most important matrix groups and the corresponding Lie algebras. Although these are defined no matter which field is involved, the Lie algebras in quantum physics have $\mathbb{K}$ is the field of real numbers of the field of complex numbers. Because exponentials can be defined for the real and complex fields, the groups have a natural differential geometric structure as differentiable manifolds; cf. Section 17.7. [2].

11.4.1 Example. The group $GL(n, \mathbb{K})$ of all invertible $n \times n$-matrices over $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$ is a linear group, The subgroup of $GL(n, \mathbb{K})$ consisting of the matrices with unit determinant is denoted by $SL(n, \mathbb{K})$. In other words, $SL(n, \mathbb{K})$ is the kernel of the map $\det : GL(n, \mathbb{K}) \to \mathbb{K}^*$, where $\mathbb{K}^*$ is the group of invertible elements in $\mathbb{K}$. The Lie algebra of $SL(n, \mathbb{K})$ is denoted by $sl(n, \mathbb{K})$ and consists of the traceless $n \times n$ matrices with entries in $\mathbb{K}$. By Theorem 11.3.1, the algebra of $n \times n$-matrices with entries in $\mathbb{K}$ is a Lie algebra the commutator as Lie product; this Lie algebra is denoted by $gl(n, \mathbb{K})$. The center of $gl(n, \mathbb{K})$ is easily seen to be the 1-dimensional subalgebra spanned by the identity matrix, $Z(gl(n, \mathbb{K})) = \mathbb{K}1 = \mathbb{K}$.

[2] For general fields, there are no exponentials, and one needs to replace the differential geometric structure inherent in Lie groups by an algebraic geometry structure, and may then interpret general matrix groups as so-called **groups of Lie type**. In particular, for finite fields, one gets the **Chevalley groups**, which figure prominently in the classification of finite simple groups.

Every subspace of a Lie algebra closed under the Lie product is again a Lie algebra. This simple recipe provides a large number of useful Lie algebras defined as Lie subalgebras of some $gl(n, \mathbb{K})$. Conversely, the (nontrivial) **theorem of Ado**, not proven here but see e.g. Jacobsen [136], states that every finite-dimensional Lie algebra is isomorphic to a Lie subalgebra of some $gl(n, \mathbb{R})$.

The group $GL(n, \mathbb{K})$ is one of the most important finite-dimensional linear groups and all finite-dimensional linear groups are isomorphic tosubgroups of $GL(n, \mathbb{K})$ for some n. If $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$ then every closed subgroup $\mathbb{G}$ of $GL(n, \mathbb{K})$ is a Lie group. These Lie groups have associated Lie algebras $\mathbb{L} = \log \mathbb{G}$ of infinitesimal generators. For any Lie subgroup G of $GL(n, \mathbb{K})$ one gets the Lie algebra by looking at the vector space of those elements X of $gl(n, \mathbb{K})$ such that $e^{\varepsilon X}$ is in G for ε small enough. This criterion is very useful since we can take ϵ so small that we only have to look at the terms linear in ϵ so that we don't have to expand the exponential series completely. If the subgroup $\mathbb{G} \subset GL(n, \mathbb{K})$ is connected and either compact or nilpotent, then the exponential map can be shown to be surjective, see e.g. Knapp [154].

The Lie algebra $sl(n, \mathbb{K})$ is the Lie subalgebra of $gl(n, \mathbb{K})$ given by the traceless matrices. The dimension is $n^2 - 1$ and we have

$$sl(n, \mathbb{K}) \cong gl(n, \mathbb{K})/\mathbb{K}\,.$$

The quotient is well defined and is a Lie algebra because $\mathbb{K}$ is the center and thus in particular an ideal.

If $\mathbb{L}$ is a Lie algebra over $\mathbb{R}$ then by taking the tensor product with $\mathbb{C}$ and extending the Lie bracket in a $\mathbb{C}$-linear way, one obtains the **complexification** of $\mathbb{L}$, denoted $\mathbb{L}^{\mathbb{C}}$. The process of complexification is also called **extension of scalars**. In particular, if we write $\mathbb{L}^{\mathbb{C}} = \mathbb{C} \otimes_{\mathbb{R}} \mathbb{L}$ then in $\mathbb{L}^{\mathbb{C}}$ the Lie bracket is given by $(\alpha \otimes x)\angle(\beta \otimes y) = \alpha\beta \otimes (x\angle y)$. The reverse process is called **realization** or **restriction of scalars**; we clarify the process of restriction of scalars by an example.

11.4.2 Example. Consider $\mathbb{L} = sl(2, \mathbb{C})$. We wish to calculate $sl(2, \mathbb{C})^{\mathbb{R}}$. A basis of $sl(2, \mathbb{C})$ is given by the elements

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

This basis is as well a basis for $sl(2, \mathbb{R})$; therefore we see $sl(2, \mathbb{C})^{\mathbb{R}} \cong sl(2, \mathbb{R}) \oplus_{\mathbb{R}} i\, sl(2, \mathbb{R})$ as real vector spaces. The Lie product of $f + ig$ and $f' + ig'$ for $f, f' \in sl(2, \mathbb{R})$ and $ig, ig' \in i\, sl(2, \mathbb{R})$ is given by

$$(f + g)\angle(f' + g') = f\angle f' - g\angle g' + i(f\angle g' + f'\angle g)\,.$$

The reader who has already some experience with Lie algebras is encouraged to verify the isomorphism $sl(2, \mathbb{C})^{\mathbb{R}} \cong so(3, 1)$.

11.4.3 Example. Suppose we have a symmetric bilinear form B on $\mathbb{K}^n$. The Lie algebra $so(n, B; \mathbb{K})$ is the subspace of all $f \in sl(n, \mathbb{K})$ satisfying

$$B(fv, w) = -B(v, fw). \tag{11.8}$$

We leave it to the reader to show that if f and g satisfy (11.8), then so does $fg - gf$; thus we have indeed a Lie algebra. In the special case where $B(v, w) = v^T w$, the Lie algebra $so(n, B; \mathbb{K})$ is called the **complex orthogonal Lie algebra** $so(n, \mathbb{K})$. In matrix language, $so(n, \mathbb{K})$ is the Lie algebra of antisymmetric matrices with entries in $\mathbb{K}$ and has dimension $n(n-1)/2$.

An **orthogonal matrix** is a matrix Q satisfying

$$Q^T Q = 1. \tag{11.9}$$

The orthogonal $n \times n$-matrices with coefficients in a field $\mathbb{K}$ form a subgroup of the group $GL(n, \mathbb{K})$, the **orthogonal group** $O(n, \mathbb{K})$. Since (11.9) implies that $(\det Q)^2 = 1$, orthogonal matrices have determinant ± 1. The orthogonal matrices of determinant one form a subgroup of $O(n, \mathbb{K})$, the **special orthogonal group** $SO(n, \mathbb{K})$. The corresponding Lie algebra is $so(n, \mathbb{K}) = \log O(n, \mathbb{K}) = \log SO(n, \mathbb{K})$, the Lie algebra of antisymmetric $n \times n$-matrices. In particular, the group $SO(3) = SO(3, \mathbb{R})$ consists of the rotations in 3-space and was discussed in some detail in Section 3.2.

For a **nondegenerate** B (i.e., one where $B(v, w) = 0$ for all v implies $w = 0$) and $\mathbb{K} = \mathbb{C}$ (or any algebraically closed field), we can always choose a basis in which the bilinear form is represented as the identity matrix. Therefore all $so(n, B; \mathbb{K})$ with nondegenerate B are isomorphic to $so(n, \mathbb{K})$.

Over $\mathbb{K} = \mathbb{R}$, symmetric bilinear forms are classified by their signature, i.e., the triple (p, q, r) consisting of the number p of positive, q of negative, and r of zero eigenvalues of the symmetric matrix A representing the bilinear form B; $B(v, w) = v^T A w$. The form B is nondegenerate if and only if $r = 0$. Bilinear forms with the same signature lead to isomorphic Lie algebras. In particular, $so(p, q)$ denotes a Lie algebra $so(p + q, B, \mathbb{R})$ where B is a nondegenerate symmetric bilinear form B on $\mathbb{R}^n$ of signature $(p, q, 0)$. The basis can always be chosen such that the representing matrix A is

$$I_{p,q} = \begin{pmatrix} 1_p & 0 \\ 0 & -1_q \end{pmatrix},$$

where 1_p and 1_q are the $p \times p$ and $q \times q$ identity matrix, respectively. In this basis, the Lie algebra $so(p, q)$ is the subalgebra of $gl(n, \mathbb{R})$ consisting of elements f satisfying

$$f^T I_{p,q} + I_{p,q} f = 0\,.$$

Note that if $f \in so(p, q)$ then

$$0 = \operatorname{tr}\left((f^T I_{p,q} + I_{p,q} f) I_{p,q}\right) = 2\operatorname{tr}(f I_{p,q}^2) = 2\operatorname{tr}(f)$$

and hence $so(p, q) \subset sl(n, \mathbb{R})$.

11.4.4 Example. Let V be a vector space over a field $\mathbb{K}$. Suppose V is equipped with a symmetric or antisymmetric nondegenerate bilinear form B. There is a symmetry group associated to the bilinear form consisting of the linear transformations $Q : V \to V$ such that

$$B(Qv, Qw) = B(v, w)$$

for all v, w in V. If B is symmetric one calls the group of these linear transformations an **orthogonal group** and denotes it by $O(B, \mathbb{K})$. The associated Lie algebra is $o(B, \mathbb{K})$. Indeed, e^{tf} transforms x, y into

$$\begin{aligned} B(e^{tf}x, e^{tf}y) &= B(e^{tf}x, e^{tf}y) \\ &= B((1+tf)x, (1+tf)y) + O(t^2) \\ &= B(x,y) + tB(fx, fy) + O(t^2). \end{aligned}$$

11.4.5 Example. When $\mathbb{K} = \mathbb{R}$, one has for symmetric bilinear forms another subdivision, since B can have a definite signature (p, q) where $p + q$ is the dimension of V. If B is of signature (p, q), this means that there exists a basis of V in which B can be represented as

$$B(v, w) = v^T A w\,, \quad \text{where} \quad A = \mathrm{diag}(\underbrace{-1, \ldots, -1}_{p \text{ times}}, \underbrace{1, \ldots, 1}_{q \text{ times}})\,.$$

The group of all linear transformations that leaves B invariant is denoted by $O(p, q)$. The subgroup of $O(p, q)$ of transformations with determinant one is the so-called **special orthogonal group** and is denoted by $SO(p, q)$. The associated real Lie algebra is denoted $so(p, q)$ and its elements are linear transformations $A : V \to V$ such that for all $v, w \in V$ we have $B(Av, w) + B(v, Aw) = 0$. The Lie product is given by the commutator of matrices.

The group of all translations in V generates together with $SO(p, q)$ the group of **inhomogeneous special orthogonal transformations**, which is denoted $ISO(p, q)$. One can obtain $ISO(p, q)$ from $SO(p, q+1)$ by performing a contraction; that is, by rescaling some generators with some parameter ϵ and then choosing a singular limit $\epsilon \to 0$ or $\epsilon \to \infty$. The group $ISO(p, q)$ can also be seen as the group of $(p+q+1) \times (p+q+1)$-matrices of the form

$$\begin{pmatrix} Q & b \\ 0 & 1 \end{pmatrix} \quad \text{with} \quad Q \in SO(p, q)\,,\ b \in V\,.$$

The Lie algebra of $ISO(p, q)$ is denoted $iso(p, q)$ and can be described as the Lie algebra of $(p+q+1) \times (p+q+1)$-matrices of the form

$$\begin{pmatrix} A & b \\ 0 & 0 \end{pmatrix} \quad \text{with} \quad A \in so(p, q)\,,\ b \in V\,.$$

Again, the Lie product in $iso(p, q)$ is the commutator of matrices.

We define the **symplectic Lie algebra** $sp(2n, \mathbb{K})$ as the Lie subalgebra of $gl(2n, \mathbb{K})$ given by the elements f satisfying

$$f^T J + J f = 0\,, \tag{11.10}$$

where J is the $2n \times 2n$-matrix given by

$$J = \begin{pmatrix} 0 & -1_n \\ 1_n & 0 \end{pmatrix}\,.$$

We leave it to the reader to verify that if f and g satisfy (11.10), then so does $fg - gf$. Another useful exercise is to prove $sl(2, \mathbb{K}) \cong sp(2, \mathbb{K})$. (Caution: The reader is warned

that in the literature there are different notational conventions concerning the symplectic Lie algebras. For example, some people write $sp(n, \mathbb{K})$ for what we and many others call $sp(2n, \mathbb{K})$.)

If B is antisymmetric in the example 11.4.4, the group is called a **symplectic group** and one writes $Sp(B, \mathbb{K})$. The associated Lie algebras is $sp(B, \mathbb{K})$. If V is of finite dimension m one writes $Sp(B, \mathbb{K}) = Sp(m, \mathbb{K})$. Note that m is necessarily even.

Other real Lie algebras that play a major role in many areas of physics are the **unitary Lie algebras** and the **special unitary Lie algebras** – called so because they are the generating algebras of the groups of (special) unitary matrices, a term that will be explained in Section 17.7. The unitary Lie algebra $u(n)$ consists of all antihermitian complex $n \times n$ matrices. The special unitary Lie algebra is defined as the antihermitian $n \times n$ complex traceless matrices and is denoted $su(n)$. It is clear that $su(n) \subset u(n)$. It might seem weird to call a Lie algebra real if it consists of complex-valued matrices. However, as a vector space the antihermitian complex $n \times n$ matrices form a real vector space. If f is a antihermitian matrix, then if is Hermitian. The dimension (as a real vector space) of $su(n)$ is $n^2 - 1$, and the dimension of $u(n)$ is n^2. It is a good exercise to check that $so(3) \cong su(2)$ since these two Lie algebras will return very often. A hint: $so(3)$ consists of anti-symmetric real 3×3 matrices, so there are only three. Choosing an obvious basis for both $su(2)$ and $so(3)$ will do the job.

11.4.6 Example. A complex matrix U is **unitary** if it satisfies

$$UU^* = 1,$$

where $(U^*)_{ij} = \bar{U}_{ji}$. Since the inverse of a matrix is unique, it follows that also $U^*U = 1$. By splitting all the matrix entries into a real and imaginary part $U_{ij} = A_{ij} + iB_{ij}$ we see that the set of $n \times n$ unitary matrices makes up a submanifold of $\mathbb{R}^{2n^2}$ of dimension n^2. The linear group of unitary $n \times n$ matrices is denoted $U(n)$.

$$U = e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k \,.$$

Then multiply A with a parameter t, take $t \to 0$ and keep only the linear terms: $U = 1 + tA + O(t^2)$. Then since U has to be unitary, we obtain

$$1 = (1 + tA + O(t^2))(1 + tA + O(t)^2)^* = 1 + t(A + A^*) + O(t)^2 \,,$$

implying that A has to be antihermitian. Thus the Lie algebra of infinitesimal generators of $U(n)$ is $u(n)$.

The subgroup of $U(n)$ of all elements with determinant 1 is denoted by $SU(n)$ and is called the **special unitary group**. The dimension of $SU(n)$ is $n^2 - 1$. For the determinant we get

$$\det(1 + tA + O(t^2)) = 1 + \operatorname{tr} tA + O(t)^2 \,,$$

and thus the trace of infinitesimal generators of $SU(n)$ has to vanish, and we see that the corresponding Lie algebra is $su(n)$. Note that the Lie algebra $u(n)$ contains all real

multiples of $i \cdot 1$, which commutes with all other elements. Hence $u(n)$ has a center, whereas $su(n)$ does not.

In the case $n = 2$ it is a nice exercise to show that each special unitary matrix U can be written as

$$U = \begin{pmatrix} x & y \\ -\bar{y} & \bar{x} \end{pmatrix}, \quad x, y \in \mathbb{C}\,,\ |x|^2 + |y|^2 = 1\,.$$

Writing $x = a + ib$ and $y = c + id$ for $a, b, c, d \in \mathbb{R}$ we see that $a^2 + b^2 + c^2 + d^2 = 1$. This implies that there is a one-to-one correspondence between $SU(2)$ and the set of points on the unit sphere S^3 in $\mathbb{R}^4$. Thus $SU(2)$ is as a manifold homeomorphic to S^3. In particular $SU(2)$ is compact. Hence every element U of $SU(2)$ can be written as the exponent of a matrix A.

Physicists prefer to work with Lie algebras defined by Hermitian matrices, corresponding to Lie $*$-algebras. In the applications, distinguished real generators typically represent important real-valued observables. Therefore they tend to replace the matrix A by iA for a Hermitian matrix A. This is one of the reasons why the structure constants for real algebras appear in the physics literature with an i, as alluded at the end of Section 11.2.

11.5 Heisenberg algebras and Heisenberg groups

A **Heisenberg algebra** is a Lie algebra $\mathbb{L}$ with a 1-dimensional center and a distinguished Lie central element 1 called **one** or **identity**, such that every $f \angle g$ is a multiple of 1 for all $f, g \in \mathbb{L}$. There is an embedding of $\mathbb{K}$ into $\mathbb{L}$ given by $\alpha \mapsto \alpha 1$ which can be used to identify the multiples of 1 with the multipliers from the field, so that $\mathbb{K} = Z(\mathbb{L}) \subset \mathbb{L}$.

When we divide out the center of a Heisenberg algebra we obtain an abelian Lie algebra. More generally, let $\mathbb{L}$ be any Lie algebra and let $\mathbb{L}'$ be another Lie algebra with a subalgebra Z contained in the center of $\mathbb{L}'$. If $\mathbb{L}'/Z$ is isomorphic to $\mathbb{L}$, one calls $\mathbb{L}'$ a **central extension** of $\mathbb{L}$.[3]

Corresponding to any Heisenberg algebra there is an alternating bilinear form $\omega : \mathbb{L} \times \mathbb{L} \to \mathbb{K}$ given by

$$f \angle g = \omega(f, g)\,.$$

[3]In more abstract terms, central extensions are conveniently described by short exact sequences. Let A_i be a set of Lie algebras and suppose that there are maps $d_i : A_i \to A_{i+1}$;

$$\ldots \longrightarrow A_{i-1} \xrightarrow{d_{i-1}} A_i \xrightarrow{d_i} A_{i+1} \longrightarrow\ . \tag{11.11}$$

We call the sequence **exact** if Ker d_i = Im d_{i-1} for all i where there are d_{i-1} and d_i. As an exercise, the reader is invited to verify the following assertion: The sequence $0 \to A \to B \to 0$ is exact if and only if $A \cong B$ and the isomorphism is the map from A to B. A short exact sequence is a sequence of maps of the form

$$0 \to A \to B \to C \to 0\,.$$

A **central extension** of $\mathbb{L}$ is then a Lie algebra $\mathbb{L}'$ such that there is an exact sequence $0 \to Z \to \mathbb{L}' \to \mathbb{L} \to 0$ with Z abelian.

Conversely, given such a form on an arbitrary vector space $\mathbb{V}$ not containing 1, this formula turns $\mathbb{L} := \mathbb{K} \oplus \mathbb{V}$ into a Heisenberg algebra. If ω is nondegenerate on $\mathbb{V}$ it defines a **symplectic form** on $\mathbb{V}$.

The Heisenberg algebra $h(n)$ is the special case where $\mathbb{K} = \mathbb{C}$, $\mathbb{V} = \mathbb{C}^{2n}$, and ω is nondegenerate. Thus $h(n)$ is a central extension of the abelian Lie algebra $\mathbb{C}^{2n}$ and has dimension $2n+1$. We can find a basis of $\mathbb{V}$ consisting of vectors p_k and q_l for $1 \leq k, l \leq n$ such that $\omega(p_k, p_l) = \omega(q_k, q_l) = 0$ for all k, l and $\omega(p_k, q_l) = \delta_{kl}$; that is, ω is then the standard symplectic form on $\mathbb{K}^{2n}$ represented by the matrix $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. Thus Heisenberg algebras encode symplectic vector spaces in a Lie algebra setting. Everything done here extends with appropriate definitions to general symplectic manifolds, and, indeed, much of classical mechanics can be phrased in terms of symplectic geometry, the geometry of such manifolds – we refer the reader to the exposition by Arnold [15] on classical mechanics and symplectic geometry.

11.5.1 Example. Let us write $t(n, \mathbb{K})$ for the Lie subalgebra of $gl(n, \mathbb{K})$ consisting of upper-triangular matrices and $n(n, \mathbb{K})$ as the Lie subalgebra of $gl(n, \mathbb{K})$ consisting of strictly upper-triangular matrices, which have zeros on the diagonal.

The Lie algebra $t(3, \mathbb{K})$ of strictly upper triangular 3×3-matrices is a Heisenberg algebra with

$$1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

since

$$\begin{pmatrix} 0 & \alpha & \gamma \\ 0 & 0 & \beta \\ 0 & 0 & 0 \end{pmatrix} \angle \begin{pmatrix} 0 & \alpha' & \gamma' \\ 0 & 0 & \beta' \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & \alpha\gamma' - \gamma\alpha' \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \alpha\gamma' - \gamma\alpha'.$$

The Lie algebra $t(3, \mathbb{C})$ is called **the Heisenberg algebra**; thus if one talks about "the" (rather than "a") Heisenberg algebra, this Lie algebra is meant and is denoted $h(1)$. Introducing names for the special matrices

$$p := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad q := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

we find that p, q and 1 form a basis of $t(3, \mathbb{C})$, and we can express the Lie product in the more compact form

$$(\alpha p + \beta q + \gamma) \angle (\alpha' p + \beta' q + \gamma') = \alpha\beta' - \beta\alpha'. \tag{11.12}$$

Defining

$$(\alpha p + \beta q + \gamma)^* := \overline{\alpha} p + \overline{\beta} q + \overline{\gamma}$$

turns the Heisenberg algebra into a Lie $*$-algebra in which p and q are Hermitian. Note that here $*$ is *not* the conjugate transposition of matrices!

(11.12) implies that p and q satisfy the so-called **canonical commutation relations**

$$p\angle q = 1\,, \quad p\angle p = q\angle q = 0. \tag{11.13}$$

Since $f\angle 1 = 0$ when 1 is Lie central, (11.13) completely specifies the Lie product. The canonical commutation relations are frequently found in textbooks on quantum mechanics, but we see that they just characterize the Heisenberg algebra.

The notation q and p is chosen to remind of position of momentum. Indeed, the canonical commutation relations arise naturally in classical mechanics. In the Lie algebra $C^\infty(\mathbb{R}\times\mathbb{R})$ constructed in Theorem 11.1.3, we consider the set of **affine functions**, that is, those that are of the form $f(p,q) = \alpha_f p + \beta_f q + \gamma_f$, with $\alpha_f, \beta_f, \gamma_f \in \mathbb{C}$. In particular, the constant functions are included with $\alpha_f = \beta_f = 0$, and we identify them with the constants $\gamma_f \in \mathbb{C}$. Given another affine function $g(p,q) = \alpha_g p + \beta_g q + \gamma_g$, we find

$$f\angle g = \alpha_f\beta_g - \beta_f\alpha_g \in \mathbb{C}\,.$$

Since $f\angle g$ is just a complex number times the function that is 1 everywhere, it is a central element, that is, it Lie commutes with all other algebra elements. Thus the affine functions form a Heisenberg subalgebra of $C^\infty(\mathbb{R}\times\mathbb{R})$, and p and q satisfy the canonical commutation relations.

Suppose that a commutative Poisson algebra $\mathbb{E}$ contains two elements p and q satisfying the canonical commutation relations (11.13). Then $\mathbb{E}$ contains a copy of the Heisenberg algebra. The algebra of polynomials in p and q is then a Poisson subalgebra of $\mathbb{E}$ in which (11.6) is valid. This follows from Proposition 12.1.5. Thus the canonical commutation relations capture the essence of the commutative Poisson algebra $C^\infty(\mathbb{R}\times\mathbb{R})$. But getting the bigger algebra requires taking limits which need not exist in $\mathbb{E}$, since with polynomials alone, one does not get all functions.

11.5.2 Example. An upper triangular $n\times n$-matrix is called **unit upper triangular** if its elements on the diagonal are 1, and **strictly upper triangular** if its elements on the diagonal are zero. It is straightforward to check that the unit upper triangular $n\times n$-matrices form a subgroup $T(n,\mathbb{K})$ of the group $GL(n,\mathbb{K})$, and the strictly upper triangular $n\times n$-matrices form a Lie subalgebra of $gl(n,\mathbb{K})$, which we denote by $t(n,\mathbb{K})$. We have $t(n,\mathbb{K}) = \log T(n,\mathbb{K})$. In the following we shall look more closely at the case $n=3$ which is especially important.

The **Heisenberg group** is the group

$$T(3,\mathbb{C}) = \left\{ \begin{pmatrix} 1 & a & c \\ 0 & 1 & b \\ 0 & 0 & 1 \end{pmatrix} \,\middle|\, a,b,c\in\mathbb{C} \right\} \tag{11.14}$$

of unit upper triangular matrices in $\mathbb{C}^{3\times 3}$; its corresponding Lie algebra is the Heisenberg algebra $t(3,\mathbb{C})$. Since the Heisenberg group is defined in terms of matrices, it comes immediately with a representation, the defining representation. Note that the defining representation is not unitary.

The relation between the Heisenberg algebra and the Heisenberg group is particularly simple since the exponential map has a simple form. Indeed, if $A \in \mathbb{C}^{n\times n}$ then

$$e^A = \sum_{k=0}^{\infty} \frac{A^k}{k!}\,, \tag{11.15}$$

where $A^0 = 1$ is the identity matrix and the series (11.15) is absolutely convergent. A note on the infinite-dimensional case: For linear operators A on a Hilbert space $\mathbb{H}$, the series converges absolutely only when A is bounded (and hence everywhere defined); for unbounded but self-adjoint A (which are only densely defined), convergence holds in a weaker sense giving

$$e^A\psi = \sum_{k=0}^{\infty} \frac{A^k}{k!}\psi \tag{11.16}$$

for a dense set of vectors $\psi \in \mathbb{H}$ that are analytic for A.

If $A \in t(3,\mathbb{C})$, then a direct calculation shows that A^2 is of the form

$$\begin{pmatrix} 0 & 0 & c \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

for some $c \in \mathbb{C}$. Hence $A^3 = 0$ and the exponential of A is simply given by $e^A = 1 + A + \frac{1}{2}A^2$. Thus if A is given by

$$A = \begin{pmatrix} 0 & \alpha & \gamma \\ 0 & 0 & \beta \\ 0 & 0 & 0 \end{pmatrix}\,,$$

the exponential is given by

$$e^A = \begin{pmatrix} 1 & \alpha & \gamma + \frac{1}{2}\alpha\beta \\ 0 & 1 & \beta \\ 0 & 0 & 1 \end{pmatrix}\,.$$

The map $A \to e^A$ is clearly bijective. The inverse map is given by the logarithm, which is for matrices defined by

$$\log(1+X) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} X^k\,, \tag{11.17}$$

so that for the Heisenberg group $\mathbb{G}$ we have

$$\log(X) = (X-1) - \tfrac{1}{2}(X-1)^2 = -2 + 2X - \tfrac{1}{2}X^2\,.$$

We are thus in the situation that both $T(3,\mathbb{C}) = \exp t(3,\mathbb{C})$ and $t(3,\mathbb{C}) = \log T(3,\mathbb{C})$. This is not special to the Heisenberg group, neither does it hold in general. But there is a class of groups for which this holds. For example, the exponential map is surjective for all connected Lie groups that are compact or nilpotent (see below), see, e.g., Helgason [124] or Knapp [154]. The Heisenberg group is a noncompact but nilpotent Lie group.

Let us shortly repeat what it means when a group is nilpotent. Given any group G, we can form the commutator subgroup $G^{(1)}$, which is generated by all elements of the form

$aba^{-1}b^{-1}$ for all $a, b \in G$. We can also consider the commutator subgroup of $G^{(1)}$ and denote it by $G^{(2)}$. Repeating this procedure we get a sequence of groups

$$G \supseteq G^{(1)} \supseteq G^{(2)} \supseteq \ldots$$

A group is nilpotent if the procedure ends in a finite number of steps with the trivial group $G^{(n)} = 1$. It is easy to see that the Heisenberg group is two-step nilpotent since $G^{(2)} = 1$.

Since the exponential map is bijective for the Heisenberg group, there exists a binary operation $\oplus$ on $t(3, \mathbb{C})$, where $A \oplus B$ is the element with

$$e^A e^B = e^{A \oplus B} \,. \tag{11.18}$$

It is not difficult to give an explicit formula for $A \oplus B$. Since A and B are strictly upper triangular, we have $A^p B^q = 0$ for $p + q \geq 3$. We thus have

$$e^A e^B = (1 + A + \tfrac{1}{2}A^2)(1 + B + \tfrac{1}{2}B^2) = 1 + A + B + \tfrac{1}{2}(A^2 + B^2 + 2AB) \,.$$

Applying (11.17) we find

$$\begin{aligned} A \oplus B &= \log\big(1 + A + B + \tfrac{1}{2}(A^2 + B^2 + 2AB)\big) \\ &= A + B + \tfrac{1}{2}(AB - BA) \,, \end{aligned}$$

hence

$$A \oplus B = A + B + \tfrac{1}{2} A \angle B \,. \tag{11.19}$$

Thus we get from (11.18) the formula $e^A e^B = e^{A+B+\frac{1}{2}A\angle B}$. Since $A\angle B$ is central, it behaves just like a complex number, and we find the **Weyl relations**

$$e^{A+B} = e^{-\frac{1}{2}A\angle B} e^A e^B \,. \tag{11.20}$$

In fact this result is also a direct consequence of the famous (but much less elementary) **Baker–Campbell–Hausdorff (BCH) formula** that gives for general matrix Lie groups a series expansion of $A \oplus B$ when A and B are not too large. Even more generally, the Baker–Campbell–Hausdorff formula applies to abstract finite-dimensional Lie groups[4] that are not necessarily matrix groups and says that for two fixed Lie algebra elements A and B and for small enough real numbers s and t there is a function C from $\mathbb{R} \times \mathbb{R}$ to the Lie algebra such that we have

$$e^{sA} e^{tB} = e^{C(s,t)} \,.$$

The function $C(s, t)$ is given by a (for small s, t absolutely convergent) infinite power series, the first terms of which are given by

$$C(s,t) = sA + tB + \frac{st}{2} A\angle B + \frac{st}{12}\left(sA\angle(A\angle B) - tB\angle(A\angle B)\right) + \ldots .$$

In fact, this series expansion may be derived from a closed form integral expression.

The Baker–Campbell–Hausdorff formula is of great importance in both pure and applied mathematics. It gives (where it applies; in particular in finite dimensions) the relation of a

[4] In infinite dimensions, additional assumptions are needed for the BCH-formula to hold.

Lie group with the associated Lie algebra. It for example says that the product of e^A and e^B for some A and B in the Lie algebra is again an element of the form e^C with C in the Lie algebra. Hence the exponents of the Lie algebra generate a subgroup of the corresponding Lie group.

For infinite-dimensional Lie algebras and groups, one has to use a refined argument centering around the Hille–Yosida theorem. Let $U(t)$ denote a one-parameter group of linear operators on a Hilbert space $\mathbb{H}$ such that $t \to U(t)$ is **strongly continuous**, which means that $t \to U(t)\varphi$ is continuous for all $\varphi \in \mathbb{H}$. Then we can differentiate $U(t)$ to obtain the strong limit

$$A = \lim_{t\to 0} \frac{U(t) - U(0)}{t} .$$

The object A is called **infinitesimal generator** of the one-parameter group $U(t)$. It turns out that A is a closed linear operator that is defined on a dense subspace in $\mathbb{H}$. The Hille–Yosida theorem gives a necessary and sufficient condition for a closed linear operator A to be the infinitesimal generator of some strongly continuous one-parameter semigroup

$$U(t) = e^{tA} ,$$

since in general one might not get a group. The Hille–Yosida theorem is very useful for analyzing the solvability of linear differential equations

$$\frac{d}{dt}\psi(t) = A\psi(t) , \quad \psi(0) = \psi_0 ,$$

examples of which are the Schrödinger equation or the heat equation. If the conditions of the Hille–Yosida theorem hold for A, the solution to this initial value problem takes the form

$$\psi(t) = e^{tA}\psi(0) .$$

For the (hyperbolic, conservative) Schrödinger equation, $A = -\frac{i}{\hbar}H$ with a self-adjoint Hamiltonian H, the solution exists for all t, and the $U(t)$ form a one-parameter group. For the (parabolic, dissipative) heat equation, $A = k\Delta$ is a positive multiple of the Laplacian $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$, the solution exists only for $t \geq 0$, and we only get a semigroup.

11.6 Lie $*$-algebras

Many Lie algebras of interest in physics have an additional structure: an adjoint mapping compatible with the Lie product.

11.6.1 Definition. A **Lie $*$-algebra** is a Lie algebra $\mathbb{L}$ over $\mathbb{C}$ with a distinguished element $1 \neq 0$ called **one** and a mapping $*$ that assigns to every $f \in \mathbb{L}$ an **adjoint** $f^* \in \mathbb{L}$ such that

$$f\angle 1 = 0,$$

$$(f+g)^* = f^* + g^*, \quad (f\angle g)^* = f^*\angle g^*,$$

$$f^{**} = f, \quad (\lambda f)^* = \bar{\lambda} f^*, \quad 1^* = 1$$

for all $f, g \in \mathbb{L}$ and $\lambda \in \mathbb{C}$. We identify the multiples of 1 with the corresponding complex numbers.

The reason why we include the 1 into the definition of a Lie $*$-algebra is that many physically relevant Lie algebras are equipped with a distinguished central element[5]. But the presence of 1 is not a restriction, since one can always adjoin a central element 1 to a Lie algebra $\mathbb{L}'$ without nonzero central element and form the direct sum $\mathbb{L} = \mathbb{L}' \oplus \mathbb{K}$.

An important Lie $*$-algebra for nonrelativistic quantum mechanics is the algebra $\mathbb{E} = \operatorname{Lin} \mathbb{H}$ of linear operators of a Euclidean space $\mathbb{H}$ (usually a dense subspace of a Hilbert space $\overline{\mathbb{H}}$). The relevant Lie product is defined by Theorem 11.3.1 with the choice

$$J := \frac{i}{\hbar} = \frac{i}{\hbar} 1_{\mathbb{H}} \in \operatorname{Lin} \mathbb{H},$$

where $1_{\mathbb{H}}$ is the identity operator on $\mathbb{H}$, and the conjugate of $f \in \mathbb{E}$ is given by the **adjoint** of f, defined as the linear mapping f^* satisfying $\phi^* f^* \psi = (f\phi)^* \psi$ for all $\phi, \psi \in \mathbb{H}$. Dropping the index J in the Lie product of Theorem 11.3.1, we get the **quantum Lie product**

$$f \angle g = \frac{i}{\hbar}(fg - gf) = \frac{i}{\hbar}[f, g] \tag{11.21}$$

of $f, g \in \operatorname{Lin} \mathbb{H}$, already familiar from (1.3). Note that the axioms require the purely imaginary factor in this formula, whereas the value of Planck's constant $\hbar$ is arbitrary from a purely mathematical point of view. In quantum field theory, a different choice of J is sometimes more appropriate.

For any Lie $*$-algebra, the set

$$\operatorname{Re} \mathbb{L} := \{f \in \mathbb{L} \mid f^* = f\}$$

is a Lie algebra over $\mathbb{R}$. When describing symmetries, physicists often work with Lie algebras over the reals; the present Lie $*$-algebras are then the complexifications of these real algebras, with a central element 1 adjoined if necessary.

The **complexification** of a real Lie algebra $\mathbb{L}$ is the Lie $*$-algebra $\mathbb{C}\mathbb{L}$ defined as follows. In case that a complex scalar multiplication is already defined on $\mathbb{L}$, one first replaces $\mathbb{L}$ by an isomorphic Lie algebra in which $if \notin \mathbb{L}$ if $f \in \mathbb{L}$ is nonzero. Then one defines

$$\mathbb{C}\mathbb{L} = \mathbb{L} \oplus i\mathbb{L},$$

extending scalar multiplication in a natural way to the complex field. That is, any element $f \in \mathbb{C}\mathbb{L}$ is of the form

$$f = f_1 + if_2$$

with $f_1, f_2 \in \mathbb{L}$, and one defines

$$\alpha(\beta f) := (\alpha\beta) f, \quad \alpha f \angle \beta g := (\alpha\beta) f \angle g$$

[5]Many such Lie algebras are realized most naturally as central extensions of semisimple Lie algebras, corresponding to projective representations of semisimple Lie algebras. By including the 1 automatically we work directly in the central extension, and avoid the cohomological technicalities associated with the formal discussion of central extensions and projective representations.

for all $f, g \in \mathbb{L}$ and $\alpha, \beta \in \mathbb{C}$. Conjugation is defined as

$$(f_1 + if_2)^* := f_1 - if_2 \quad \text{for } f_1, f_2 \in \mathbb{L};$$

The axioms for a Lie $*$-algebra are easily established if $1 \in \mathbb{L}$. Note that the real dimension of $\mathbb{L}$ equals the complex dimension of $\mathbb{C}\mathbb{L}$. It is easy to check that

$$\operatorname{Re} \mathbb{C}\mathbb{L} \cong \mathbb{L}.$$

Conversely, for a Lie $*$-algebra $\mathbb{L}$,

$$\mathbb{C} \operatorname{Re} \mathbb{L} \cong \mathbb{L}.$$

If a complex Lie algebra $\mathbb{L}'$ is isomorphic to $\mathbb{C}\mathbb{L}$ as a Lie algebra, one says that $\mathbb{L}$ is a **real form** of the complex Lie algebra $\mathbb{L}'$.

We leave it as an exercise to verify $\mathbb{C}su(n) \cong sl(n, \mathbb{C})$ and $\mathbb{C}so(p, q) = so(p + q, \mathbb{C})$. In general, a complex Lie algebra has more than one real form as we can see since for $p \neq q, n-q$ the Lie algebras $so(p, n - p)$ and $so(q, n - q)$ are not isomorphic.

An **involutive Lie algebra** (Neeb [199]) is a Lie algebra $\tilde{\mathbb{L}}$ with Lie product $[\cdot, \cdot]$ and with an involutive, antilinear anti-automorphism σ, i.e., a mapping $\sigma : \tilde{\mathbb{L}} \to \tilde{\mathbb{L}}$ satisfying

$$\sigma(\alpha f) = \alpha^* \sigma f, \quad \sigma(f \angle g) = \sigma g \angle \sigma f$$

for $\alpha \in \mathbb{C}, f, g \in \tilde{\mathbb{L}}$. Associated to an involutive Lie algebra $\tilde{\mathbb{L}}$ is the **real form** $\tilde{\mathbb{L}}_{\mathbb{R}} = \left\{ x \in \tilde{\mathbb{L}} \mid \sigma x = -x \right\}$. Our definition of a Lie $*$-algebra is closely related and obtained as follows, after adjoining to $\tilde{\mathbb{L}}$ a central element 1 if necessary. We define $\mathbb{L}$ as the vector space $\tilde{\mathbb{L}}$ equipped with the Lie product $\angle$ defined by $x \angle y = \frac{i}{\hbar}[x, y]$. Then the mapping $x \mapsto i\hbar x$, with $\hbar$ a positive real constant (in physical applications Planck's constant) is an isomorphism of Lie algebras. The map σ induces the conjugation $x^* = -\sigma x$ and $\operatorname{Re} \mathbb{L} = \tilde{\mathbb{L}}_{\mathbb{R}}$.

11.6.2 Remarks.
(i) The nomenclature of Lie $*$-algebras is a bit tricky. If $\mathbb{L}$ is a Lie $*$-algebra, we therefore denote it (usually) with the name of the real Lie algebra $\operatorname{Re} \mathbb{L}$. To avoid confusion, it is important to keep track of whether we are discussing real Lie algebras, complex Lie algebras or Lie $*$-algebras.

(ii) In the physics literature, one often sees the defining relations (11.1) for real Lie algebras written in terms of complex structure constants,

$$X_j \angle X_k = \sum_l i c_{jkl} X_l \,.$$

where $i = \sqrt{-1}$ and the c_{jkl} are real. That is, the Lie product takes values outside of the real Lie algebra! What is done by the physicists is that – as in the above definition of a Lie $*$-algebra from an involutive Lie algebra – they multiply all elements in the Lie algebra by i. The reasons for making this seemingly difficult construction mainly has historical reasons. One is that in some real algebras the elements are antihermitian matrices. By multiplying with i one obtains Hermitian matrices and in quantum mechanics, observable quantities are represented as Hermitian operators.

The converse process of complexification is **realization**. Given a complex Lie algebra $\mathbb{L}$, one regards it as a real Lie algebra $\mathbb{L}^{\mathbb{R}}$ by restricting scalar multiplication to real factors. Since f and the imaginary scalar multiple if are linearly independent over $\mathbb{R}$, the real dimension of $\mathbb{L}^{\mathbb{R}}$ is twice the complex dimension of $\mathbb{L}$. In the finite-dimensional case, a convenient way to obtain the realization is as follows: Choose a basis $t_1, \ldots, t_n$ of $\mathbb{L}$ and then form the elements $s_j = it_j$ for all j. All real linear combinations of s_j and t_j make up $\mathbb{L}^{\mathbb{R}}$. Given two elements f, g in $\mathbb{L}^{\mathbb{R}}$ one calculates their Lie product as if they were elements of $\mathbb{L}$; the result can be written as

$$f \angle g = \sum (\alpha_j + i\beta_j) t_j \,.$$

The Lie product of f and g in $\mathbb{L}$ is then defined as

$$f \angle g = \sum \alpha_j t_j + i \sum \beta_j s_j \,.$$

See also Example 11.4.2.

Chapter 12

Mechanics in Poisson algebras

This chapter brings more physics into play by introducing Poisson algebras, i.e., associative algebras with a compatible Lie algebra structure. These are the algebras in which it is possible to define Hamiltonian mechanics. Poisson algebras abstract the algebraic features of both Poisson brackets and commutators, and hence serve as a unifying tool relating classical and quantum mechanics. In particular, we discuss classical Poisson algebras for oscillating and rotating systems.

12.1 Poisson algebras

Many algebras that we will encounter have both an associative product and a Lie product, which are compatible in a certain sense. Such algebras are **Poisson algebras**, our definition of which is the noncommutative version discussed, e.g., in Farkas & G. Letzter [86]. (In contrast, in classical mechanics on Poisson manifolds, one usually assumes Poisson algebras to be always commutative.)

12.1.1 Definition. A **Poisson algebra** $\mathbb{E}$ is a Lie algebra with an associative and distributive **multiplication** which associates with $f, g \in \mathbb{E}$ its **product** fg, and an **identity** 1 with respect to multiplication, such that the compatibility condition

$$f\angle(gh) = (f\angle g)h + g(f\angle h) \tag{12.1}$$

holds. Equation (12.1) is also called the **Leibniz identity**.

In expressions involving the associative product and the Lie product, the binding of the associative product is stronger than the Lie product, i.e., $f\angle gh$ is interpreted as $f\angle(gh)$, and $fg\angle h$ as $(fg)\angle h$.

12.1.2 Remarks. Since Poisson algebras have two products, neither of which is assumed to be commutative, we reserve the notation $[f, g]$ for the **commutator**

$$[f, g] := fg - gf$$

with respect to the associative product. If $[f,g]=0$ we say that f and g **commute**. If $f\angle g=0$ we say that f and g **Lie commute**. An element which commutes (Lie commutes) with every element in $\mathbb{E}$ is called **central (Lie central)**.

12.1.3 Example. We take $C^\infty(\mathbb{R}\times\mathbb{R})$ where the associative product is given by ordinary multiplication of functions, and where the Lie product is given by $f\angle g=f_pg_q-f_qg_p$. To see that the Leibniz condition is satisfied we write

$$\begin{aligned} f\angle gh &= f_p(gh)_q-f_q(gh)_p \\ &= f_pg_qh+f_pgh_q-f_qg_ph-f_qgh_p \\ &= (f\angle g)h+g(f\angle h)\,. \end{aligned}$$

Thus $C^\infty(\mathbb{R}\times\mathbb{R})$ is a commutative Poisson algebra.

12.1.4 Example. For a Euclidean space $\mathbb{H}$ we consider the space $\operatorname{Lin}\mathbb{H}$ of continuous linear operators on $\mathbb{H}$. The Lie product is given by

$$f\angle g=\frac{i}{\hbar}[f,g]=\frac{i}{\hbar}(fg-gf)\,.$$

We have

$$\begin{aligned} f\angle gh &= \frac{i}{\hbar}\Big(fgh-ghf\Big) \\ &= \frac{i}{\hbar}\Big(fgh-gfh+gfh-ghf\Big) \\ &= \frac{i}{\hbar}\Big([f,g]h+g[f,h]\Big)\,. \end{aligned}$$

Hence $\operatorname{Lin}\mathbb{H}$ is a non-commutative Poisson algebra. In particular, taking $\mathbb{H}=\mathbb{C}^n$, we find that $\mathbb{C}^{n\times n}$ is a non-commutative Poisson algebra.

These examples are prototypical for the application in physics. Indeed, the Poisson algebras relevant for classical mechanics are commutative and are defined via differential operators, while the Poisson algebras relevant for qunatum mechanics are noncommutative and typically defined via a commutator.

We note some immediated consequences of the axioms, which show that the Lie product has close similarities with differentiation.

12.1.5 Proposition. *Let $\mathbb{E}$ be a Poisson algebra. Then*

$$f\angle 1=0,$$

and

$$f\angle g^n=ng^{n-1}(f\angle g)\quad \text{if}\ \ [f\angle g,g]=0\,.$$

Proof. We first take $n=0$ and calculate

$$f\angle 1=f\angle(1\cdot 1)=(f\angle 1)1+1(f\angle 1)=2(f\angle 1)\,,$$

from which it follows that $f\angle 1 = 0$. Let us therefore suppose that the proposition is true for all k with $0 \leq k \leq n$, then for $k = n+1$ we have

$$f\angle(g^{n+1}) = (f\angle g^n)g + g^n(f\angle g) = ng^{n-1}(f\angle g)g + g^n(f\angle g) = ng^n(f\angle g)\,.$$

□

12.1.6 Definition. A **Poisson $*$-algebra** is a Poisson algebra that as a Lie algebra is a Lie $*$-algebra (defined in Definition 11.6.1) satisfying the additional rule

$$(fg)^* = g^* f^*\,.$$

Note the change of order in $(fg)^* = g^* f^*$, while the ordering of the Lie product is preserved under the involution $*$.

12.1.7 Example. The commutative Poisson algebra $C^\infty(\mathbb{R}\times\mathbb{R})$ is made into a Poisson $*$-algebra by defining

$$f^*(p,q) := \overline{f(p,q)}.$$

We have $(f^*)_p(p,q) = \overline{f_p(p,q)}$, and

$$(fg)^*(p,q) = \overline{fg}(p,q) = \overline{f(p,q)}\;\overline{g(p,q)} = (f^*g^*)(p,q),$$

hence $(fg)^* = f^*g^* = g^*f^*$ since the algebra is commutative. From these considerations it follows immediately that $C^\infty(\mathbb{R}\times\mathbb{R})$ is a Poisson $*$-algebra.

12.1.8 Example. We make $\mathrm{Lin}\,\mathbb{H}$ with the quantum Lie product (11.21) into a non-commutative Poisson $*$-algebra by defining A^* to be the adjoint conjugate transpose of A, which is defined as the linear operator A^* such that

$$\langle A\phi,\psi\rangle = \langle \phi, A^*\psi\rangle\,, \qquad \text{for all } \phi,\psi\in\mathbb{H}\,,$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product on $\mathbb{H}$. In particular, if $\mathbb{H}=\mathbb{C}^n$ then $\langle\phi,\psi\rangle = \phi^*\psi$ and A^* is the conjugate transpose of the matrix $A\in\mathbb{C}^{n\times n}$. For general $\mathbb{H}$, we have

$$\langle AB\phi,\psi\rangle = \langle B\phi, A^*\psi\rangle = \langle\phi, B^*A^*\psi\rangle\,,$$

from which we read off that $(AB)^* = B^*A^*$. Then it follows that

$$\begin{aligned} A\angle B &= \left(\frac{i}{\hbar}[A,B]\right)^* = -\frac{i}{\hbar}((AB)^* - (BA)^*) = -\frac{i}{\hbar}(B^*A^* - A^*B^*) \\ &= \frac{i}{\hbar}(A^*B^* - B^*A^*) = \frac{i}{\hbar}[A^*,B^*] = A^*\angle B^*\,. \end{aligned}$$

Hence $\mathrm{Lin}\,\mathbb{H}$ is a Poisson $*$-algebra.

12.2 Rotating rigid bodies

The spinning top is the classical model of a spinning particle. Like a football, the top can be slightly deformed but when the external force is released it jumps quickly back to its equilibrium state. Molecular versions of a football are the fullerenes, the most football-like fullerene being a molecule with 60 carbon atoms arranged in precisely the same manner as the vertices that can be seen in the corners between the patches on the surface of an official football. In a reasonable approximation, the deformability can be neglected; the spinning top, and also the fullerene soccer ball, is most often treated as a rigid body.

The spinning top is treated in most undergraduate courses in mechanics; hence there is a rich literature on the topic.[1] Due to the abundance of classical treatments of the spinning top we pursue here a nonstandard approach based on Poisson algebras, which shows how it is a special prototypical case of a uniform algebraic approach to mechanical systems.

A rigid body can be moving as a whole, that is, its center of mass can have a nonzero velocity, but changing to comoving coordinates via a time-dependent translation, one may assume that the center of mass is not moving. The coordinate system in which the center of mass of the rigid body is fixed is in physics literature called the **center of mass coordinate system**. Without loss of generality we then assume the center of mass is at the origin $(0,0,0)$.

Having fixed the center of mass the rigid body can still rotate, but after rotating the coordinate system to the body-fixed one, no freedom is left. This means that the **pose** of a rigid body with fixed center of mass is completely described by a rotation $Q(t) \in SO(3)$.

Thus $Q(t)$ satisfies $Q(t)Q(t)^T = Q(t)^T Q(t) = 1$ and $\det Q(t) = 1$. Differentiating we get

$$\dot{Q}(t)Q(t)^T + Q(t)\dot{Q}(t)^T = 0\,.$$

Calling $\Omega(t) = \dot{Q}(t)Q(t)^T = \dot{Q}(t)Q(t)^{-1}$ we thus have

$$\Omega(t)^T = -\Omega(t)\,,$$

that is Ω is antisymmetric. We can therefore parameterize Ω as

$$\Omega = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}.$$

We then have $\Omega\mathbf{v} = \omega \times \mathbf{v}$, where ω is the vector $(\omega_1, \omega_2, \omega_3)^T$. We view $\Omega(t)$ as a matrix $X(\omega(t))$ depending on the vector $\omega(t)$, called the **angular velocity**.

A rigid body in a conserved system has an energy that can depend on the position determined by $Q(t)$ and the velocity $\dot{Q}(t)$. Since $\dot{Q} = \Omega Q^{-T} = \Omega Q = X(\omega)Q$, the energy thus depends on Q and ω: the Hamiltonian $H = H(Q, \omega)$ is a function of Q and ω.

[1] Good accounts of the standard approach can be found, e.g., in Arnold [15], Marion & Thornton [183], or Goldstein [106].

For a **freely rotating body**, the Hamiltonian only depends on the kinetic energy and is quadratic in the angular velocity;

$$H = H(\omega) = \frac{1}{2}\omega^T I \omega\,,$$

and we can always take I symmetric, $I = I^T$. The 3×3-matrix I, called the **tensor of moments of inertia**, or just **inertia tensor**, has the meaning of an **angular mass matrix** analogous to the mass matrix M given in Chapter 5 for the case of an oscillating particle, where the kinetic energy was given by $H = \frac{1}{2}\mathbf{v}^T M \mathbf{v}$. The reason why it is called a tensor and not a matrix is because I is in fact a bilinear form.[2] Under a coordinate change I does transform as a bilinear form and not as a matrix. Indeed, under the change of coordinates $\omega \mapsto \tilde{Q}\omega$ for some $\tilde{Q} \in SO(3)$, the Hamiltonian is invariant and thus I transforms as $I \mapsto Q^{-T} I Q^{-1}$, that is, by a congruence transformation. In contrast, a matrix A transforms as $A \mapsto QAQ^{-1}$, which is a similarity transformation. By a coordinate change I can be made diagonal, so that we may assume that

$$H = \frac{1}{2}\sum_{k=1}^{3} I_k \omega_k^2\,.$$

The coefficients I_k are called the **principal moments of inertia**. To have a Hamiltonian that is bounded from below we require $I_i \geq 0$. In practice one has $I_k > 0$ for all $k = 1, 2, 3$; then I is invertible.

In analogy to the linear momentum $p = Mv = \frac{\partial H}{\partial v}$ for an oscillating particle with kinetic energy $H = \frac{1}{2}v^T M v$, we define the **angular momentum J** by

$$\mathbf{J} := \frac{\partial H}{\partial \omega} = I\omega\,.$$

We rewrite the Hamiltonian as a function of $\mathbf{J}$;

$$H = \frac{1}{2}\mathbf{J}^T I^{-1} \mathbf{J}\,, \tag{12.2}$$

in analogy to the formula $H = \frac{1}{2}\mathbf{p}^T M^{-1}\mathbf{p}$ for the oscillating particle. We have

$$\frac{\partial H}{\partial \mathbf{J}} = I^{-1}\mathbf{J} = \omega, \tag{12.3}$$

in analogy with $\mathbf{v} = \frac{\partial H}{\partial \mathbf{p}} = M^{-1}\mathbf{p}$.

12.3 Rotations and angular momentum

In Section 3.4, we used the J_k as generators of the rotations; they are basis elements of the Lie algebra $\mathbb{L} = so(3)$. The J_k correspond to the angular momenta of a spinning particle (see

[2]The same holds for the mass matrix – but there the terminology has become traditional.

Section 12.2). Thus there is a more physical interpretation; the J_k correspond to measurable quantities, the components of the angular momentum. We denote the observable that corresponds to J_k with the same symbol J_k. Purely classical, the state of a rigid rotating body in its rest frame is defined by specifying a numerical value for $\mathbf{J} = (J_1, J_2, J_3)^T$, called the **angular momentum** of the rigid body.

The dynamics of a rigid body is determined by the equation $\dot{\mathbf{J}} = \mathbf{J} \times \omega$, where $\omega = I^{-1}\mathbf{J}$ is the angular velocity of the rigid body and I is the constant inertia tensor.

Thus the state at a given time determines uniquely its value at any time, and therefore the value of every classical observable $f(\mathbf{J})$, i.e., every function of the angular momentum, such as the angular velocity or the **total angular momentum** $\mathbf{J}^2$. In analogy with the case of a single particle, we therefore consider the manifold $\mathbb{R}^3$ of possible states $\mathbf{J}$ to be the phase space of the rotating rigid body.

To study the observables, i.e., functions of $\mathbf{J}$, we begin with polynomials. We write $\operatorname{Pol}\mathbb{L}$ for the **polynomial algebra** generated by 1 and the J_i, and give this algebra the structure of a Poisson algebra. The recipe obtained will then be further generalized to cover arbitrary C^∞-functions of $\mathbf{J}$.

Motivated by the $so(3)$ structure we define a product $\angle$ recursively, starting with the commutation relations of $so(3)$ with 1 adjoined,

$$1\angle J_k = 0\,, \quad J_k\angle J_l = \sum_m \epsilon_{klm} J_m\,.$$

With the abbreviation $a_1J_1 + a_2J_2 + a_3J_3 = a\cdot\mathbf{J}$, this gives

$$1\angle a\cdot\mathbf{J} = 0\,, \quad a\cdot\mathbf{J}\angle b\cdot\mathbf{J} = (a\times b)\cdot\mathbf{J}\,.$$

Having given the product on the generators of $\operatorname{Pol}\mathbb{L}$, the product is completely determined by the Leibniz rule

$$a\cdot\mathbf{J}f(\mathbf{J})\angle b\cdot\mathbf{J} = (a\cdot\mathbf{J}\angle b\cdot\mathbf{J})f(\mathbf{J}) + a\cdot\mathbf{J}(f(\mathbf{J})\angle b\cdot\mathbf{J})$$

for $f \in \operatorname{Pol}\mathbb{L}$.

12.3.1 Lemma. *We have the identity*

$$f(\mathbf{J})\angle b\cdot\mathbf{J} = (b\times\mathbf{J})\cdot\frac{\partial f(\mathbf{J})}{\partial\mathbf{J}}\,,$$

where $\mathbf{J}$ *as a vector in* $(\operatorname{Pol}\mathbb{L})^3$ *means* $(J_1, J_2, J_3)^T$*, with components* $J_k \in \operatorname{Pol}\mathbb{L}$.

Proof. The proof is by induction. For degree of f zero the statement is trivial. For degree 1 we have

$$a\cdot\mathbf{J}\angle b\cdot\mathbf{J} = (a\times b)\cdot\mathbf{J} = (b\times\mathbf{J})\cdot a = (b\times\mathbf{J})\cdot\frac{\partial a\cdot\mathbf{J}}{\partial\mathbf{J}}\,.$$

Here we use a vector notation, that is, we consider $\mathrm{Pol}\,\mathbb{L}$. Now suppose the statement is true for some $n \geq 1$, then we consider next a homogeneous polynomial of degree $n+1$ and write it as $a \cdot \mathbf{J} f(\mathbf{J})$ (or a linear sum of such). Next we consider on the one hand

$$a \cdot \mathbf{J} f(\mathbf{J}) \angle b \cdot \mathbf{J} = (a \times b) \cdot \mathbf{J} f(\mathbf{J}) + a \cdot \mathbf{J} b \times \mathbf{J} \cdot \frac{\partial f(\mathbf{J})}{\partial \mathbf{J}}\,,$$

and on the other hand

$$\begin{aligned}(b \times \mathbf{J}) \cdot \frac{\partial}{\partial \mathbf{J}}\Big(a \cdot \mathbf{J} f(\mathbf{J})\Big) &= (b \times \mathbf{J}) \cdot a f(\mathbf{J}) + a \cdot \mathbf{J}(b \times \mathbf{J}) \cdot \frac{\partial}{\partial \mathbf{J}} f(\mathbf{J}) \\ &= (a \times b) \cdot \mathbf{J} f(\mathbf{J}) + a \cdot \mathbf{J}(b \times \mathbf{J}) \cdot \frac{\partial}{\partial \mathbf{J}} f(\mathbf{J})\,,\end{aligned}$$

and by inspection the two expressions are the same. □

12.3.2 Lemma. *The product $\angle$ satisfies*

$$f(\mathbf{J}) \angle g(\mathbf{J}) = \Big(\frac{\partial g(\mathbf{J})}{\partial \mathbf{J}} \times \mathbf{J}\Big) \cdot \frac{\partial f(\mathbf{J})}{\partial \mathbf{J}} = \mathbf{J} \cdot \Big(\frac{\partial f(\mathbf{J})}{\partial \mathbf{J}} \times \frac{\partial g(\mathbf{J})}{\partial \mathbf{J}}\Big)\,. \tag{12.4}$$

Proof. We again proceed by induction, this time on the degree of g. For degree ≤ 1 of g, the previous lemma gives the result. Now suppose the result holds for polynomials up to degree $n \geq 1$. Now consider the polynomials of degree $n+1$ and write such a polynomial as a sum of terms $g(\mathbf{J})h(\mathbf{J})$ where g and h both have degree $\leq n$. Then for each such term we have

$$\begin{aligned}f(\mathbf{J}) \angle \Big(g(\mathbf{J})h(\mathbf{J})\Big) &= \Big(f(\mathbf{J}) \angle g(\mathbf{J})\Big) h(\mathbf{J}) + g(\mathbf{J}) \Big(f(\mathbf{J}) \angle h(\mathbf{J})\Big) \\ &= \Big(\frac{\partial g}{\partial \mathbf{J}} \times \mathbf{J}\Big) \cdot \frac{\partial f}{\partial \mathbf{J}} h(\mathbf{J}) + g(\mathbf{J}) \Big(\frac{\partial h}{\partial \mathbf{J}} \times \mathbf{J}\Big) \cdot \frac{\partial f}{\partial \mathbf{J}} \\ &= \Big(\frac{\partial (gh)}{\partial \mathbf{J}} \times \mathbf{J}\Big) \cdot \frac{\partial f}{\partial \mathbf{J}} = \mathbf{J} \cdot \Big(\frac{\partial f}{\partial \mathbf{J}} \times \frac{\partial (gh)}{\partial \mathbf{J}}\Big)\,.\end{aligned}$$

□

Note that although (12.4) was derived only for polynomials, its right hand side makes sense for arbitrary C^∞ functions of $\mathbf{J}$ Thus we take it as the definition of a Lie product on $C^\infty(\mathbb{R}^3)$:

12.3.3 Proposition. *The algebra $\mathbb{E} = C^\infty(\mathbb{R}^3)$ and its subalgebra $Pol(\mathbb{L})$ are Poisson algebras. That is, the product* (12.4) *is a Lie product satisfying the Leibniz identity.*

Proof. The antisymmetry of the product $\angle$ is obvious on the generators, for the other cases we use Lemma 12.3.1 and Lemma 12.3.2 together with the observation that $u \cdot \mathbf{J} \times w = w \cdot u \times \mathbf{J} = -w \cdot \mathbf{J} \times u$. The Leibniz identity is a direct consequence of the product rule for partial derivatives. The Jacobi identity is a bit tedious to check. Using the notation $f_k = \frac{\partial f}{\partial J_k}$ and

the Levi–Cività symbol, one writes the outer product for vectors as $(u\times v)_k = \sum_{lm} \epsilon_{klm} u_l v_m$. Then we find for the Lie product

$$f\angle g = \sum_{klm} \epsilon_{klm} J_l f_m g_k \,,$$

from which the antisymmetry follows immediately. Using the identity

$$\sum_m \epsilon_{klm}\epsilon_{mnp} = \delta_{kn}\delta_{lp} - \delta_{kp}\delta_{ln} \,,$$

one obtains after some algebraic calculations

$$(f\angle g)\angle h = \sum h_k f_k J_k g_l - h_k g_k J_l f_l + \sum \epsilon_{klm}\epsilon_{abc} J_m J_c h_l (f_a g_{bk} + f_{ak} g_b) \,,$$

where the summations are over all present indices. When summing over the cyclic permutations of f, g and h the first summation is easily seen to give zero. We write the second sum as

$$\epsilon_{klm}\epsilon_{abc} J_m J_c \Big(f_a g_{bk} h_l + f_{ak} g_b h_l + g_a h_{bk} f_l + g_{ak} h_b f_l + h_a f_{bk} g_l + h_{ak} f_b g_l \Big),$$

and focus on the term with two derivatives on f

$$\begin{aligned} \epsilon_{klm}\epsilon_{abc} J_m J_c \Big(f_{ak} g_b h_l + h_a f_{bk} g_l \Big) &= \epsilon_{klm}\epsilon_{abc} J_m J_c \Big(f_{ak} g_b h_l + h_k f_{la} g_b \Big) \\ &= \epsilon_{klm}\epsilon_{abc} J_m J_c \Big(f_{ak} g_b h_l - h_l f_{ka} g_b \Big) \\ &= 0 \,. \end{aligned}$$

The other terms cancel similarly. □

12.4 Classical rigid body dynamics

Many books on classical mechanics, see for example Marion and Thornton [183], Arnold [15] or Goldstein [106], present the standard approach to the dynamics of a spinning rigid body, resulting in the **Euler equations**. We take an alternative route, exploiting the Lie algebra structure corresponding to the rotation group. We write down the Lie product that determines the mechanics. We then derive the Euler equations and reproduce the same equations of motion. Thus we are giving an equivalent description.

The motivation for the form of the Lie product is determined by symmetry considerations. We have seen that the algebra of infinitesimal rotations – which must be involved in the differential equations describing the state of the spinning object – is $so(3)$, the Lie algebra of real, antisymmetric 3×3-matrices. In Section 12.5, we shall see that we can obtain a Lie–Poisson algebra out of any Lie algebra; in particular, we construct the Lie–Poisson algebra of $so(3)$ in Example 12.5.3. Since the dynamical observables of a physical system form

a Poisson algebra, we consider the Lie–Poisson algebra of arbitrarily often differentiable functions on $\mathbb{R}^3$, with coordinates J_1, J_2 and J_3, equipped with the Lie product given in Section 12.3

$$f\angle g := \left(\mathbf{J} \times \frac{\partial f}{\partial \mathbf{J}}\right) \cdot \frac{\partial g}{\partial \mathbf{J}}$$

for $f, g \in C^\infty(\mathbb{R}^3)$.

Now that we have the Poisson algebra and the Hamiltonian (12.2) for the classical mechanics of the spinning top, we can apply the usual recipe. For an observable f the time-evolution is given by

$$\dot{f} = H\angle f\,.$$

In particular, for the angular momentum we have from (12.3)

$$\dot{J}_k = H\angle J_k = \left(\mathbf{J} \times \frac{\partial H}{\partial \mathbf{J}}\right) \cdot \hat{e}_k = (\mathbf{J} \times \omega)_k\,,$$

where $\hat{e}_k$ is the unit vector in the direction k, and where we use $\partial H/\partial \mathbf{J} = I^{-1}\mathbf{J} = \omega$. We thus have

$$\dot{\mathbf{J}} = \mathbf{J} \times \omega\,.$$

Further, since $\mathbf{J} = I\omega$ we find $I\dot{\omega} = I\omega \times \omega$. Writing this out in components we find

$$\begin{pmatrix} I_1\dot{\omega}_1 \\ I_2\dot{\omega}_2 \\ I_3\dot{\omega}_3 \end{pmatrix} = \begin{pmatrix} I_1\omega_1 \\ I_2\omega_2 \\ I_3\omega_3 \end{pmatrix} \times \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix} = \begin{pmatrix} \omega_2\omega_3(I_2 - I_3) \\ \omega_1\omega_3(I_2 - I_1) \\ \omega_1\omega_2(I_1 - I_2) \end{pmatrix} \tag{12.5}$$

The equations (12.5) are the **Euler equations** for the spinning rigid body. The spinning direction is given by the vector $\mathbf{n} := \omega/|\omega|$ and the spinning speed is given by $|\omega|$. Thus knowing the trajectory of $\omega(t)$ in the phase space $\mathbb{R}^3$ at all times implies knowing everything about the direction and speed of the spinning motion.

We claim that $\mathbf{J}^2 = \mathbf{J} \cdot \mathbf{J}$ is a Casimir of the Lie algebra $so(3)$. Indeed, from (3.43) we have $J_1\angle J_2 = J_3$ and the other commutation relations can be obtained by cyclic permutation. But then

$$J_1\angle \mathbf{J}^2 = J_1\angle J_2^2 + J_1\angle J_3^2 = J_3J_2 + J_2J_3 - J_2J_3 - J_3J_2 = 0\,,$$

and for the other generators the results are similar. Since $\mathbf{J}^2$ is a Casimir of the Lie algebra, it is conserved by the dynamics. Indeed, calculating the time-derivative of $\mathbf{J}^2$ we find

$$(\mathbf{J}^2)^\bullet = 2\mathbf{J} \cdot \dot{\mathbf{J}} = 2\mathbf{J} \cdot \mathbf{J} \times \omega = 0\,.$$

Hence the motion preserves surfaces of constant $\mathbf{J}^2$, which are spheres. The radius of the sphere is determined by the initial conditions.

Note that the angular momentum phase space $\mathbb{R}^3$ cannot be symplectic since it is not even-dimensional. However, since we have a Poisson algebra, it is a Poisson manifold as described in Section 18.1.

In the present case, the symplectic leaves (co-adjoint orbits) are the surfaces where the Casimir $\mathbf{J}^2$ has a constant value; hence they are the spheres on which the motion takes

place. Indeed, 2-dimensional spheres in $\mathbb{R}^3$ have a natural symplectic manifold structure, on which the rotation group $SO(3)$ acts as a group of symplectic transformations.

Since the Hamiltonian is conserved (although for completely different reasons), the motion also preserves surfaces of constant $E = \frac{1}{2}\mathbf{J}^T I^{-1}\mathbf{J}$, which are ellipsoids. If I is not a multiple of the identity, this forces the motion to be on curves of constant $\mathbf{J}^T I^{-1}\mathbf{J}$ on the co-adjoint orbit, i.e., on the intersection of the sphere defining the co-adjoint orbit with the ellipsoid $\mathbf{J}^T I^{-1}\mathbf{J} = 2E$, where E is again determined by the initial conditions. Then only the speed along these curves needs to be determined to specify the motion. Thus the free spinning rigid body motion is exactly solvable.

Let us consider affine functions on the Poisson algebra of the classical spinning top. We calculate (for $a, b \in \mathbb{C}^3$ and $\alpha, \beta \in \mathbb{C}$)

$$(\alpha + a \cdot \mathbf{J})\angle(\beta + b \cdot \mathbf{J}) = (a \times \mathbf{J}) \cdot b = (b \times a) \cdot \mathbf{J}\,,$$

which describes the Lie algebra $u(2)$. Looking only at linear functions, that is, the linear subspace spanned by $\mathbf{J}$, we find the Lie algebra $so(3)$. The two Lie algebras only differ by the center of $u(2)$ and thus $u(2) \cong su(2) \oplus \mathbb{R} \cong \mathbb{R} \oplus so(3)$. This coincidence is due to the sporadic isomorphism $so(3) \cong su(2)$.

12.5 Lie–Poisson algebras

In the above section we started from a the Lie algebra structure of $so(3)$ to construct an associated Poisson algebra. This program can be repeated for arbitrary real Lie algebras.

The formulation closest to the physical applications is in terms of a Lie $*$-algebra $\mathbb{L}$. It applies to arbitrary real Lie algebras such as so(3) by taking their complexification and adding, if necessary, a central element 1, thus extending the dimension of the Lie algebra by one. As usual, we write $\mathbb{C}$ for the complex linear subspace spanned by the element 1. In case that $\mathbb{L}$ is infinite-dimensional, we assume $\mathbb{L}$ to be equipped with a topology in which all operations are continuous and that $\mathbb{L}$ is reflexive (see below); in finite dimensions this is automatic.

We consider the dual space $\mathbb{L}^*$ of continuous linear maps from $\mathbb{L}$ to $\mathbb{C}$, and the bidual space $\mathbb{L}^{**}$ of continuous linear maps from the dual space $\mathbb{L}^*$ to $\mathbb{C}$. For finite-dimensional vector spaces we have canonically $\mathbb{L}^{**} = \mathbb{L}$, for infinite-dimensional vector spaces in general only $\mathbb{L} \subseteq \mathbb{L}^{**}$; in both cases we have an injective map $\mathbb{L} \to \mathbb{L}^{**}$ given by

$$\delta \in \mathbb{L}\,, \quad \xi \in \mathbb{L}^* : \quad \delta(\xi) := \xi(\delta)\,.$$

A normed vector space is called reflexive if $\mathbb{L}^{**} \cong \mathbb{L}$. We need $\mathbb{L}$ to be reflexive for the construction that follows. We thus assume $\mathbb{L}^{**} \cong \mathbb{L}$ in the following.

For any real number λ (we shall need $\lambda = 0$ and $\lambda = 1$), we define the family of parallel affine hyperplanes

$$M_\lambda := \{\xi \in \mathbb{L}^* \mid \xi(f^*) = \xi(f)^* \quad \text{for all } f \in \mathbb{L},\ \xi(1) = \lambda\}\,.$$

One should note that M_0 is a real linear subspace in $\mathbb{L}^*$. The affine hyperplane M_1 carries the structure of a real submanifold, with the tangent space at each point being isomorphic to M_0.

If $\mathbb{L}$ is the complexification of a real Lie algebra $\mathbb{L}'$, so that we have $\mathbb{L} = \mathbb{L}' \otimes_{\mathbb{R}} \mathbb{C}$, then the elements of M_0 are the linear functionals ξ on $\mathbb{L}'$ that are zero on the element 1, and are extended to linear forms on $\mathbb{L}$ by linearity: $\xi(a + bi) = \xi(a) + i\xi(b)$ for $a, b \in \mathbb{L}'$. So we can identify M_0 in this case with the dual of the quotient Lie algebra $\mathbb{L}'/\mathbb{R}$, where $\mathbb{R}$ denotes the real subspace spanned by the distinguished central element 1. Therefore the dual of M_0 is again $\mathbb{L}'/\mathbb{R}$. In the general case M_0 is a real subspace in $(\mathbb{L}/\mathbb{C})^*$, so that $M_0\mathbb{C} = M_0 + iM_0$ satisfies $(M_0\mathbb{C})^* \cong \mathbb{L}/\mathbb{C}$.

We consider for a non-empty open subset M of M_1 the commutative algebra $\mathbb{E} = C^\infty(M)$. We define for every $f \in \mathbb{E}$ and $\xi \in M$ a linear map $df(\xi) : M_0 \to \mathbb{C}$ by

$$df(\xi)v = \lim_{t\to 0} \frac{f(\xi + tv) - f(\xi)}{t} \quad \text{for all } v \in M_0\,.$$

So we have $df(\xi) \in \mathrm{Lin}(M_0, \mathbb{C})$. Extending by $\mathbb{C}$-linearity we can view $df(\xi)$ as an element of $\mathrm{Lin}(M_0\mathbb{C}, \mathbb{C})$. Hence $df(\xi)$ defines an element in $(M_0\mathbb{C})^* \cong \mathbb{L}/\mathbb{C}$. We can find an element $Df(\xi)$ in $\mathbb{L}$ such that under the projection $\mathbb{L} \to \mathbb{L}/\mathbb{C}$ the element $Df(\xi)$ goes to $df(\xi)$. The choice of $Df(\xi)$ is not unique, but another choice $D'f(\xi)$ differs from $Df(\xi)$ by an element in $\mathbb{C}$, which is contained in the center.

We now show how the object $Df(\xi)$ can be chosen. We choose an arbitrary element $\omega \in \mathbb{L}^*$ with $\omega(1) = 1$. Then we can write $\mathbb{L}^*$ as a direct sum $\mathbb{L}^* = M_0\mathbb{C} \oplus W$ (as a complex vector space), where $W = \mathbb{C}\omega := \{\alpha\omega \mid \alpha \in \mathbb{C}\}$ is the 1-dimensional span of ω. Indeed, for an arbitrary element of $\xi \in \mathbb{L}^*$, the element $\xi' := \xi - \xi(1)\omega$ satisfies $\xi'(1) = 0$. Now ξ' can be written as a linear combination $u + iv$ of two elements $u, v \in M_0$. Thus $\xi = u + iv + \xi(1)\omega \in M_0\mathbb{C} \oplus W$. For any fixed choice of ω we define $Df(\xi)$ by

$$Df(\xi)u := df(\xi)(u - u(1)\omega)\,. \tag{12.6}$$

Note that $u - u(1) \in M_0\mathbb{C}$. The extended $Df(\xi)$ lies thus in $\mathbb{L}^{**}$. But $\mathbb{L}$ was assumed to be reflexive, hence we have $Df(\xi) \in \mathbb{L}$.

We are now in a position to define a Lie product on $\mathbb{E}$ by

$$(f\angle g)(\xi) = (Df(\xi)\angle Dg(\xi))(\xi) \quad \text{for all } \xi \in M \subset M_1\,,$$

where the Lie product on the right-hand side is that of $\mathbb{L}$. The left-hand side above is the complex number obtained by evaluating the function $h := f\angle g$ for the argument $\xi \in M \subseteq M_1 \subset \mathbb{L}^*$. The right-hand side is the complex number obtained from the bilinear pairing between $df(\xi)\angle dg(\xi) \in \mathbb{L}$ and the same ξ. Since the derivative of a smooth function is again smooth, $f\angle g$ is again an element of $\mathbb{E}$.

We see that the Lie product $f\angle g$ is independent of the choice of $Df(\xi)$ and $Dg(\xi)$, or equivalently, of the choice of ω in (12.6). Indeed, any other choice would differ only by an element in the center. But taking the Lie product in $\mathbb{L}$ the dependence of the central element drops out.

We have the following theorem:

12.5.1 Theorem. *The algebra $\mathbb{E}$ with the Lie product $\angle$ defined above is a Poisson algebra, called the* ***Lie–Poisson algebra*** *over $\mathbb{L}$. The restriction of the Lie product of $\mathbb{E}$ to affine functions coincides with the Lie product of $\mathbb{L}$.*

Proof. (Sketch): The definition of $\angle$ is independent of ω. The antisymmetry of $\angle$ is clear, and the Jacobi identity follows from that of $\mathbb{L}$, using the fact that partial derivatives commute. The Leibniz identity follows from the Leibniz property of differentiation. The injection $\mathbb{L} \to \mathbb{L}^{**}$ gives a map from the Lie algebra to the affine functions. We therefore regard the Lie algebra as a subalgebra of the affine functions. Since we assumed the Lie algebra $\mathbb{L}$ to be reflexive the affine functions represent elements of the Lie algebra. Indeed, for an affine function f we obtain a linear function by subtracting $f(0)$ and thus defines an element $f'$of $\mathbb{L}$. But $f(0)$ is a multiple of 1 and thus also an element of the Lie algebra, therefore $f = f' + f(0) \in \mathbb{L}$. □

We give two important examples.

12.5.2 Example. Consider $\mathbb{L} = h(1)$, the Heisenberg algebra, which is spanned by generators p, q and 1, with $p\angle q = 1$ and all other Lie products between the generators vanishing. We identify the dual $\mathbb{L}^*$ with $\mathbb{C}^3$ as follows,

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} (\alpha p + \beta q + \gamma) = x\alpha + y\beta + z\gamma\,,$$

for any choice α, β, and γ in $\mathbb{C}$. The affine hyperplane M_0 is in this case given by

$$M_0 = \left\{ \begin{pmatrix} x \\ y \\ 0 \end{pmatrix} \;\middle|\; x, y \in \mathbb{R} \right\},$$

and similarly, for M_1 we find

$$M_1 = \left\{ \begin{pmatrix} x \\ y \\ 1 \end{pmatrix} \;\middle|\; x, y \in \mathbb{R} \right\}.$$

If f is a smooth function on M_1, it is a smooth function $\mathbb{R}^2 \to \mathbb{R}$. For $df(\xi)$, $\xi = (x, y, 1)^T$ and $v = (a, b, 0)^T$ we find

$$df(\xi)v = \frac{\partial f(x,y)}{\partial x} a + \frac{\partial f(x,y)}{\partial y} b\,.$$

The simplest choice for $Df(\xi)$ corresponding to writing $h(1) = \mathbb{C}p \oplus \mathbb{C}q \oplus \mathbb{C}$, is

$$Df(\xi) = \frac{\partial f(x,y)}{\partial x} p + \frac{\partial f(x,y)}{\partial y} q\,.$$

If g is another smooth function $\mathbb{R}^2 \to \mathbb{R}$ we have

$$Df(\xi)\angle Dg(\xi) = \frac{\partial f(x,y)}{\partial x}\frac{\partial g(x,y)}{\partial y} - \frac{\partial f(x,y)}{\partial y}\frac{\partial g(x,y)}{\partial x} \in \mathbb{C} \subset h(1)\,,$$

and thus

$$(f\angle g)(\xi) = \frac{\partial f(x,y)}{\partial x}\frac{\partial g(x,y)}{\partial y} - \frac{\partial f(x,y)}{\partial y}\frac{\partial g(x,y)}{\partial x}\,,$$

which precisely corresponds to the Lie product associated to the dynamics of a single particle in one dimension.

More generally, an arbitrary Heisenberg algebra leads to general symplectic Poisson algebras on convenient vector spaces.

12.5.3 Example. We now show that for the choice $so(3)$ we recover the Lie product (12.4). We identify the real Lie algebra $so(3)$ with $\mathbb{R}^3$ equipped with the vector product. We adjoin a central element to obtain $so(3)\oplus 1$ and call $\mathbb{L}$ the complexification of $so(3)\oplus 1$. We write an element of $\mathbb{L}$ as (v,a) where $v\in\mathbb{C}^3$ and $a\in\mathbb{C}$, so that the Lie product is given by

$$(v,a)\angle(w,b) = (v\times w, 0)\,.$$

Of course, $v\times w$ is defined by extending the vector product on $\mathbb{R}^3$ by $\mathbb{C}$-linearity. We identify $\mathbb{L}^*$ with $\mathbb{C}^4$ as follows

$$\begin{pmatrix} x\\ y\\ z\\ t\end{pmatrix}(v,a) = xv_1+yv_2+zv_3+ta\,,\quad v=\begin{pmatrix} v_1\\ v_2\\ v_3\end{pmatrix}.$$

Thus we find that M_λ consists of the vectors $(x,y,z,\lambda)^T$ with x, y and z real numbers. A smooth function on M_1 is just a smooth function $\mathbb{R}^3\to\mathbb{R}$. For any smooth $f:\mathbb{R}^3\to\mathbb{R}$, and $\xi=(x,y,z,1)$ we define

$$\nabla f(\xi) = \Big(\frac{\partial f(\xi)}{\partial x},\frac{\partial f(\xi)}{\partial y},\frac{\partial f(\xi)}{\partial z}\Big)^T,$$

where we identify the vector $\xi=(x,y,z,1)$ in M_1 with the vector (x,y,z) in $\mathbb{R}^3$. We see that we can choose $Df(\xi)=(\nabla f(\xi),0)$ and the Lie product on $\mathbb{E}$ is then given by

$$f\angle g(\xi) = \xi\cdot(\nabla f(\xi)\times\nabla g(\xi))\,,$$

which is precisely (12.4); $(x,y,z)^T$ corresponds to $(J_1,J_2,J_3)^T$.

The attentive reader might have noticed that in Example 12.5.3, the central element 1 played no role at all. As mentioned before, when a Lie algebra has no distinguished central element one can always add one. However, in this case one can also proceed directly as follows. For a real Lie algebra $\mathbb{L}$, we consider the dual $\mathbb{L}^*$ and the algebra $\mathbb{E}$ of real-valued smooth functions on $\mathbb{L}^*$. Let $f\in\mathbb{E}$ and $\xi\in\mathbb{L}^*$. The 1-form $df(\xi)$ is an element of the dual of the tangent space at ξ. Since $\mathbb{L}^*$ is a vector space and $\mathbb{L}$ is assumed to be reflexive, the dual of the tangent space at ξ is again $\mathbb{L}$. Hence $df(\xi)$ defines an element of the Lie algebra, which we also denote by $df(\xi)$. Then we define the Lie product on $\mathbb{E}$ for $f,g\in\mathbb{E}$ as follows $(f\angle g)(\xi)=\xi(df(\xi)\angle dg(\xi))$, that is, to get $(f\angle g)(\xi)$ the function ξ is evaluated at the Lie algebra element $df(\xi)\angle dg(\xi)$. We leave it as an exercise that this gives the same result for real Lie algebras that do not have a distinguished central element.

It turns out that the majority of commutative Poisson algebras relevant in physics are Lie–Poisson algebras constructible from a suitable Lie algebra, or natural quotients of such algebras. In particular, this holds for the Poisson algebra of classical symplectic geometry in $\mathbb{R}^N$, which come from general Heisenberg algebras, and for all but one of the Poisson algebras for nonequilibrium thermodynamics constructed in Beris and Edwards [33].

12.6 Classical symplectic mechanics

A conservative physical system is completely characterized by three main ingredients: the kinematical algebra, the Hamiltonian, and the state. The **kinematical algebra** of the system is a Lie $*$-algebra $\mathbb{L}$ which defines the kinematics, i.e., the structure of the quantities whose knowledge determines the system. The **Hamiltonian** H defines the dynamics. It is a Hermitian quantity in an associative algebra $\mathbb{E}$ carrying a particular representation of the kinematical algebra, a Poisson representation in the classical case, and a unitary representation in the quantum case. The state encodes all properties of the physical state of an individual realization of the system at a fixed time.

The kinematical algebra determines the kinematical symmetries of a whole class of systems which differ in Hamiltonian and state. This means that applying a transformation of the corresponding symmetry group transforms a system of this class into another system of the same class, usually with a different Hamiltonian. Those (often few) symmetries which preserve a given Hamiltonian are called symmetries of the system; applying a symmetry of the system changes possible state space trajectories of the system into other possible trajectories, usually affecting the states. Those (even fewer) symmetries which preserve the Hamiltonian and the state are symmetries of the particular realization of the system, and hence directly measurable.

The kinematical algebra may admit (up to isomorphism) one or many Poisson representations for classical systems, and one or many unitary representations for the corresponding quantum systems. For example, a Heisenberg algebra with finitely many degrees of freedom admits only one unitary representation, which is the content of the Stone–Von Neumann theorem.

In the nonrelativistic case, the Hamiltonian is an element of the Poisson algebra for classical systems, and for quantum systems the Hamiltonian is an element of the universal enveloping algebra of the Lie $*$-algebra.

Let $\mathbb{E}$ be the algebra determined by the physical system, that is, either $\mathbb{E}$ is the Lie–Poisson algebra of the classical system, or $\mathbb{E} = \operatorname{Lin}\mathbb{H}$ for a Euclidean space $\mathbb{H}$ whose closure is a Hilbert space. Both the Lie algebra $\mathbb{L}$ and the space-time symmetry group are represented inside $\mathbb{E}$.

We now consider the special case of classical N-particle systems describing the motions of a molecule.] The algebra $\mathbb{E}$ consists of the complex-valued functions on phase space M

and each point $z \in M$ in phase space determines a state $\langle \cdot \rangle_z$ by

$$\langle f \rangle_z := f(z),$$

called a **classical pure state**. Note that evaluation at a point $z \in M$ is more than a linear functional; an evaluation gives an algebra homomorphism $C^\infty(M;\mathbb{R}) \to \mathbb{R}$ since $(fg)(z) = f(z)g(z)$; hence we have a character of the commutative algebra $\mathbb{E}$. If the phase space M is an open subset of $\mathbb{R}^n$, the evaluations are the only characters of $\mathbb{E}$. This can be seen as follows. Take any algebra homomorphism $\varphi : C^\infty(M) \to \mathbb{R}$. Let $x_1, \ldots, x_n$ be coordinates on M and denote by $a_i = \varphi(x_i)$ the images of the coordinate functions. The homomorphism φ thus determines a point $z = (a_1, \ldots, a_n)$ in $\mathbb{R}^n$. We have to show $z \in M$. Suppose $z \notin M$, then

$$f(x_1, \ldots, x_n) = \sum_j (x_j - a_j)^2$$

is a function that does not vanish on M, and thus is an invertible element of $C^\infty(M)$. If an element x is invertible, then so is its image under any homomorphism. Indeed, if $xy = 1$, then $\varphi(xy) = \varphi(x)\varphi(y) = \varphi(1) = 1$. But the function f is mapped to zero under φ and hence cannot be invertible. Hence we arrive at a contradiction and the assumption $z \notin M$ is false.

A mixed classical state is a weighted mixture of pure classical states. That is, there is a real-valued function ρ on the phase space M, called the **density**, taking nonnegative values and integrating to one

$$\int_M \rho(z) d\mu(z) = 1\,,$$

such that

$$\langle f \rangle = \int_M \rho(z) f(z) d\mu(z)\,. \tag{12.7}$$

The integration measure $d\mu$ depends on the application. In symplectic mechanics, the symplectic Poisson bracket determines the Lie product, one uses the **Liouville measure**, defined in local coordinates (q, p) by

$$d\mu(z) = dq_1 \cdots dq_n dp_1 \cdots dp_n.$$

Consider a system containing N particles. Then each particle has a momentum and a position. Hence phase space is $6N$-dimensional. The Lie algebra is given by the relations $p_{ia} \angle q_{jb} = \delta_{ij}\delta_{ab}$ where p_{ia} is the ath component of the momentum of the ith particle and q_{jb} is the bth component of the position of the jth particle. The obtained Lie algebra is the Heisenberg algebra $h(N)$.

In molecular mechanics, the Hamiltonian is of the simple form[3]

$$H = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_i} + V(\mathbf{q}_1, \ldots, \mathbf{q}_N)\,,$$

[3]The more general form $H = \frac{1}{2}\sum_{i,j=1}^N G_{ij}(\mathbf{q}_1, \ldots, \mathbf{q}_N)\mathbf{p}_i\mathbf{p}_j + V(\mathbf{q}_1, \ldots, \mathbf{q}_N)$, where G is a configuration-dependent inverse mass matrix, appears at various places in physics. When the potential V is constant (so that we can put it to zero), the physical system is sometimes called a **σ-model**. Such models play an important role in modern high-energy physics and cosmology. Some authors prefer to include a potential into the definition of a σ-model.

where the **potential** $V(\mathbf{q}_1, \ldots, \mathbf{q}_N)$ describes the potential energy of the configuration with positions $(\mathbf{q}_1, \ldots, \mathbf{q}_N)$.

The states in symplectic mechanics are precisely the states of the form (12.7). If the system is such that we can measure at one instant of time all positions and momenta exactly (obviously an idealization), the configuration is precisely given by the point $z = (\mathbf{q}_1, \ldots, \mathbf{q}_N, \mathbf{p}_1, \ldots, \mathbf{p}_N)$ in phase space, and $\langle f \rangle = f(z)$ for all $f \in \mathbb{E}$. Thus the density degenerates to a product of delta functions of each phase space coordinate. Thus classical pure states are equivalent to points z in phase space, marking position and momentum of each point of interest, such as the centers of mass of the stars, planets, and moons making up a celestial system.

12.7 Molecular mechanics

Consider a molecule consisting of N atoms. The molecule is chemically described by assigning bonds between certain pairs of atoms, reflecting the presence of chemical forces that – in the absence of chemical reactions which may break bonds – hold these atoms close together. Thus a molecule may be thought of as a graph embedded in 3-dimensional space, in which some but usually not all atoms are connected by a bond. The chemical structure of the molecule is thus described by a connected graph, the **formula** of the molecule. (In the following, we ignore multiple bonds, which are just a way to indicate stronger binding than for single bonds, reflected in the interaction potential.) We write $i \sim j$ if there is a bond between atom i and atom j and similarly we write $i \sim j \sim k$ if there is a bond connecting i and j and there is a bond connecting j and k. The notation is extended to longer chains: $i \sim j \sim k \sim l \sim \ldots$.

The interactions between the atoms in a molecule are primarily through the bonds, and to a much smaller extent through forces described by a pair potential and through multibody forces for joint influences of several adjacent bonds.

The geometry is captured mathematically by assigning to the jth atom a 3-dimensional coordinate vector

$$q_j = \begin{pmatrix} q_{j1} \\ q_{j2} \\ q_{j3} \end{pmatrix}$$

specifying the position of the atom in space. If two atoms with labels j and k are joined by a chemical bond, we consider the corresponding **bond vector** $q_j - q_k$, with **bond length** $\|q_j - q_k\|$. At room temperature, the bonds between adjacent atoms i and j are quite rigid, meaning that the deviation from the average distance r_{ij} is generally small and the force that tries to maintain the atoms at distance r_{ij} is strong. In chemistry this is modeled by a term

$$V_{\text{bond}}(q_1, \ldots, q_N) = \sum_{i \sim j} \frac{a_{ij}}{2} (\|q_i - q_j\| - r_{ij})^2$$

in the Hamiltonian, where the a_{ij} are **stiffness constants**, parameters determined by the particular chemical structure.

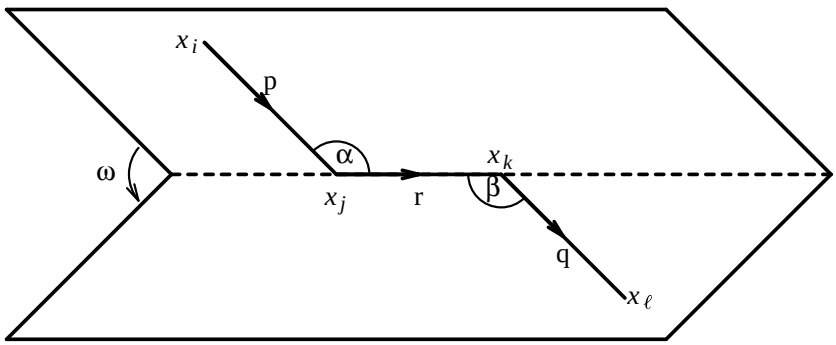


Figure 12.1: Bond vectors, bond angles, and the dihedral angle

Consider two adjacent bonds $i \sim j$ and $k \sim l$. The **bond angle** α is the angle between the bond vectors $q_j - q_i$ and $q_l - q_k$. The bond angle α can then be computed from the formulas

$$\cos\alpha = \frac{(q_i - q_j)\cdot(q_k - q_j)}{\|q_i - q_j\|\|q_k - q_j\|}, \quad \sin\alpha = \frac{\|(q_i - q_j)\times(q_k - q_j)\|}{\|q_i - q_j\|\|q_k - q_j\|},$$

and is thus invariant under the simultaneous action of the group $ISO(3)$ on all 3 vectors. In most molecules the bond angles are determined from the interaction between the atoms in the molecule. There is thus an $ISO(3)$-invariant term

$$V_{\text{angle}}(q_1, \ldots, q_N) = \sum_{i\sim j\sim k} a_{ijk}\Phi(q_i, q_j, q_k)$$

in the potential with $\Phi : (\mathbb{R}^3)^3 \to \mathbb{R}$ an $ISO(3)$-invariant function, and a_{ijk} are some parameters.

Finally, the **dihedral angle** $\omega = \sphericalangle(i \sim j \sim k \sim l)$ (or the complementary **torsion angle** $2\pi - \omega$) measures the relative orientation of two adjacent angles in a chain $i \sim j \sim k \sim l$ of atoms. It is defined as the angle between the normals through the planes determined by the atoms i, j, k and j, k, l, respectively, and can be calculated from

$$\cos\omega = \frac{(q_i - q_j)\times(q_k - q_j)\cdot(q_j - q_k)\times(q_l - q_k)}{\|(q_i - q_j)\times(q_k - q_j)\|\|(q_j - q_k)\times(q_l - q_k)\|},$$

and

$$\sin\omega = \frac{|(q_i - q_j)\times(q_l - q_k)\cdot(q_k - q_j)|\,\|q_k - q_j\|}{\|(q_i - q_j)\times(q_k - q_j)\|\|(q_j - q_k)\times(q_l - q_k)\|}.$$

Again, the angle between the planes is $ISO(3)$-invariant and therefore described by an $ISO(3)$-invariant function $\Psi : (\mathbb{R}^3)^4 \to \mathbb{R}$ of the positions of the four atoms. Hence to model the molecule there is a term

$$V_{\text{dihedral}}(q_1, \ldots, q_N) = \sum_{i\sim j\sim k\sim l} a_{ijkl}\Psi(q_i, q_j, q_k, q_l)$$

in the Hamiltonian, with again a_{ijkl} parameters. The total Hamiltonian is then taken to be

$$H = \sum_i \left(\frac{p_i^2}{2m_i} + V_{\text{bond}}(q_1, \ldots, q_N) + V_{\text{angle}}(q_1, \ldots, q_N) + V_{\text{dihedral}}(q_1, \ldots, q_N)\right).$$

The above Hamiltonian is of a special type; it is a member of the family of Hamiltonians of the form

$$H = \sum_i \frac{p_i^2}{2m_i} + V(q_1, \ldots, q_N)\,.$$

This family of Hamiltonians is favorable since there are no mixed terms between the momenta and the positions. Therefore, in the quantum theory there is no ambiguity in how the quantum mechanical Hamiltonian has to be written, since the momenta commute among themselves and the positions commute among themselves, too.

The group $ISO(3)$ plays an important role here purely on symmetry grounds; how and where a molecule is located in $\mathbb{R}^3$ does not determine the chemical properties. Hence the Hamiltonian should depend on $ISO(3)$-invariant quantities only.

From the above we see that the one in practice is given a representation $j : G \to GL(V)$ of some group in a vector space. The construction of a suitable Hamiltonian can be facilitated by knowing the invariants in the tensor representations $V \otimes V$, $V \otimes V \otimes V$ and so on. If V is irreducible, V might contain one or more one-dimensional subrepresentations on which G acts trivially; these are precisely the invariants in V. Hence knowing the irreducible representations of G is of great importance.

Now suppose that G has an irreducible representation j on V. Then $g \in G$ acts on $V \otimes V$ as follows: $g : v \otimes w \mapsto j(g)v \otimes j(g)w$, and similarly for higher order tensor products. It is almost never the case that the representation of G in tensor products of irreducible representations is again irreducible. But, in many cases, the decomposition of $V \otimes V$, $V \otimes V \otimes V$, etc. into irreducible representations is known.

In the case of $ISO(3)$ the representation is in $\mathbb{R}^3$, which contains no invariants since all points of $\mathbb{R}^3$ form a single orbit. But, as we have shown in Section 12.7, $V \otimes V$, $V \otimes V \otimes V$ and $V \otimes V \otimes V \otimes V$ do have invariants: distances and angles.

12.8 An outlook to quantum field theory

Quantum field theory is the area in physics where fields are treated by quantum mechanics. The way physicists think of this is more or less as follows. As we have seen in Chapter 5, classical linear field equations, such as the Maxwell equations, can be seen as describing a family of harmonic oscillators labeled by a continuum of pairs $(\mathbf{p}, s)$ of momenta $\mathbf{p}$ and spin or helicity s. Therefore, what has been treated above is nice, but for quantum field theory it is not enough. One needs an infinite number of oscillators. Treating such a system becomes mathematically sophisticated, because topological details start playing a dominant role. A way to deal with this heuristically, often employed by physicists, is by discretizing space-time in a box. On each point of the lattice one places a harmonic oscillator; then there are just a finite number of oscillators. To get the quantum field theory, one considers the limit in which the size of the box goes to infinity and the spacing of the lattice goes to zero. Then the oscillators are not described by operators a_k and a_k^+ that are labeled by

vectors k, but by operators $a(x)$ and $a^+(x)$ that are labeled by the continuous four-vector index x. The limit might not exist. . . .

In two space-time dimensions the limit is well-defined for interacting field theories, that is, for field theories where the different fields can interact. In case of four dimensions, the correct limit is only known for non-interacting field theories. From experience we know that there is interaction, of course, so our description shows serious shortcomings. After the preceding description of representations, it is interesting to note that,- in the field theory limits, the metaplectic representations still exist.

For 2-dimensional field theories with one space and one time dimension, this leads to satisfactory quantum field theories (such as conformal field theory) . But for 4-dimensional field theories, the metaplectic representation is restricted to a class of operators not flexible enough for capturing the physics. This is the main mathematical obstacle for formulating a consistent framework for 4-dimensional quantum field theories.

Chapter 13

Representation and classification

13.1 Poisson representations

Consider the Heisenberg algebra $h(n)$ with the usual generators 1, p_i, and q_i, and the corresponding Lie–Poisson algebra $\mathbb{E}(h(n))$. The subalgebra of all polynomials in q_i, p_j is closed under the Lie product, and hence a Poisson subalgebra. More interestingly, there are several Lie subalgebras of low degree polynomials, which we shall now explore. We write z for the $2n$-tuple

$$z = \begin{pmatrix} p \\ q \end{pmatrix}$$

of all the generators except 1. All linear polynomials without constant term can be written as $a \cdot z$ for some $a \in \mathbb{C}^{2n}$. On $\mathbb{C}^{2n}$ we introduce the antisymmetric bilinear form ω, represented in the given basis by the matrix J:

$$\omega(a, b) = a^T J b\,, \quad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\,,$$

where the entries in J are $n \times n$-matrices, i.e., $1 = 1_n$, etc.. The bilinear form ω is nondegenerate and antisymmetric, and we have

$$a \cdot z \angle b \cdot z = \omega(a, b)\,. \tag{13.1}$$

Any quadratic expression in $\mathbb{E}(h(n))$ is a linear sum of expressions of the form

$$(a \cdot z)(b \cdot z)\,.$$

We consider two such expressions and calculate their Lie product, using the Leibniz rule twice.

$$\begin{aligned}
(a \cdot z)(b \cdot z) \angle (c \cdot z)(d \cdot z) &= a \cdot z((b \cdot z) \angle (c \cdot z)(d \cdot z)) + (a \cdot z \angle (c \cdot z)(d \cdot z)) b \cdot z \\
&= (b \cdot z)(c \cdot z)\omega(a, d) + (b \cdot z)(d \cdot z)\omega(a, c) \\
&\quad + (a \cdot z)(c \cdot z)\omega(b, d) + (a \cdot z)(d \cdot z)\omega(b, c)\,,
\end{aligned}$$

which is a quadratic expression. Hence the homogeneous quadratic polynomials form a Lie subalgebra of $\mathbb{E}(h(n))$. We show below that this Lie algebra is related to $sp(2n,\mathbb{C})$. We proceed in physicist's fashion by looking at a conveniently chosen basis. In Section 21.4 we give a second derivation in a coordinate independent fashion, which generalizes to the fermionic case and gives Lie algebras related to the real orthogonal groups.

The generators of $h(n)$ are 1, p_i and q_i. Consider the elements

$$Q_{ij} = q_i q_j\,, \quad P_{ij} = p_i p_j\,, \quad E_{ij} = \frac{1}{2}(q_i p_j + p_j q_i)\,,$$

of the universal enveloping algebra. We have $Q_{ij} = Q_{ji}$ and $P_{ij} = P_{ji}$. We find the commutation relations:

$$\begin{aligned}
Q_{ij}\angle Q_{kl} &= 0\,, \quad P_{ij}\angle P_{kl} = 0\,,\\
E_{ij}\angle E_{kl} &= -\delta_{il}E_{kj} + \delta_{jk}E_{il}\,,\\
E_{ij}\angle Q_{kl} &= \delta_{jl}Q_{ik} + \delta_{jk}Q_{il}\,,\\
E_{ij}\angle P_{kl} &= -\delta_{il}P_{jk} - \delta_{ik}P_{jl}\,,\\
Q_{ij}\angle P_{kl} &= -\delta_{ik}E_{jl} - \delta_{jk}E_{il} - \delta_{jl}E_{ik} - \delta_{il}E_{jk}\,.
\end{aligned}$$

The Lie algebra $sp(2n,\mathbb{C})$ is given by the complex $2n\times 2n$-matrices that preserve the above given J:

$$X \in sp(2n,\mathbb{C}) \;\Leftrightarrow\; X^T J + JX = 0\,.$$

Taking X in block form as

$$X = \begin{pmatrix} A & B \\ C & D \end{pmatrix}\,,$$

we find $X \in sp(2n,\mathbb{C})$ if and only if $C = C^T$, $B = B^T$ and $D = -A^T$. If we introduce the $n\times n$-matrices e_{ij} that are 1 on the ij-entry and zero elsewhere, we have $e_{ij}e_{kl} = \delta_{jk}e_{il}$ and the matrices

$$A_{ij} = \begin{pmatrix} e_{ij} & 0 \\ 0 & -e_{ji} \end{pmatrix}\,, \quad B_{ij} = \begin{pmatrix} 0 & e_{ij}+e_{ji} \\ 0 & 0 \end{pmatrix}\,, \quad C_{ij} = \begin{pmatrix} 0 & 0 \\ e_{ij}+e_{ji} & 0 \end{pmatrix}\,,$$

form a basis for $sp(n,\mathbb{C})$. We find the commutation rules

$$\begin{aligned}
B_{ij}\angle B_{kl} &= 0\,, \quad C_{ij}\angle C_{kl} = 0\,,\\
A_{ij}\angle A_{kl} &= -\delta_{il}A_{kj} + \delta_{jk}A_{il}\,,\\
E_{ij}\angle B_{kl} &= \delta_{jl}B_{ik} + \delta_{jk}B_{il}\,,\\
A_{ij}\angle C_{kl} &= -\delta_{il}C_{jk} - \delta_{ik}C_{jl}\,,\\
B_{ij}\angle C_{kl} &= \delta_{ik}E_{jl} + \delta_{jk}E_{il} + \delta_{jl}E_{ik} + \delta_{il}E_{jk}\,.
\end{aligned}$$

Sending Q_{ij} to $-B_{ij}$, P_{ij} to C_{ij} and E_{ij} to A_{ij} we have an isomorphism between the algebras.

We now allow for inhomogeneous quadratic polynomials by adjoining the linear forms of the algebra $\mathbb{E}(h(n))$ to this Lie algebra. Everything commutes with the central element 1,

so we will not write down the commutation relations with 1. The commutation relations of the other basis elements are found to be

$$\begin{aligned} Q_{ij}\angle q_k &= P_{ij}\angle p_k = 0\,, \\ Q_{ij}\angle p_k &= -\delta_{ik}q_j - \delta_{jk}q_i\,, \\ P_{ij}\angle q_k &= -\delta_{ik}p_j - \delta_{jk}p_i\,, \\ E_{ij}\angle q_k &= \delta_{ik}q_j\,, \\ E_{ij}\angle p_k &= -\delta_{jk}p_i\,. \end{aligned}$$

We define the Lie subalgebra $\mathbb{L}'$ of $\mathbb{E}(h(n))$ as the Lie subalgebra of quadratic expressions in the generators and we define $\mathbb{L} = \mathbb{L}'/\mathbb{C}$, so that in $\mathbb{L}$ we have $q_i\angle p_j = 0$. Using the previously established isomorphism with $sp(2n,\mathbb{C})$ it is not too hard to see that $\mathbb{L}$ is isomorphic to the Lie algebra $isp(2n,\mathbb{C})$, which is defined as the Lie algebra of all $(2n+1)\times(2n+1)$-matrices of the form

$$\begin{pmatrix} A & r \\ 0 & 0 \end{pmatrix},$$

with A a $2n\times 2n$-matrix in $sp(2n,\mathbb{C})$ and r a $2n$-vector. We have thus shown that $\mathbb{L}'$ is a central extension of $isp(2n,\mathbb{C})$.

13.2 Linear representations

Of great interest in quantum mechanics are certain realizations of Lie algebras and of Lie groups by means of operators on vector spaces. We therefore address the concept of a representation of a Lie algebra. In the previous chapter we have already given a short discussion of finite-dimensional representations of finite-dimensional Lie algebras.

13.2.1 Definition.
(i) A **(linear) representation** of a Lie algebra $\mathbb{L}$ in an associative algebra $\mathbb{E}$ is a linear map $J:\mathbb{L}\to\mathbb{E}$ such that

$$J(f\angle g) = J(f)J(g) - J(g)J(f) \quad \text{for all } f,g\in\mathbb{L}.$$

The representation is called **faithful** if J is injective. A **linear representation** on a (finite- or infinite-dimensional) vector space $\mathbb{H}$ is a representation in the algebra $\mathbb{E} = \mathrm{Lin}\,\mathbb{H}$. In the case that $\mathbb{E}$ is the algebra of $n\times n$ matrices with entries in $\mathbb{K}$ one obtains the definition of Section 13.3. A linear representation is called **irreducible** when the only subspaces closed under multiplication by linear mappings of the form $J(f)$ are 0 and $\mathbb{H}$.

(ii) A **unitary representation** of a Lie $*$-algebra $\mathbb{L}$ is a linear map $J:\mathbb{L}\to\mathbb{E}$ in the $*$-algebra $\mathbb{E} = \mathrm{Lin}\,\mathbb{H}$ of continuous linear operators of a Euclidean space $\mathbb{H}$ (with $*$ being the adjoint), satisfying

$$J(1) = 1\,, \quad J(f^*) = J(f)^*\,, \quad J(f\angle g) = \frac{i}{\hbar}\Big(J(f)J(g) - J(g)J(f)\Big).$$

Note that by Proposition 11.2.3, an associative algebra $\mathbb{E}$ becomes in a natural way a Lie algebra by defining $f\angle g = [f,g] = fg - fg$. Hence a representation of a Lie algebra $\mathbb{L}$ in an algebra $\mathbb{E}$ is a Lie algebra homomorphism from $\mathbb{L}$ to $\mathbb{E}$, with $\mathbb{E}$ regarded as a Lie algebra. If the representation is faithful, the image of $\mathbb{L}$ is a Lie subalgebra of $\mathbb{E}$ isomorphic to $\mathbb{L}$. In this case, one often identifies the elements of $\mathbb{L}$ with their images, and then speaks of an **embedding** of $\mathbb{L}$ into $\mathbb{E}$. By the Theorem of Ado mentioned in Section 11.4, every finite-dimensional real Lie algebra has a faithful representation.

The enveloping algebra. In a representation, the elements of $\mathbb{L}$ are represented by matrices or linear operators. From a given set of matrices we can form the algebra that these matrices generate, containing the unit matrix, all finite products and their linear combinations. This motivates us to consider an object that already encompasses this algebra for all representations: the universal enveloping algebra of a Lie algebra $\mathbb{L}$. In general it is constructed by considering the tensor algebra $T(\mathbb{L})$, which is given by

$$T(\mathbb{L}) = \mathbb{K} \oplus \mathbb{L} \oplus (\mathbb{L} \otimes \mathbb{L}) \oplus (\mathbb{L} \otimes \mathbb{L} \otimes \mathbb{L}) \oplus \ldots = \bigoplus_{i=0}^{\infty} \mathbb{L}^{\otimes i} .$$

One makes $T(\mathbb{L})$ into an associative noncommutative algebra over the complex numbers by defining the product ab to be the tensor product $a \otimes b$.

Within $T(\mathbb{L})$ we consider the ideal $\mathcal{J}$ generated by all elements of the form

$$x \otimes y - y \otimes x - [x,y]$$

for all x, y in $\mathbb{L}$. Thus an element in $\mathcal{J}$ is a sum of elements of the form

$$a \otimes (x \otimes y - y \otimes x - [x,y]) \otimes b ,$$

for some $a, b \in T(\mathbb{L})$. The **universal enveloping algebra** of $\mathbb{L}$ is then defined as the associative noncommutative algebra $\mathcal{U}(\mathbb{L})$ over the complex numbers given by

$$\mathcal{U}(\mathbb{L}) = T(\mathbb{L})/\mathcal{J} .$$

Another view on the universal enveloping algebra $\mathcal{U}(\mathbb{L})$ would be as follows. One chooses a basis $\{t_i\}$ for $\mathbb{L}$ and considers the associative noncommutative polynomial algebra in the generators while imposing the relation

$$t_i t_j - t_j t_i = [t_i, t_j] .$$

Thus we consider the associative algebra generated by 1 and by the generators of $\mathbb{L}$ and impose the Lie product, which in this case is the commutator, by hand. The algebra we obtain in this way is canonically isomorphic to the universal enveloping algebra $\mathcal{U}(\mathbb{L})$.

The universal enveloping algebra thus contains the Lie algebra, i.e. envelopes the Lie algebra. This approach is very practical and therefore often used by physicists. There exists a more sophisticated definition, using a so-called universal property. One then proves that such an object is unique and that the given definition above has this universal property.

We do not expand on the definition using the universal property but refer to the literature, see, e.g., JACOBSEN [136], KNAPP [154], or FUCHS & SCHWEIGERT [95]. It is because of this universal property that $\mathcal{U}(\mathbb{L})$ is usually called the universal enveloping algebra, and not just the enveloping algebra.

The main reason to define the universal enveloping algebra is to study the representations of the Lie algebra. Every representation of the Lie algebra induces a unique representation of the *associative* universal enveloping algebra, and conversely, every representation of the universal enveloping algebra induces a representation of the Lie algebra itself. In a sense, all finite-dimensional representations are maps of the associative universal enveloping algebra to the associative algebra of $n \times n$-matrices for some n.

Casimir elements. An element $C \in \mathcal{U}(\mathbb{L})$ in the center of the universal enveloping algebra, i.e. that commutes with all other elements of $\mathcal{U}(\mathbb{L})$, is called a **Casimir element**, or just Casimir and sometimes also Casimir operator. If $\mathbb{L}$ has a representation in a vector space V, then for any $c \in \mathbb{K}$ the subspace $V_c = \{v \in V | Cv = cv\}$ is invariant under the action of $\mathbb{L}$, precisely because C is in the center of $\mathcal{U}(\mathbb{L})$. Hence if the representation V is irreducible, V_c must be the whole of V for some c and the other V_c are zero. That means, C acts diagonally in irreducible representations.

The classical analogue of the universal enveloping algebra is the Lie–Poisson algebra discussed in Chapter 12.5.

13.3 Finite-dimensional representations

We have already seen in Section 11.4 that the Lie algebra $gl(n, \mathbb{K})$ has many interesting Lie subalgebras. Given an arbitrary Lie algebra $\mathbb{L}$ it is interesting to see how we can represent $\mathbb{L}$ as a Lie algebra of matrices. In this section we consider finite-dimensional Lie algebras and finite-dimensional representations in more detail.

For any vector space V over $\mathbb{K}$ we denote $gl(V)$ the Lie algebra of linear maps from V to V with the Lie product given by the commutator $f \angle g = fg - gf$. If V is identified with $\mathbb{K}^n$ we write $gl(V) = gl(n, \mathbb{K})$ (see Section 11.4). A Lie algebra homomorphism $\phi : \mathbb{L} \to gl(V)$ is called a **finite-dimensional representation** of $\mathbb{L}$; the vector space V is then called an $\mathbb{L}$**-module**. We call the representation complex if $\mathbb{K} = \mathbb{C}$ and real if $\mathbb{K} = \mathbb{R}$. We have already seen that $su(n)$ has a complex representation, since it is defined as a (real) subalgebra of $gl(n, \mathbb{C})$.

Given a representation $\phi : \mathbb{L} \to gl(V)$ we call W an **invariant subspace** of V if $\phi(f)w \in W$ for all $f \in \mathbb{L}$ and all $w \in W$. The representation is called **irreducible** if the only invariant subspaces are 0 and V. We call the representation **decomposable** or **fully reducible**, if for any invariant subspace W there is a complementary invariant subspace W' such that $V = W \oplus W'$.

If $\phi_1 : \mathbb{L} \to gl(V_1)$ and $\phi_2 : \mathbb{L} \to gl(V_2)$ are representations of $\mathbb{L}$ we can form the direct sum

representation $\phi_{1\oplus 2} : \mathbb{L} \to gl(V_1 \oplus V_2, \mathbb{K})$ by defining

$$\phi_{1\oplus 2}(f)(v_1 + v_2) = \phi_1(f)(v_1) + \phi_2(f)(v_2)$$

for $f \in \mathbb{L}$ and $v_1 \in V_1$, $v_2 \in V_2$. It is easy to check the representation property. In terms of matrices, the direct sum representation corresponds to the map given by

$$f \mapsto \begin{pmatrix} \phi_1(f) & 0 \\ 0 & \phi_2(f) \end{pmatrix}$$

in block matrices.

If $\phi_1 : \mathbb{L} \to gl(V)$ and $\phi_2 : \mathbb{L} \to gl(W)$ are representations of $\mathbb{L}$ we can form the tensor product representation $\phi_{1\otimes 2}$ as follows: Each element f in $\mathbb{L}$ is sent to the linear map

$$\phi_{1\otimes 2}(f)(v \otimes w) = (\phi_1(f)v) \otimes w + v \otimes (\phi_2(f)w) \tag{13.2}$$

for all $v \in V$ and $w \in V$. It is easy to check that (13.2) defines a representation.

In Section 13.5 we have already mentioned the adjoint representation $\mathrm{ad} : \mathbb{L} \to gl(\mathbb{L})$ defined by

$$\mathrm{ad}_f : g \mapsto [f, g]\,.$$

The map ad is clearly linear, and from the Jacobi identity we see

$$\mathrm{ad}_x \mathrm{ad}_y(z) - \mathrm{ad}_y \mathrm{ad}_x(z) = \mathrm{ad}_{[x,y]}(z)\,,$$

hence

$$[\mathrm{ad}_x, \mathrm{ad}_y] = \mathrm{ad}_{[x,y]}.$$

We can now rephrase the definition of the ideal (see Section 13.5) as follows: $I \subset \mathbb{L}$ is an ideal if and only if I is an invariant subspace of the adjoint representation.

13.4 Representations of Lie groups

Lie group representations have a similar definition as Lie algebra representations.

13.4.1 Definition. A representation of a Lie group $\mathbb{G}$ in an associative algebra $\mathbb{E}$ with identity 1 is a map $U : \mathbb{G} \to \mathbb{E}$ such that

$$U(fg) = U(f)U(g), \quad U(1) = 1.$$

The representation is called **faithful** if U is injective. If $\mathbb{E} = \mathrm{Lin}\,\mathbb{H}$, one speaks again of a **linear representation** on $\mathbb{H}$. A linear representation is called **irreducible** if the only subspaces closed under multiplication by linear mappings of the form $U(f)$ are 0 and $\mathbb{H}$. A **unitary representation** of a Lie group $\mathbb{G}$ is a linear representation in the $*$-algebra $\mathbb{E} = \mathrm{Lin}\,\mathbb{H}$ of continuous linear operators of a Euclidean space $\mathbb{H}$, satisfying

$$U(f)^* U(f) = 1.$$

It is easy to see that $U(f^{-1}) = U(f)^{-1}$, and in the unitary case, $U(f^{-1}) = U(f)^{-1} = U(f)^*$.

Note that the invertible elements of $\mathbb{E}$ form a group and a Lie group representation of $\mathbb{G}$ in $\mathbb{E}$ is a group homomorphism of $\mathbb{G}$ into this group. Again, if the representation is faithful, one may identify group elements with their images under the representation, and then has an **embedding** of $\mathbb{G}$ into the algebra $\mathbb{E}$. Thus if $\mathbb{E}$ is the algebra of $n \times n$ matrices with entries in $\mathbb{K}$ we get a group homomorphism of $\mathbb{G}$ into $GL(n, \mathbb{K})$. For $\mathbb{K} = \mathbb{C}$ the representation is unitary if the image of $\mathbb{G}$ lies inside $U(n)$.

If a Lie algebra representation $J : \mathbb{L} \to \mathbb{E}$ is an embedding, we can get something that is close to a representation of the Lie group by exponentiation, i.e., by defining

$$U(e^f) := e^{J(f)} = \sum_{k=0}^{\infty} \frac{J(f)^k}{k!},$$

provided this converges for all $f \in \mathbb{L}$ in the topology of $\mathbb{E}$. In Subsection 13.4 we go deeper into the question of how to get a Lie group representation from a Lie algebra representation and the problems one encounters. On the other hand, given a representation U of a Lie group $\mathbb{G}$ with Lie algebra $\mathbb{L}$ we can get a representation J of the Lie algebra by differentiation, i.e., by defining

$$J(X) := \frac{d}{dt} U(e^{tX})\Big|_{t=0},$$

provided the derivative always exists. In finite dimensions, both constructions work generally; in infinite dimensions, suitable assumptions are needed to make the constructions work.

The group $\mathbb{G}$ acts on the Lie algebra $\mathbb{L}$. We will discuss this shortly for groups of matrices. For every element $g \in \mathbb{G} \subset GL(n, \mathbb{K})$ we define $\mathrm{Ad}(g)$ which is a linear transformation of $\mathbb{L}$ given by

$$\mathrm{Ad}(g) : X \mapsto gXg^{-1}.$$

It holds that $\mathrm{Ad}(g)X \in \mathbb{L}$, which we will not prove. The interested reader is referred to Knapp [154], Helgason [124], Frankel [91], or Kirillov [151]. For all the examples discussed so far, the reader can check it by hand. The map $\mathrm{Ad} : g \to \mathrm{Ad}(g)$ clearly satisfies $\mathrm{Ad}(gh) = \mathrm{Ad}(g)\mathrm{Ad}(h)$ and is thus a representation, which is called the **adjoint** representation of the group $\mathbb{G}$.

Universal covering group. For Lie algebra representations an important construct is the universal enveloping algebra. For Lie groups there is an analogue. Above we mentioned that by differentiating a representation of a Lie group, one obtains a representation for the corresponding Lie algebra. By exponentiating a representation of the Lie algebra one gets a representation for those group elements that can be written as exponents. If a group is not connected, one does not obtain a representation of the group in this way.

Other problems arise when the group is not simply connected. For example $SO(3)$ is not simply connected and therefore certain representations of the Lie algebra cannot be lifted

to representations of the Lie group; the spin representations become multivalued. Even other problems arise when two Lie groups that are fundamentally different have isomorphic Lie algebras. Consider for example the group $U(1)$ of complex numbers of absolute value 1. As a manifold $U(1)$ is just the circle S^1. The Lie group of $U(1)$ is the one-dimensional abelian Lie algebra (there is only one). Now consider the Lie group $\mathbb{R}$ where the group operation is addition $a \cdot b = a + b$. Then $\mathbb{R}$ is a one-dimensional abelian Lie group with a one-dimensional Lie algebra. The Lie algebras of $U(1)$ and $\mathbb{R}$ are isomorphic, but the Lie groups are totally different. When we want to lift a Lie algebra representation of either of them to a Lie group representation, which group do we choose then?

These topological considerations lead one to the question whether there is a unique simply connected Lie group for a given Lie algebra. The answer is positive: for every real finite-dimensional Lie algebra $\mathbb{L}$ there is a unique simply connected Lie group $\mathbb{G}$ with Lie algebra $\mathbb{L}$. So given a Lie group $\mathbb{H}$ with Lie algebra $\mathbb{L}$ one can construct a unique simply connected Lie group $\mathbb{G}$ with Lie algebra $\mathbb{L}$. The group $\mathbb{G}$ is called the **universal covering group** of $\mathbb{H}$. Then $\mathbb{H}$ and $\mathbb{G}$ are locally isomorphic; there are small neighborhoods of the origin in both groups on which $\mathbb{H}$ and $\mathbb{G}$ are diffeomorphic to each other. The Lie group $\mathbb{H}$ is then a quotient of $\mathbb{G}$; $\mathbb{H} \cong \mathbb{G}/D$ for some discrete normal subgroup D of $\mathbb{G}$.

The exponential map $\mathbb{L} \to \mathbb{G}$ is in general not surjective, however, the image of the exponential map generates an interesting subgroup of $\mathbb{G}$, the connected component of $\mathbb{G}$, denoted $\mathbb{G}_0$. If $g \in \mathbb{G}$ lies in the connected component, we can write $g = e^{f_1} \cdots e^{f_r}$ for some Lie algebra elements $f_1, \ldots, f_r$. Given a Lie algebra representation we can uniquely lift it to a representation of the connected component of the Lie group $\mathbb{G}_0$ if $\mathbb{G}_0$ is simply connected. Therefore, in this case, the representations of the Lie algebra $\mathbb{L}$ are in a one-to-one correspondence with the representations of the universal covering group corresponding to $\mathbb{L}$.

Now let $\mathbb{H}$ be a Lie group with Lie algebra $\mathbb{L}$ and with universal covering group $\mathbb{G}$ such that $\mathbb{H} \cong \mathbb{G}/K$ for some normal subgroup K of $\mathbb{G}$. Given a Lie algebra representation of $\mathbb{L}$, we get a Lie group representation of $\mathbb{G}$. If the normal subgroup K is in the kernel of the representation, we get a well-defined representation of $\mathbb{H}$ as well. Conversely, given a representation of $\mathbb{H}$, we get a representation of $\mathbb{G}$ by first projecting to $\mathbb{G}/K$, so that K is in the kernel. Hence, representations of $\mathbb{H}$ are in one-to-one correspondence with representations of $\mathbb{G}$ that map K to the unit matrix.

13.5 Finite-dimensional semisimple Lie algebras

For finite-dimensional Lie algebras a lot is known about the general structure; here we give an overview over the results most useful in physics. Since no details are given, this section may be skipped on first reading.

Classifying all finite-dimensional Lie algebras is in a certain sense possible; all finite-dimensional Lie algebras are a semidirect product of a semisimple and a solvable Lie algebra (to be defined below). The classification of all semisimple real and complex Lie algebras

is completely understood. It turns out that the semisimple complex Lie algebras can be classified by studying certain root systems. The semisimple real Lie algebras are obtained by applying the classification of complex Lie algebras to the complexified Lie algebras and then finding all ways of turning the resulting complex Lie algebras into a Lie $*$-algebra; their real parts then give all semisimple real Lie algebras.

In the semisimple case, every representation is faithful; hence a representation is nothing more than an embedding into a matrix Lie algebra $gl(n, \mathbb{C})$, realizing the Lie algebra elements by matrices. Every Lie algebra $\mathbb{L}$ comes with a canonical representation, the **adjoint representation**, denoted ad, which maps an element f to the Hamiltonian derivative ad_f in direction f, introduced in Section 11.2. Thus to each Lie algebra element f we assign a linear operator on a vector space. The vector space is the Lie algebra itself and an element f of the Lie algebra is represented by the linear transformation ad_f that maps an element $g \in \mathbb{L}$ to $f \angle g$. In the mathematical literature, one often writes the Lie product as a commutator. Then the definition takes the form

$$ad_x(y) = [x, y] \,.$$

Due to the Jacobi identity this indeed defines a representation. For finite-dimensional Lie algebras, there is a canonical symmetric bilinear form called the **(Cartan–)Killing form**, which we write as B_{CK} and defined by

$$B_{CK}(x, y) = \mathrm{tr}(ad_x ad_y) \,.$$

Due to the Jacobi identity, the Killing form is invariant,

$$B_{CK}([x, z], y) = B_{CK}(x, [z, y]) \,.$$

Recall that an ideal of a Lie algebra $\mathbb{L}$ is a subspace I in $\mathbb{L}$ such that $\mathbb{L} \angle I \subseteq I$. Thus an ideal is an invariant subspace under the adjoint action of the Lie algebra on itself. A Lie algebra $\mathbb{L}$ is called **simple** if it is not one-dimensional and has no nontrivial ideals (distinct from 0 and $\mathbb{L}$). Thus the adjoint action of $\mathbb{L}$ on itself has no nontrivial invariant subspace. A Lie algebra is **semisimple** if it is a direct sum of simple Lie algebras. There is a convenient criterion for a Lie algebra to be semisimple:

13.5.1 Theorem. ***(Lemma of Cartan)***
A Lie algebra is semisimple if and only if its Killing form is nondegenerate.

Proof. The proof can be found in many Lie algebra textbooks such as Jacobsen [136], Humphreys [131], Knapp [154], or Fulton & Harris [96]. □

A finite-dimensional real Lie algebra $\mathbb{L}$ is called **compact** if its Killing form is negative definite. In this case, the Lemma of Cartan implies that $\mathbb{L}$ is semisimple. For example, the Lie algebra $so(3)$ is compact, whereas $so(2, 1)$ is noncompact. However, note that Lie algebras are vector spaces and therefore not compact as topological spaces in the usual topology.

For a given Lie algebra one may form the so-called **lower central series** (or **derived series**) of ideals:

$$\mathbb{L}_0 = \mathbb{L}\,, \quad \mathbb{L}_{n+1} = \mathbb{L}_n \angle \mathbb{L}_n\,, \quad n \geq 0\,.$$

The Lie algebra $\mathbb{L}$ is called **solvable** if there is an n such that $\mathbb{L}_n = 0$. A theorem of Levi says that every Lie algebra is a semidirect sum of a semisimple part P and a solvable ideal S (that is, S is a solvable Lie subalgebra that is an ideal in $\mathbb{L}$), such that $P \cong \mathbb{L}/S$. It follows that an important part of the classification of all Lie algebras is the classification of the simple Lie algebras.

The classification of the finite-dimensional complex simple Lie algebras can be done by classifying certain objects called finite **root systems**, associated to a choice of maximal commutative subalgebras called **Cartan subalgebras**. Associated to each root system is a finite **reflection group**, i.e., a group generated by elements whose square is 1. The finite reflection groups (also called **Coxeter groups**) which are not direct products of nontrivial smaller reflection groups arise as symmetry groups of regular polytopes. They have all been classified by Coxeter, and fall into five infinite families denoted by A_n (simplices), B_n, C_n, D_n (all three related to cubes and crosspolytopes), and I_n (polygons), and a few sporadic cases denoted by E_6, E_7, E_8, F_4, H_3, and H_4 (H_3 is the symmetry group of the dodecahedron and the icosahedron).

Most of the finite reflection groups are also realized as symmetry groups of a root system. All root systems give rise to semisimple Lie algebras, and irreducible root systems lead to simple Lie algebras. The classification says there are four infinite series of Lie algebras denoted A_n, B_n, C_n for $n \geq 1$ and D_n for $n \geq 4$ and five exceptional Lie algebras called E_6, E_7, E_8, G_2 and F_4. The corresponding reflection groups have the same labels, except for G_2 which corresponds to the hexagon I_6. It is a highly nontrivial result – and one of the most beautiful pieces of mathematics – that this gives a complete classification of the finite-dimensional semisimple complex Lie algebras.

The four infinite series of Lie algebras, called the **classical Lie algebras**, are realized geometrically as infinitesimal symmetry groups of certain bilinear forms, i.e., Lie algebras of linear transformations with zero trace whose exponentials leave the form invariant. The Lie algebras A_n are isomorphic to the **special linear** Lie algebras $sl(n+1,\mathbb{C})$ of $(n+1)\times(n+1)$-matrices with complex entries and trace zero. The Lie algebras B_n and D_n are the odd and even **special orthogonal** Lie algebras $so(m,\mathbb{C})$ ($m = 2n+1$ and $m = 2n$, respectively), consisting of complex antisymmetric $m \times m$-matrices. For the C-series we have $C_n = sp(2n,\mathbb{C})$, where the **symplectic** Lie algebras $sp(2n,\mathbb{C})$ are given by the complex $2n \times 2n$-matrices X satisfying $X^T J + JX = 0$ where J is the antisymmetric $2n \times 2n$-matrix given in block form by

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\,.$$

For each complex Lie algebra $\mathbb{L}$ of the A-, B-, C- or D-series, there is an associated (simply connected) Lie group denoted by the same, but capitalized letters, whose complexified tangent space at the identity coincides with the Lie algebra $\mathbb{L}$.

There is some redundancy in the nomenclature for low-dimensional Lie algebras: $A_1 \cong B_1 \cong C_1$, $B_2 \cong C_2$. It is easy to check that $sp(2,\mathbb{C}) \cong sl(2,\mathbb{C}) \cong so(3,\mathbb{C})$. The Lie algebra

$so(2)$ is one-dimensional (and hence abelian) and therefore not simple. The Lie algebra $so(4,\mathbb{C})$ is in fact semisimple, $so(4,\mathbb{C}) \cong so(3,\mathbb{C}) \oplus so(3,\mathbb{C})$, and not simple since each $so(3,\mathbb{C})$-factor is a nontrivial ideal. The Lie algebra $so(6,\mathbb{C})$ is isomorphic to $sl(4,\mathbb{C})$. For the just mentioned reasons, one starts the D-series for $n \geq 4$; $so(8,\mathbb{C})$ is the first in the series that is not isomorphic to any other. In fact, $so(8,\mathbb{C})$ is very special in that it has a large automorphism group (related to **triality**). For the exceptional simple Lie algebras E_6, E_7, E_8, F_4 and G_2, there is no simple geometric description as for those in the A-, B-, C- and D-series. However, the exceptional simple Lie algebras can be realized as infinitesimal symmetry groups of some algebraic structure. And to each exceptional Lie algebra $\mathbb{L}$ one can associate a Lie group, such that $\mathbb{L}$ is the complexification of the tangent space at the identity.

It is important to keep in mind over which field the Lie algebra is considered. For example, over the real numbers the Lie algebras $so(p,q) \equiv so(p,q;\mathbb{R})$ are non-isomorphic, apart from the trivial isomorphism $so(p,q) \cong so(q,p)$. Over the complex numbers we have $so(p,q;\mathbb{C}) \cong so(p+q,\mathbb{C})$, since over the complex numbers the sign of a nondegenerate symmetric bilinear form is not invariant. Even more severe things are dependent of the field; the real Lie algebra $so(1,3)$, which is extremely important in physics, is simple, but extending the field to the complex numbers we have $so(1,3;\mathbb{C}) \cong so(4,\mathbb{C}) \cong so(3,\mathbb{C}) \oplus so(3,\mathbb{C})$, which is not simple. (For applications to physics, this is actually an advantage.) However, this is as bad as it can get from the structural point of view; if a Lie algebra is semisimple over some field $\mathbb{K}$, then it is semisimple over all fields containing $\mathbb{K}$. This follows from the Lemma of Cartan 13.5.1: If the Killing form is nondegenerate over some field, then extending the field does not change this property.

The (semi-)simple real Lie algebras can also be classified, albeit the classification is a bit more complicated. See for example the books of Gilmore [104] (or, for the more mathematically minded, Helgason [124] or Knapp [154]). If a real Lie algebra $\mathbb{L}$ is simple, the complex extension – letting the scalars be complex – is either simple or of the form $S \oplus S$ for a simple complex Lie algebra S. Hence the classification of the real simple Lie algebras is still 'close' to the classification of the simple complex Lie algebras in the sense that no completely new structures appear. It is an amusing historical fact that Élie Cartan provided the classification of the complex simple Lie algebras and his son, Henri Cartan, finished the project so to say by classifying the real simple Lie algebras.

As we shall see in Chapter 20, the unitary representations of different real forms of the same complex Lie algebra can be quite different. The Lie algebra $so(2,1)$ does not admit a finite-dimensional unitary representation, whereas $so(3)$ does. All compact Lie algebras admit a unitary representation, and in fact, the adjoint representation is already unitary. The main difficulty in the proof of this lies in establishing that all compact Lie algebras admit a Lie $*$-algebra structure; this requires more theory and will not be discussed here. Since finite-dimensional unitary groups are compact, noncompact semisimple Lie algebras cannot have finite-dimensional unitary representations, apart from the trivial one which maps everything to zero.

13.6 Automorphisms and coadjoint orbits

The adjoint and coadjoint representations of a Lie algebra $\mathbb{L}$ extend to elements $g \in \operatorname{Aut}\mathbb{L}$ by defining

$$\delta^g := g\delta g^{-1} = \operatorname{Ad}_g \delta \quad \text{for } \delta \in \mathbb{L}$$

$$\omega^g = \operatorname{Ad}^*_{g^{-1}}\omega \quad \text{for } \omega \in \mathbb{L}^*$$

with the properties

$$(\delta\angle\varepsilon)^g = \delta^g\angle\varepsilon^g,$$

$$(\delta\angle\omega)^g = \delta^g\angle\omega^g, \quad (\omega\angle\delta)^g = \omega^g\angle\delta^g,$$

$$\delta^g(\omega^g) = \delta(\omega)$$

and for continuous motions $g \in C^1([0,1], \operatorname{Aut}\mathbb{L})$,

$$\frac{d}{d\tau}\delta^{g(\tau)} = \frac{dg}{d\tau}(\tau)\angle\delta^{g(\tau)},$$

$$\frac{d}{d\tau}\omega^{g(\tau)} = \frac{dg}{d\tau}(\tau)\angle\omega^{g(\tau)};$$

in short,

$$(\delta^g)^\bullet = \dot{g}\angle\delta^g, \quad (\omega^g)^\bullet = \dot{g}\angle\omega^g.$$

A set $\Omega \subseteq V$ is called **$\mathbb{L}$-invariant** (in a given representation Q of $\mathbb{L}$ on V) if, for all $\delta \in C([0,1], \mathbb{L})$ and all $\omega_0 \in \Omega$ there is a unique $\omega \in C^1([0,1], \Omega)$ such that

$$\dot{\omega}(\tau) = Q(\delta(\tau))\omega(\tau), \quad \omega(0) = \omega_0. \tag{13.3}$$

The set of points $\omega(1)$ reachable from a fixed ω_0 in this way is called the **orbit** $\operatorname{Orb}(\omega_0)$ of ω_0. The orbits partition V, and Ω is invariant iff it is a union of orbits. The **coadjoint orbits** are the orbits in the coadjoint representation on $\mathbb{L}^*$. Apparently, $\Omega = \operatorname{Orb}(\omega)$ is a manifold homeomorphic to $\operatorname{Aut}\mathbb{L}/\operatorname{Stab}(\omega)$, and the tangent space at ω is

$$T_\omega\Omega = \{Q(\delta)\omega \mid \delta \in \mathbb{L}\}.$$

The coadjoint orbits correspond to maximal subgroups and are symplectic manifolds with closed 2-form $\omega(f,g) := \operatorname{tr}\rho(f\angle g)$ The set of all $\omega \in \mathbb{L}^*$ for which a fixed set of casimirs takes fixed values is always invariant.

Part IV

Nonequilibrium thermodynamics

Chapter 14

Markov Processes

Part IV discusses the dynamics of nonequilibrium phenomena, i.e., processes where the expectation changes with time, in as far as no fields are involved.

It should be complemented (in a later stage of the book) by a treatment of space-time dependent thermodynamics, and its derivation from quantum field theory.

We first develop a formal mathematical language for representing the physical concepts related to experiments with quantum systems in an unambiguous way, such that the relations between the mathematical concepts precisely mirror the relations between the corresponding physical concepts. In particular, we define sources, activities, processes, observers, protocols and observables.

In this way, phenomenological quantum physics gets a formal representation in the Platonic world of precise ideas, in the same way as it has been custumary for centuries for mathematics.

A general formal framework for phenomenological quantum mechanics is given that allows a concise formulation of the problems of observation, in a way close to real life.

It makes the ideas developed in quantum measurement theory, and in particular the theory of positive operator valued measures (POVM's) intuitive and useful for actual modeling.

We then take the continuum limit of the present framework; it results in the traditional Lindblad theory of dissipative quantum processes. However, we shall put the latter in the broader framework of Markov processes.

The most important class of nonequilibrium processes are the memory-less Markov processes. But by disregarding some variables in a Markov process, one also finds a natural dynamics for processes with memory. Since it can be argued that the memory in any physical process is due to hidden variables, Markov processes can be regarded as the fundamental processes, and we shall concentrate on the latter.

A Markov process is characterized in our set-up by a linear operator with properties resembling those of a derivation, and hence called a **forward derivation**. We shall discuss forward derivations in Section 14.4, general Markov processes in Section 14.5.

The building blocks of phenomenological (classical or quantum) objects are *sources*, i.e., physical objects producing a definite state. For example, in optical experiments, a source is typically an object or arrangement that produces one or several light beams of a certain kind. On the formal level, sources are represented by certain monotone linear functionals.

Part of experimental physics consists in the art of devising real arrangements that *prepare* a source, i.e., that produce output whose ensemble properties agree with that of a formal source.

Sources are further modified by *conditioning*, i.e., subjecting them to one or several *activities* that change the output of a source. For example, in optical experiments, an activity may be passing a light beam through a beam splitter or an optical filter. On the formal level, activities are represented by certain monotone linear operators. Activities and how they condition sources are discussed in Section 14.1.

Informally, a *process* is a description of everything that may happen to the output of a source while passing through an arrangement of physical equipment. Since experiments are not completely reproducible, they need a stochastic description; thus, we describe processes by a (classical) probability distribution on the possible activities that characterize the corresponding possible changes.

The relation between activities and real-life observations is established by an *observer* who classifies the activities according to more or less objective principles, resulting in classical *records*. Further processing of the records according to established scientific standards yields *protocols* that can be communicated by classical means. Associated to each protocol is a set of *observables* defined by the protocol. Processes, observers, and protocols are discussed in Section 14.2.

14.1 Activities

The building blocks of phenomenological (classical or quantum) objects are *sources*, i.e., physical objects producing a state. For example, in optical experiments, a source is typically an object or arrangement that produces one or several light beams of a certain kind. On the formal level, sources are represented by certain monotone linear functionals.

A **source** is a monotone $*$-linear functional E on the space $\mathbb{E}$ of quantities, i.e., a mapping $E : \mathbb{E} \to \mathbb{C}$ satisfying

$$E(f+g) = E(f) + E(g), \quad E(\lambda f) = \lambda E(f),$$

$$E(f^* f) \geq 0, \quad E(f^*) = E(f)^*.$$

A source is **proper** if it has a finite and positive **partition function**

$$Z := E(1) \in \ ]0, \infty[.$$

(This is a function $Z(\theta)$ only when the source $E = E_\theta$ is parameterized by one or several control variables, collected in the vector θ.)

Typical examples of sources are:

$$E(f) = f(\omega) \quad \text{(pure classical source)}$$

if f is a quantity from an algebra $\mathbb{E}$ of functions of a set Ω and $\omega \in \Omega$,

$$E(f) = \psi^* f \psi \quad \text{(pure quantum source)}$$

if f is a quantity from the algebra $\mathbb{E}$ of linear operators on a Hilbert space $\mathbb{H}$ and $\psi \in \mathbb{H}$,

$$E(f) = \int e^{-\beta H} f \quad \text{(canonical thermal source)}$$

for an arbitrary Hermitian Hamiltonian $H \in \mathbb{E}$ and an inverse temperature β such that $Z = \int e^{-\beta H}$ is finite.

The **ensemble** associated with a proper source is defined by the expectation functional $\langle E \cdot \rangle$ that associates with a quantity f the **expectation**

$$\langle Ef \rangle := E(f)/E(1).$$

Sources that are multiples of each other are equivalent and define the same ensemble. Sources form a closed convex set:

14.1.1 Proposition. *Let E_α be a family of sources.*

(i) For any directed set order on the α, the limit $E = \lim_\alpha E_\alpha$ defined by

$$E(f) = \lim_\alpha E_\alpha(f),$$

is again a source.

(ii) For any probability measure $d\mu(\alpha)$ (with $\int d\mu(\alpha) = 1$), the ***convex combination*** *$E = \int d_\mu(\alpha) E_\alpha$ of the E_α, defined by*

$$E(f) = \int d\mu(\alpha) E_\alpha(f),$$

is again a source. In particular, if p_α are nonnegative numbers with sum 1 then the weighted sum $E = \sum p_\alpha E_\alpha$ of sources is a source.

Proof. Straightforward. □

Part of experimental physics consists in the art of devising real arrangements that *prepare* a source, i.e., that produce output whose ensemble properties agree with that of a formal

source E. If a family of sources E_α is already available, arbitrary convex combinations of these sources can be realized in practice by randomizing the selection of sources in sufficiently narrow time intervals.

Sources are further modified by *conditioning*, i.e., subjecting them to one or several *activities* that change the output of a source. For example, in optical experiments, an activity may be passing a light beam through a beam splitter or an optical filter such as a polarizer or an absorber. On the formal level, activities are represented by certain monotone linear operators.

An **activity** is a monotone *-linear mapping $A : \mathbb{E} \to \mathbb{E}$

$$A(1) \leq 1;$$

$A(1)$ is called the **effect** of A. An activity is called **conservative** if it is invertible and

$$A(fg) = A(f)A(g) \forall f, g \in \mathbb{E};$$

i.e., if it is a $*$-automorphism of $\mathbb{E}$. An activity is called **autonomous** if

$$A(f) = E_A(f) g_A, \quad 0 \leq g_A \leq E_A(1)^{-1} \tag{14.1}$$

for some source E_A and some $g_A \in \mathbb{E}$, and **primitive** if

$$A(f) = L^* f L \tag{14.2}$$

for some quantity $L \in \mathbb{E}$ with

$$L^* L \leq 1,$$

called the **Lindblad operator** of the activity. (Nonprimitive activities have no associated Lindblad operator.) A **von-Neumann activity** is an activity with $A^2 = A$, e.g., a primitive activity whose Lindblad operator is a projector L (satisfying $L^2 = L$).

A primitive activity with Lindblad operator L is conservative iff L is unitary, and a von-Neumann activity iff L is idempotent, $L^2 = L$.

Primitive activities with Lindblad operators

$$L = e^{-\iota t H}$$

with a Hermitian **Hamiltonian** H describe conservative unitary evolution (simply passing time).

A **screen** is an orthogonal projector to an invariant subspace of the position operator, i.e., to the closed subspace spanned by some Borel set of position eigenstates. For classical algebras, the corresponding Lindblad operator is a characteristic function, for quantum algebras an orthogonal projector. Thus (displaying on) a screen is a von-Neumann activity.

In real applications to quantum systems (for quantum optical devices, see, e.g., Leonhardt & Neumaier [174]), we typically have dissipative systems described by **dissipative Lindblad operators** of the form

$$L = e^a \quad \text{where} \quad a \in \mathbb{E}, \ \operatorname{Re} a \leq 0.$$

Note that $\operatorname{Re} a \le 0$ implies $L^*L \le 1$: From

$$\frac{d}{dt}(e^{ta})^* e^{ta} = (e^{ta})^*(a + a^*)e^{ta} \le 0,$$

we see that $b(t) := (e^{ta})^* e^{ta}$ is monotone decreasing; hence $L^*L = b(1) \le b(0) = 1$.

14.1.2 Theorem.

(i) If A is an activity then its ***transpose*** *A^T, defined by $A^T(f) = A(f)^T$, is an activity.*

(ii) The product $A = A_1 \dots A_n$ of a sequence $A_1, \dots, A_n$ of activities is again an activity.

(iii) Activities form a closed convex set.

(iv) When $\mathbb{E}$ is the algebra of bounded linear operators on a Hilbert space then all activities are convex combinations of primitive activities, transposed primitive activities and autonomous activities.

Proof. (i)–(iii) are straightforward, and (iv) follows from a well-known classification theorem; see, e.g., Davies [71, Section 3.1]. □

(For classical $\mathbb{E}$, the analogue of (iv) is wrong.)

For any source E and any activity A, the product EA is again a source, the source E **conditioned** by A. The associated ensemble has the **conditional expectation**

$$\langle EAf \rangle = EA(f)/EA(1).$$

For an autonomous activity (14.1), $\langle EAf \rangle = \langle E_A(f) \rangle$ independent of the source E. Thus autonomous activities wipe out the information in the input.

A source E can be conditioned by a sequence $A_1, \dots, A_n$ of activities, resulting in the **conditioned source** $EA_1 \dots A_n$. Except for von-Neumann activities, conditioning by repeating an activity generally gives results different from conditioning by the single activity, $EAA \ne EA$ (e.g., when applying several absorbers in turn to an optical system).

Activities can be considered in the pictures of Heisenberg and von Neumann:

$$f \to L^* f L = E(f), \quad \psi \to L\psi, \quad \rho \to L\rho L^* = E^*(\rho).$$

Primitive activities (which preserve or reduce the rank) can also be considered in the Schrödinger picture; nonprimitive activities have no associated Schrödinger picture.

In physics, one frequently passes from a fundamental description in terms of microscopic quantities to coarse-grained description in terms of certain effective quantities of interest. The effective quantities form a subalgebra, and we may look at the consequences of restricting attention to such a subalgebra.

A **restriction** is an idempotent $*$-linear mapping Π from $\mathbb{E}$ onto a subalgebra E_Π of $\mathbb{E}$. Typical examples are

$$\Pi(f \otimes g) = f$$

(projecting away so-called *heat bath* quantities g),

$$\Pi(f) = \text{Diag}\ (f)$$

(projecting quantum observables to corresponding classical observables in the maximal commuting subalgebra of diagonal operators). The latter may be combined with a basis change, giving

$$\Pi(f) = P\text{Diag}\ (P^* f P)P^* \quad \text{for } P : \mathbb{H}' \to \mathbb{H}, \quad P^*P = 1.$$

To each source E of $\mathbb{E}$ we associate the **restricted source** E_Π on $\mathbb{E}_\Pi$ with

$$E_\Pi(f) = E\Pi(f) = E(f) \quad \text{for } f \in \mathbb{E}_\Pi,$$

and to each activity on $\mathbb{E}$ the **restricted activity** A_Π on $\mathbb{E}_\Pi$ with

$$A_\Pi(f) = \Pi A \Pi(f) = \Pi A(f) \quad \text{for } f \in \mathbb{E}_\Pi.$$

Note that $(EA)_\Pi \neq E_\Pi A_\Pi$ in general, whence the composition of activities (and sources) depends on the context in which they are described!

Over an algebra $\mathbb{E} = \mathbb{E}_\Pi \oplus \mathbb{E}_{\text{env}}$, **separable** activities are those satisfying

$$A(f \otimes g) = A_\Pi f \otimes A_{\text{env}} g.$$

They behave well under restriction,

$$(EA)_\Pi(f) = EA(f \otimes 1) = E(A_\Pi f \otimes 1) = EA_\Pi(f) = E_\Pi A_\Pi(f).$$

Nonseparable activities are *entangled* and their restriction has no simple description.

However, *primitivity is not preserved* by restriction, whence restriction generally cannot produce truly pure sources.

14.2 Processes

Informally, a *process* is a description of everything that may happen to the output of a source while passing through an arrangement of physical equipment. Since (as far as human observations are concerned) nature is not deterministic, we describe processes by a (classical) probability distribution on the possible activities that characterize the corresponding possible changes.

A **process** $\mathcal{A}$ changes a source E into the conditioned source EA_α with probability density $d\mu(\alpha)EA_\alpha(1)/E\overline{A}(1)$, cf. Figure 14.1. Here the A_α are activities indexed by **labels** α, and $d\mu(\alpha)$ is a probability measure on the set of labels, and the expression

$$\overline{A} := \int d\mu(\alpha) A_\alpha \tag{14.3}$$

Figure 14.1: Conditioning a source by a process

$$E \longrightarrow \boxed{\mathcal{A}} \longrightarrow EA_\alpha$$

is the **mean activity** of the process. A process is called **complete** if $\overline{A} = 1$. (Traditionally, a complete process is referred to as a *positive operator-valued measure*, or POVM; see, e.g., Davies [71]. We prefer to use the above more intuitive terminology.)

The relation between activities and real-life observations is established by an *observer* who classifies the activities according to more or less objective principles, resulting in classical *records* that can be objectively processed.

An (ideal) **observer** is a mapping r that associates with each label α a **record** $r(\alpha) \in R$; here R is an arbitrary set containing the possible records. The expression

$$\overline{A}_r := \int d\mu(\alpha)\chi_{r(\alpha)=r}A_\alpha$$

is called the **mean activity** corresponding to record r.

14.2.1 Proposition. *Given a source E and a process $\mathcal{A}$, the distribution of the observed records is described by the expectation*

$$\langle f(r)\rangle = \int d\mu(\alpha)EA_\alpha(f(r(\alpha)))/E\overline{A}(1) \tag{14.4}$$

for classical *functions $f : R \to \mathbb{C}$, hence is a classical probability distribution.*

(14.4) follows from the definition of the change a process causes, and defines an expectation since $\langle 1\rangle = 1$ by (14.3). *Proof.*

□

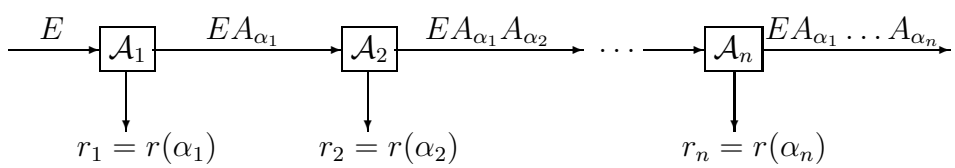
A **composite process** with **subprocesses** $\mathcal{A}_1, \ldots, \mathcal{A}_n$ is the family of activities

$$A_{(\alpha_1\ldots,\alpha_n)} := A_{\alpha_1}\ldots A_{\alpha_n}(A_{\alpha_s} \in \mathcal{A}_s)$$

with associated product measure $d\mu(\alpha_1, \ldots, \alpha_n) = d\mu_1(\alpha_1)\ldots d\mu_n(\alpha_n)$. A corresponding sequence $(r_1, \ldots, r_n) = (r(\alpha_1)\ldots, r(\alpha_n))$ is called a **history**, cf. Figure 14.2.

Note that things happening at the same time (e.g., in quantum entanglement experiments) are considered to be part of a *single* activity of a composite process. This is an expression of the nonlocality of quantum mechanics, and assumes a preferred time axis (given in the relativistic case by the 4-momentum of the observer).

Figure 14.2: History generation by observing a composite process



Further processing of the records according to established scientific standards yields *protocols* that can be communicated by classical means. Associated to each protocol is a set of *observables* defined by the protocol.

A **protocol** is a mapping $v : R \to \mathbb{C}^n$ that assigns to each record r a vector $v(r)$, and hence (given an observer), to each label α the vector $v_\alpha = v(r(\alpha))$. For any protocol v with values in $D \subseteq \mathbb{R}^n$ and any function $\phi : D \to \mathbb{R}^m$, we define the protocol $\phi(v)$ with

$$\phi(v)_\alpha := \phi(v_\alpha).$$

Each protocol v defines a vector of **observables**

$$\widehat{v} := \int d\mu(\alpha) A_\alpha(v_\alpha).$$

14.2.2 Theorem. *For an arbitrary source E, the (observable) record expectation $\langle v(r)\rangle$ is related to the (computable) ensemble expectation $\langle E\widehat{v}\rangle$ by*

$$\langle v(r)\rangle = \langle E\widehat{v}\rangle / \langle E\widehat{1}\rangle.$$

Proof. We have

$$E\widehat{v} = E\int d\mu(\alpha) A_\alpha(v_\alpha) = \int d\mu(\alpha) E A_\alpha(v(r(\alpha))) = \langle v(r)\rangle E\overline{A}(1)$$

by (14.4), hence

$$\langle E\widehat{v}\rangle = E\widehat{v}/E1 = \langle v(r)\rangle E\overline{A}(1)/E1 = \langle v(r)\rangle\langle E\overline{A}(1)\rangle.$$

Since $\overline{A}(1) = \widehat{1}$, the result follows. □

Thus $\langle E\widehat{1}\rangle = \langle E\overline{A}(1)\rangle \in [0,1]$ is the **efficiency** of a source E for a given process. If the process is complete, all sources are 100% efficient.

Note that the $A_\alpha(1)$ need not commute (randomize the decision of what to measure); thus we can jointly measure noncommuting quantities.

Scientific or industrial standards carefully define protocols for objectively observing key observables. The art of experimental design consists in finding protocols whose associated

observables approximate a desired vector quantity $f \in \mathbb{E}^n$ as closely as possible. Note that generally $\widehat{\phi(v)} \neq \phi(\widehat{v})$, so that operations on protocols are only approximately matched by the corresponding operations on the associated observables.

Conjecture. (in the 2-norm w.r. to E or in the ∞-norm? Is there a related result in terms of protocols?)

$$[\tilde{f}, \tilde{g}] = 0 \qquad \Rightarrow \quad \|f - \tilde{f}\| \, \|g - \tilde{g}\| \geq \mathrm{unc}(f, g)$$

One way to measure the quality of the approximation of a quantity f by an observable $\widehat{v}$ is in terms of the **maximal deviation**

$$\|\widehat{v} - f\|$$

which is defined independent of sources. Numerically, this leads to a semidefinite programming problem that can be approximately solved with high efficiency (see, e.g., [8, 125, 279, 293]), namely

$$\begin{array}{ll} \min & \lambda \\ \text{s.t.} & -\lambda \leq \sum_r v(r) f_r - f \leq \lambda, \end{array}$$

where

$$f_r = \int d_\mu(\alpha) \chi_{r(\alpha)=r} A_\alpha(1).$$

If the source is known, we may instead minimize the empirical expectation of the **surprise** (Neumaier [204])

$$s = \frac{1}{n}(v(r) - f)^* \, \mathrm{Cov}(f)(v(r) - f)$$

where

$$\overline{f} = \langle Ef \rangle, \quad \mathrm{Cov}(f) = \langle E(f - \overline{f})(f - \overline{f})^* \rangle.$$

This defines a least squares problem. Note that $\langle s \rangle \geq 1$, with equality iff $\widehat{v} = f$.

14.3 Forward morphisms and quantum dynamical semigroups

This section is still incomplete.

Dissipative quantum systems are described by quantum dynamical semigroups and their associated evolution equations (often called Lindblad equations). The former are characterized in terms of what we shall call **forward morphisms**, satisfying a relaxed version of the laws for a homomorphisms; the latter are defined in terms of what we shall call **forward derivations**, which relax the property of a derivation, and are discussed in the next section.

14.3.1 Definition. Let $\mathbb{E}$ be a Euclidean *-algebra and $\mathbb{H}$ a Euclidean space. A *-linear map $A \in \mathrm{Lin}(\mathbb{E}, \mathrm{Lin}\,\mathbb{H})$ is called **completely positive** if a **Stinespring factorization**

$$A(f) = L^* U(f) L \quad \text{for } f \in \mathbb{E}$$

holds for some Euclidean space $\mathbb{F}$, some linear mapping $L : \mathbb{H} \to \mathbb{F}$, and some homomorphism $U : \mathbb{E} \to \mathrm{Lin}\,\mathbb{F}$ (satisfying $U(1) = 1$, $U(f^*) = U(f)^*$, and $U(fg) = U(f)U(g)$).

14.3.2 Proposition. *If A is completely positive then, for every $n = 1, 2, \ldots$ and every positive semidefinite $F \in \mathbb{E}^{n\times n}$, the matrix $A(F) \in \mathrm{Lin}(\mathbb{H})^{n\times n}$ with component $A(F)_{jk} = A(F_{jk})$ is positive semidefinite, in the sense that for all $u \in \mathbb{C}^n$, the operator $\sum_{j,k} u_j^* A(F_{jk}) u_k^*$ is positive semidefinite.*

If all $f \in \mathbb{E}$ are bounded, these conditions are equivalent (Stinespring's theorem); then the latter property may be taken to be the definition of complete positivity.

14.3.3 Definition. A **forward morphism** on a Euclidean *-algebra $\mathbb{E}$ is a *-linear functional $E : \mathbb{E} \to \mathbb{C}$ such that

$$E(f^* f) \geq E(f)^* E(f) \tag{14.5}$$

$$E(f^* f) \geq E(f)^* f + f^* E(f) - f^* E(1) f \tag{14.6}$$

hold for all bounded $f \in \mathbb{E}$.

14.3.4 Proposition. *(i) The identity mapping is a forward morphism.*

(ii) Convex combinations of forward morphisms are forward morphisms.

(iii) If E is a forward morphism on $\mathbb{E}$ and $P \in \mathrm{Lin}\,\mathbb{E}$ satisfies $PP^* \leq 1$ then the mapping $E_P : \mathbb{E} \to \mathbb{C}$ defined by $E_P(f) := P^* E(f) P$ is a forward morphism.

Apparently, the set of forward morphisms is the smallest set with the properties stated in this proposition. This can be proved in case $\mathbb{E}$ is finite-dimensional.

14.3.5 Proposition. *If E is a forward morphism on $\mathbb{E}$ and $P \in \mathrm{Lin}\,\mathbb{E}$ satisfies $PP^* \leq 1$ then the mapping $E_P : \mathbb{E} \to \mathbb{C}$ defined by $E_P(f) := P^* E(f) P$ is a forward morphism.*

14.4 Forward derivations

Let $\mathbb{E}$ be an Euclidean *-algebra.

14.4.1 Definition. A mapping $D : \mathbb{E} \to \mathbb{E}$ is called a **derivation** if it satisfies
(D1) $D(\alpha f + \beta g) = \alpha Df + \beta Dg$ for $\alpha, \beta \in \mathbb{C}$, $f, g, \in \mathbb{E}$,
(D2) $D(f^*) = (Df)^*$ for $f \in \mathbb{E}$,
(D3a) $D(fg) = (Df)g + f(Dg)$ for $f, g \in \mathbb{E}$,
and a **forward derivation** if $(D1), (D2)$ hold and
(D3) $D(f^* f) \geq (Df)^* f + f^*(Df)$ for $f \in \mathbb{E}$

14.4.2 Proposition. *For a forward derivation, $D1 \leq 0$, and for a derivation, $D1 = 0$.*

Proof. Insert $f = 1$ into $(D3)$ and $f = g = 1$ into $(D3_0)$. □

14.4.3 Examples.

(i) If $\mathbb{E} = C^\infty(\mathbb{R})$ then $Df(x) := f'(x)$ defines a derivation. This example is responsible for the name.

(ii) If $\mathbb{E} = C(\mathbb{R}^n)$, $h \in \mathbb{R}^n$ and $\varepsilon > 0$ then the **coarse-grained directional derivative**

$$D_h f(x) := \frac{f(x + \varepsilon h) - f(x)}{\varepsilon}$$

defines a forward derivation. Indeed, $(D1)$ and $(D2)$ are trivial, and since $D_h(ff^*)$ maps x to

$$\begin{aligned} D_h(ff^*)(x) &= \frac{f(x+\varepsilon h)f^*(x+\varepsilon h) - f(x)f^*(x)}{\varepsilon} \\ &= \frac{(f(x) + \varepsilon D_h f(x))(f^*(x) + \varepsilon D_h f^*(x)) - f(x)f^*(x)}{\varepsilon} \\ &= D_h f(x) f^*(x) + f(x) D_h f^*(x) + \varepsilon D_h f(x)(D_h f(x))^*, \end{aligned}$$

we find

$$D_h(ff^*) - (D_h f)f^* - f(D_h f^*) = \varepsilon (D_h f)(D_h f)^* \geq 0$$

since $\varepsilon > 0$. Therefore, $(D3)$ holds.

(iii) If B is an arbitrary quantity then

$$Df := 2BfB^* - BB^*f - fBB^*$$

defines a forward derivation; $(D3)$ follows from [details?]

$$D(ff^*) - (Df)f^* - f(Df^*) = 2[B, f][B, f]^* \geq 0.$$

(iv) If B is a quantity such that $B + B^* \geq 0$ then

$$Df := -Bf - fB^*$$

defines a forward derivation. Again, only $(D3)$ is nontrivial and follows from

$$\begin{aligned} &D(ff^*) - (Df)f^* - f(Df^*) \\ &= -Bff^* - ff^*B^* + (Bf + fB^*)f^* + f(Bf^* + fB^*) \\ &= f(B + B^*)f^* \geq 0. \end{aligned}$$

(v) If H is a Hermitian quantity then

$$Df := i[H, f] = i(Hf - fH)$$

defines a derivation. Indeed, $(D1)$ is trivial, $(D2)$ follows from

$$(Df)^* = -i(Hf - fH)^* = -i(f^*H - Hf^*) = i(Hf^* - f^*H) = Df^*,$$

and $(D3)$ from

$$\begin{aligned} &D(H^*) = i(Hff^* - ff^*H) = i((Hf - fH)f^* + f(Hf^* - f^*H)) \\ &= (Df)f^* + f(Df^*). \end{aligned}$$

(vi) If D is a derivation then D^2 is a forward derivation. Indeed, $(D1)$ and $(D2)$ are trivial, and

$$D^2(ff^*) = D(D(ff^*)) = D((Df)f^* + f(Df^*))(D^2f)f^* +_2 (Df)(Df)^* + f(D^2f^*)$$

so that

$$D^2(ff^*) - (D^2f)f^* - f(D^2f^*) = 2(Df)(Df)^* \geq 0.$$

In particular, $Df(x) := f''(x)$ is a forward derivation.

(vii) Clearly, a nonnegative linear combinaton of forward derivations is again a forward derivation.

The fact that the derivation (v) is the special case $B = -iH$ of (iv), where $B + B^* = 0$ can be extended to the following result.

14.4.4 Proposition. *If D and $-D$ are forward derivations then D is a derivation.*

Proof. Under our assumptions, $(D3)$ holds with equality. Therefore

$$\begin{aligned} &D(ff^*) + \alpha D(gf^*) + \alpha^* D(fg^*) + \alpha\alpha^* D(gg^*) \\ &= D((f + \alpha g)(f + \alpha g)^*) = (D(f + \alpha g))(f + \alpha g)^* + (f + \alpha g)D(f + \alpha g)^* \\ &= (Df)f^* + \alpha(Dg)f^* + \alpha^*(Df)g^* + \alpha\alpha^*(Dg)g^* \\ &\quad + f(Df^*) + \alpha g(Df^*) + \alpha^* f(Dg^*) + \alpha\alpha^* g(Dg^*). \end{aligned}$$

Again, since $(D3)$ holds with equality, this simplifies to

$$\alpha D(gf^*) + \alpha^* D(fg^*) = \alpha((Dg)f^* + g(Df^*)) + \alpha^*((Df)g^* + f(Dg^*)),$$

If we add this equation for $\alpha = 1$ and i times for $\alpha = i$, we find

$$(1 + i)D(fg^*) = (1 + i)(Df)g^* + (1 + i)f(Dg^*),$$

and this implies $(D3_0)$. □

14.4.5 Definition. A quantity $c \in \mathbb{E}$ is called **conserved** if

$$Dc = 0 \tag{14.7}$$

and

$$D(cf) = c(Df), \quad D(fc) = (Df)c \quad \text{for all } f \in \mathbb{E}. \tag{14.8}$$

The forward derivation D is called **dissipative** if every quantity c satisfying

$$D(c^*c) = (Dc)^*c + c^*(Dc) \tag{14.9}$$

is conserved, and **primitive** if it is dissipative and only constants are conserved.

The conserved quantities form a *-subalgebra of $\mathbb{E}$ containing $\mathbb{C}$. Indeed, $D\alpha = 0$ for $\alpha \in C$ follows from (14.8) for $f = \alpha$, and closure under addition, multiplication and conjugation is straightforward. Therefore any algebraic expression f involving only conserved quantities is conserved, too. In particular, we automatically have (14.9) for conserved quantities.

14.5 Single-time, autonomous Markov processes

To motivate our abstract concept of a (single-time, autonomous) Markov process, we first consider two special cases: a classical deterministic dynamics and the quantum Schrödinger dynamics.

14.5.1 Example. (**Deterministic processes**) Let $x : \mathbb{R} \to \mathbb{R}^n$ be a solution of the differential equation

$$\dot{x}(t) = F(x(t), t), \tag{14.10}$$

and

$$E = C^1(\mathbb{R}^n), \quad \operatorname{tr} f = \int dx^n f(x).$$

If we define

$$\langle f \rangle_t := f(x(t), t) \tag{14.11}$$

then

$$\begin{aligned} \tfrac{d}{dt}\langle f \rangle_t = \tfrac{d}{dt} f(x(t), t) &= \partial_x f(x(t), t) \cdot \dot{x}(t) + \partial_t f(x(t), t) \\ &= \partial_x f(x(t), t) \cdot F(x(t), t) + \partial_t f(x(t), t) \\ &= \langle \partial_x f \cdot F + \partial_t f \rangle_t = \langle D_F f + f \rangle_t, \end{aligned}$$

where D_F, defined by

$$D_F f = F \cdot \partial_x f \tag{14.12}$$

is the **Lie derivative** with respect to F. Clearly, D_F is a derivation on $\mathbb{E}$. Thus (14.16) holds with $D = D_F$, and we have a reversible Markov process. The general solution of (14.16) with initial condition

$$\langle f \rangle_{t_0} = \int dz \rho_0(z) f(z, t_0) \tag{14.13}$$

is easily seen to be

$$\langle f \rangle_t = \int dz \rho_0(z) f(x(z, t), t), \tag{14.14}$$

where $x(z,t)$ is the solution of (14.10) with $x(z,t_0) = z$. The particular solution (14.11) corresponds to the density $\rho_0(z) = \delta(z - x(t_0))$, and has vanishing variance

$$\langle (f - \langle f\rangle_t)^2\rangle_t = (f(x(t),t) - \langle f\rangle_t)^2 = 0,$$

as one would expect from a deterministic process. However, unsharp initial conditions (14.13) lead to solutions (14.14) with, in general, nonzero, variance.

14.5.2 Example. (**Reversible classical mechanics**) If we specialize the preceding example to an autonomous Hamiltonian system, defined by

$$\dot q = \frac{\partial}{\partial p} H(p,q), \qquad \dot p = -\frac{\partial}{\partial q} H(p,q), \tag{14.15}$$

for a Hamiltonian $H : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, we find (for time-independent f) the reversible dynamics

$$\frac{d}{dt}\langle f\rangle_t = \langle Df\rangle_t \qquad \text{for } t \in \mathbb{R}, f \in \mathbb{E}, \tag{14.16}$$

with the **Poisson bracket**

$$Df = \{f, H\} := \sum_\nu \left(\frac{\partial f}{\partial q_\nu}\frac{\partial H}{\partial p_\nu} - \frac{\partial f}{\partial p_\nu}\frac{\partial H}{\partial q_\nu} \right) \tag{14.17}$$

as associated derivation.

14.5.3 Example. (Reversible quantum mechanics)

Let ψ be a solution of the time-dependent Schrödinger equation,

$$i\hbar \frac{d}{dt}\psi = H\psi, \tag{14.18}$$

defined in a Hilbert space $\mathbb{H}$ for a Hermitian Hamilton operator H, and let $\mathbb{E}$ be the algebra of linear operators on $\mathbb{H}$, with standard trace. If we define

$$\langle f\rangle_t := \psi^* f \psi \tag{14.19}$$

then

$$\begin{aligned}
\tfrac{d}{dt}\langle f\rangle_t &= \psi^* f\psi) = \dot\psi^* \dot f \psi + \psi^* \dot f \psi + \psi^* f \dot\psi \\
&= \left(\tfrac{H\psi}{i\hbar}\right)^* f\psi + \psi^* \dot f \psi + f \tfrac{H}{i\hbar}\psi \\
&= \psi^* \left(-\tfrac{H}{i\hbar} f + \dot f + f \tfrac{H}{i\hbar} \right) \psi = \langle \tfrac{i}{\hbar}[H,f] + \dot f\rangle_t \\
&= \langle Df + \dot f\rangle_t,
\end{aligned}$$

where

$$Df = \frac{i}{\hbar}[H,f] \tag{14.20}$$

is a commutator. As we have seen, D is a derivation on $\mathbb{E}$, and (14.16) holds again. The general solution of (14.16) can be expressed in terms of solutions of the Schrödinger equation, see below .

We now discuss an axiomatic irreversible dynamics, of which our reversible examples are particular cases.

14.5.4 Definition. A (single-time, autonomous) **Markov process** is a flow on the set of states of a Euclidean *-algebra $\mathbb{E}$ such that (14.16) holds with a forward derivation D on $\mathbb{E}$. We use a dot to denote differentiation with respect to time. The process is called **reversible** if D is a derivation, and **dissipative** if D is dissipative.

A **stationary state** of the process (14.16) is a state with $\langle Df \rangle = 0$.

14.5.5 Remarks. (i) In (14.16), it is assumed that f is independent of t; otherwise, the correct dynamics is given instead by

$$\frac{d}{dt}\langle f(t)\rangle_t = \langle (Df)(t) + \frac{d}{dt}f(t)\rangle_t \qquad \text{for } t \in \mathbb{R},\ f \in C^1(\mathbb{R}, \mathbb{E}). \tag{14.21}$$

(ii) For a reversible Markov process, the backward dynamics is also a Markov process.

(iii) A stationary state is invariant under the dynamics (14.16). The expectation of conserved quantities satisfies $\frac{d}{dt}\langle f\rangle_t = 0$, and hence is time-invariant also for nonstationary states.

In reversible quantum mechanics (Example 14.5.3), the conserved quantities are precisely the quantities commuting with H.

14.5.6 Proposition. *(**Schrödinger picture and Liouville equation**)*

$$\dot{\rho} = D^* \rho.$$

14.6 to be done

- Markov chains. This is the case $\mathbb{E} = \mathbb{C}^n$ with pointwise operations
- Conservative classical and quantum mechanics. Here $\mathbb{E}$ is a Poisson algebra and $Df = H \angle f$ for some Hamiltonian H.
- General properties of Markov processes (the second law)
- Low noise approximation (drift and diffusion)

Chapter 15

Diffusion processes

In this chapter we describe an important class of classical primitive Markov processes, characterized by their drift vector and their diffusion matrix. As particular cases we obtain **damped Hamiltonian systems**, which are shown to converge towards the canonical ensemble, and another important case, the exactly solvable **Ornstein-Uhlenbeck processes**, which describe coupled damped harmonic oscillators.

Our Euclidean *-algebra is $\mathbb{E} = \mathbb{E}_0 = \mathcal{S}(\mathbb{R}^n)$, the Schwartz space of rapidly decaying C^∞ functions, and the trace is integration over $\mathbb{R}^n$ Partial integration then gives $\nabla^* = -\nabla$.

15.1 Stochastic differential equations

15.1.1 Theorem. *Let v be a vector field and let G be a symmetric tensor field on $\mathbb{R}^n$, $G(x)$ positive semidefinite (v and G may be time dependent). Then*

$$Df := v \cdot \nabla f + \frac{1}{2} G : \nabla^2 f$$

defines a forward derivation on $E_0 = C^\infty(\mathbb{R}^n)$, with drift vector v and diffusion matrix G.

Moreover, if G is definite then D is primitive.

Proof. *-Linearity is clear, and

$$\begin{aligned} D(f,g) : &= D(fg^*) - (Df)g^* - f(Dg^*) \\ &= u \cdot (\nabla(fg^*) - (\nabla f)g^* - f\nabla g^*) \\ &\quad + \frac{1}{2} G : \nabla^2(fg^*) - \frac{1}{2}(G : \nabla^2)g^* - \frac{1}{2} f(G : \nabla^2 g) \\ &= \frac{1}{2} G : (\nabla^2(fg^*) - (\nabla^2 f)g^* - f\nabla^2 g^*) \\ &= G : (\nabla f)(\nabla g) = (\nabla f)^T G(\nabla g). \end{aligned}$$

In particular, $D(f, f^*) \geq 0$. Moreover if G is positive definite then $D(f, f^*) > 0$ unless $\nabla f = 0$, i.e., unless f is a constant. Hence in this case D is primitive.

Finally, the drift vector is $Dx = v \cdot \nabla x = v$ and the diffusion matrix is $D(x, x^*) = (\nabla x)^T G(\nabla x) = G$. □

15.1.2 Definition. The Markov process

$$\frac{d}{dt}\langle f\rangle = \langle v \cdot \nabla f + \frac{1}{2}G : \nabla^2 f\rangle \tag{15.1}$$

is called the **diffusion process** with drift vector v and diffusion matrix G.

We note that the low noise approximation of any Markov process is determined by drift vector and diffusion matrix, hence any Markov process can be approximated by a diffusion process when the noise is sufficiently small. (This is the first approximation of the **Kramers-Moyal**, or **system size expansion** and gives a more accurate approximation than the low noise approximation. The diffusion approximation treats slow time scales as infinitely slow; hence metastable states appear to be stable.) This accounts for the importance of diffusion processes as approximations of more complex Markov processes.

15.1.3 Proposition. *The Liouville equation for a diffusion process is the* **Fokker-Planck equation**

$$\dot{\rho} = D^*\rho = -\nabla \cdot (v\rho) + \frac{1}{2}\nabla^2 : (G\rho).$$

Proof. By integration by parts of (15.1). □

15.1.4 Remark. Associated with the diffusion process (15.1) is the **stochastic Ito differential equation**

$$dx = v(t, x)dt + B(t, x)dW(t), \tag{15.2}$$

where BB^T is an arbitrary factorization of G. Here $W(t)$ denotes the **Wiener process**, i.e., the special process (15.1) with $v = 0$, $G = 1$, and x is defined by (15.2) via stochastic integration. We shall not use this, and refer to Gardiner (4.3.18) and (4.3.3) for the equivalence of (15.1) and (15.2). To avoid the arbitrariness in the choice of B we shall write (15.2) as

$$dx = vdt + (Gdt)^{\frac{1}{2}} = vdt + d\varepsilon, \quad d\varepsilon \sim N(0, Gdt), \tag{15.3}$$

which is suggestive in view of

$$\begin{aligned}\langle f(x(t+dt))\rangle = \langle f(x+dx)\rangle &= \langle f + \nabla f \cdot dx + \frac{1}{2}\nabla^2 f : (dx)^2\rangle \\ &= \langle f\rangle + \langle \nabla f \cdot v + \frac{1}{2}\nabla^2 f : G\rangle dt = \langle f\rangle + d\langle f\rangle\end{aligned}$$

if we note that $\langle ud\varepsilon\rangle = 0$, $\langle A : (d\varepsilon)^2\rangle = A : G$, and $d\varepsilon^3 = d\varepsilon dt = dt^2 = 0$. We shall see that the definition (15.1) is very satisfactory, and we need no integrals; these are needed for questions of existence and other, more mathematical developments.

15.1.5 Remark. Stochastic integrals from diffusion processes: In $\hat{\mathbb{E}}$ (the extended algebra of Heisenberg operators, with fixed $\langle\cdot\rangle = \langle\cdot\rangle_0$), we **define** the relation (15.3) with **arbitrary** operators v, G (possibly unrelated to the operator x to be equivalent with

$$\frac{d}{dt}\langle f(t,x)\rangle = \langle \partial_t f(t,x) + v\cdot\nabla f(t,x) + \frac{1}{2}G : \nabla^2 f(t,x)\rangle$$

for all expolynomials f (together with a multitime Markov property). Then it is meaningful to ask for solutions of stochastic differential equations (where now a relation between x, v, G is **prescribed**), and we can consider an existence and uniqueness theory. Clearly things are linear, and

$$dx = v(t)dt,\ x(0) = x_0$$

is solved by

$$x = x_0 + \int_0^t v(t)v(t)dt$$

so one has to give a meaning to $\int_0^t (Gdt)^{\frac{1}{2}}$ which is an Ito-stochastic integral. With this as **definition**, it is easy to show that the **Ito transformations formula** holds:

$$df(x) = (v\cdot\nabla f + \frac{1}{2}G : \nabla^2 f)dt + \big((\nabla f)^T G(\nabla f)dt\big)^{\frac{1}{2}} \qquad \text{where } \nabla f = (f')^T.$$

15.1.6 Proposition. *(Ito transformation formula)*

If functions of x satisfy the Markov process (15.1) *then functions of $\bar{x} = \xi(x)$ satisfy the Markov process* ($\bar{1}$) *with*

$$\bar{v} = \xi' v + \frac{1}{2}\xi'' : G, \quad \bar{G} = \xi' G \xi'^T. \tag{15.4}$$

Thus, the Ito differential equation transforms according to

$$d\xi(x) = (\xi' v + \frac{1}{2}\xi'' : G)dt + d\eta, \quad d\eta \sim N(0, \xi' G \xi'^T dt). \tag{15.5}$$

Proof. Differentiation of $\bar{f}(\bar{x}) = \bar{f}(\xi(x)) = f(x)$ gives

$$(\nabla f)^T = (\overline{\nabla}\bar{f})^T \xi' \Rightarrow \nabla f = \xi'^T \overline{\nabla}\bar{f} \tag{15.6}$$

and hence

$$v\cdot\nabla f = v\cdot\xi'^T\overline{\nabla}\bar{f} = \xi' v\cdot\overline{\nabla}\bar{f}.$$

Differentiating (15.6) *again gives*

$$\nabla^2 f = \nabla(\xi'^T\overline{\nabla}\bar{f}) = \xi''\overline{\nabla}\bar{f} + \xi'^T\nabla(\overline{\nabla}\bar{f}) = \xi''\overline{\nabla}\bar{f} + \xi'^T\xi'^T\overline{\nabla}^2\bar{f}.$$

Therefore, $G : \nabla^2 f = (\xi'' : G)\overline{\nabla}\bar{f} + \xi' G \xi'^T : \overline{\nabla}^2 f$, so that

$$v\cdot\nabla f + \frac{1}{2}G : \nabla^2 f = (\xi' v + \frac{1}{2}\xi'' : G)\overline{\nabla}\bar{f} + \frac{1}{2}\xi' G \xi'^T : \overline{\nabla}^2 f.$$

□

15.1.7 Corollary. *(Covariant form)*

We may rewrite the Markov process (15.1) *as*

$$\frac{d}{dt}\langle f\rangle = \langle u\cdot\nabla f + \frac{1}{2}\nabla\cdot(G\nabla f)\rangle \tag{15.7}$$

with the **covariant drift**

$$u^T = v^T - \frac{1}{2}\nabla\cdot G; \tag{15.8}$$

then u transforms under $\bar{x} = \xi(x)$ according to

$$\bar{u} = \xi' u. \tag{15.9}$$

[but $\langle dx - udt\rangle \neq 0$ in general.]

Proof.

$$\begin{aligned}\bar{u}^T &= \bar{v}^T - \frac{1}{2}\overline{\nabla}\cdot\bar{G} = v^T\xi'^T + \frac{1}{2}G:\xi'' - \frac{1}{2}\overline{\nabla}\cdot\xi' G\xi'^T \\ &= v^T\xi'^T + \frac{1}{2}G:\xi'' - \frac{1}{2}\nabla\cdot(G\xi'^T) = (v^T - \frac{1}{2}\nabla\cdot G)\xi'^T = u^T\xi'^T.\end{aligned}$$

□

One can also derive the **Stratonovic transformation formula**. The **Stratonovic drift**

$$w^T := u^T + \frac{1}{2}(\nabla\cdot B)B^T, \text{ where } G = BB^T,$$

transforms by

$$\begin{aligned}\bar{w}^T &= (\xi' u)^T + \frac{1}{2}(\nabla\cdot\xi' B)(\xi' B)^T \\ &= u^T\xi'^T + \frac{1}{2}(\xi'^T\nabla\cdot B)(B^T\xi'^T) \\ &= (u^T + \frac{1}{2}(\overline{\nabla}\cdot B)B^T)\xi'^T = w\xi'^T,\end{aligned}$$

hence according to standard rules. However, it depends on the factorization of G and hence is less useful than the covariant form (15.7).

Note: The equation $w^T = v^T - \frac{1}{2}B:(\nabla B^T)$ gives the traditional translation between the Ito version and the Stratonovic version of a stochastic process.

15.1.8 Proposition. *The Liouville equation for a diffusion process is a* **continuity equation**

$$\dot{\rho} + \nabla\cdot j = 0, \tag{15.10}$$

with the current

$$j = u\rho - \tilde{G}(\nabla\rho), \tag{15.11}$$

where $\tilde{G}$ is an arbitrary (possibly x-dependent) matrix with $G = \tilde{G} + \tilde{G}^T$.

Proof. We have $\dot{\rho} = D^*\rho$ and by symmetry, $D = u \cdot \nabla + \frac{1}{2}\nabla \cdot \tilde{G}\nabla$. □

In particular, for the Wiener process ($u = 0, \tilde{G} = \frac{1}{2}G = \kappa$, constant) we get the **diffusion equation**

$$\dot{\rho} = \frac{1}{2}\nabla \cdot G\nabla\rho = \kappa\Delta\rho.$$

In general, the current is composed of a streaming part (velocity u times density ρ) and a diffusion part.

15.1.9 Proposition. *The relative entropy increases, and takes its maximum at the equilibrium.*

Proof. For any convex Φ which is bounded below, and

$$f := \rho^{-1}\rho_0,$$

we have

$$\begin{aligned}
\frac{d}{dt}\operatorname{tr}(\rho\Phi f)) &= \operatorname{tr}(\dot{\rho}\Phi(f) + \rho\dot{f}\Phi'(f)) = \operatorname{tr}(\dot{\rho}[\Phi(f) - f\Phi'(f)] + \dot{\rho}_0\Phi'(f)) \\
&= \operatorname{tr}(\rho D[\Phi(f) - f\Phi'(f)] + \rho_0 D[\Phi'(f)]) \\
&= \operatorname{tr}(\rho\{D[\Phi(f) - f\Phi'(f)] + fD[\Phi'(f)]\}).
\end{aligned}$$

Now the part in curly brackets simplifies to

$$\begin{aligned}
&-\Phi''(f)(\nabla f)^T G(\nabla f) \\
-\int d\nu w(\nu,t,x)[\Phi(f(t,x+\nu)) - \Phi(f(t,x)) &- (f(t,x+\nu) - f(t,x))\Phi'(f(t,x+\nu))].
\end{aligned}$$

For convex Φ, this is nonpositive. In particular, and

$$\left.\begin{array}{l}\Phi(s) = s - 1 - \log s \\ \Phi(s) = 1 - s + s\log s\end{array}\right\} \to \text{ standard relative entropy} \left\{\begin{array}{l}\rho\ \log(\rho/\rho_0) \\ \rho_0\log(\rho_0/\rho)\end{array}\right.$$

□

15.2 Closed diffusion processes

We consider **closed systems** at constant temperature T. Closed systems are characterized by the fact that there is a current which vanishes at equilibrium. Thus any equilibrium state ρ_{eq} is given by the solution if

$$u\rho_{eq} = \tilde{G}(\nabla\rho_{eq}), \quad \operatorname{tr}\rho_{eq} = 1. \tag{15.12}$$

It is traditional to write some positive equilibrium state in terms of a **thermodynamic potential** Φ (with units of energy) as

$$\rho_{eq} = Z^{-1} e^{-\beta\Phi}, \qquad \beta = (\hbar T)^{-1}$$

with a constant Z, the **partition function** determined by the normalization condition to

$$Z = \operatorname{tr} e^{-\beta\Phi}.$$

Equation (15.12) then becomes

$$u = -\beta \tilde{G} \nabla \Phi.$$

In terms of the **transport matrix**

$$L := \beta \tilde{G}$$

and the **thermodynamics force**

$$F := \nabla \Phi$$

(named so in analogy with the ordinary force and a mechanical potential) we find as covariant drift

$$u = -LF, \tag{15.13}$$

and the diffusion matrix becomes

$$G = \hbar T (L + L^T). \tag{15.14}$$

Two cases are particularly important:

(i) For **closed systems with fixed boundary** (i.e., at constant T, V), the thermodynamic potential is called the **Helmholtz potential**, and $Z =: e^{-\beta U}$ determines the **internal energy** $U = \Phi - TS = -\hbar T \log Z$.

(ii) For **closed systems with free boundary** (i.e., at constant T, P), the thermodynamic potential is the **Gibbs potential**, and $Z =: e^{-\beta H}$ determines the **enthalpy** $H = \Phi - TS = -\hbar T \log Z$. (Actually, since we ignore space coordinates, we describe only well-mixed systems, and "diffusion" is here in the space $\mathbb{R}^n$ of species densities, not in physical space.)

(15.13)–(15.14) allow one to obtain the parameters of a diffusion process from macroscopic measurements: The thermodynamical potential can be obtained from measurements at equilibrium, and the transport matrix from measuring the response of the system to small external forces.

15.2.1 Theorem. *Let the transport matrix L be positive semidefinite. Then the diffussion process with covariant drift $u = -LF$ and diffusion matrix $G = \hbar T(L + L^T)$ can be written in the* **canonical form**

$$\frac{d}{dt}\langle f \rangle = \langle (\hbar T \nabla - F) \cdot L^T \nabla f \rangle. \tag{15.15}$$

For **closed** *systems, i.e., if the thermodynamic force F has the form*

$$F = \nabla \Phi \tag{15.16}$$

with a thermodynamical potential Φ*, then the process* (15.15) *has an equilibrium state*

$$\rho_{eq} = Z^{-1}e^{-\beta\Phi}, \qquad \beta = (\hbar T)^{-1}, \tag{15.17}$$

with the partition function $Z = \operatorname{tr} e^{\beta\Phi}$*. The equilibrium state is unique if* L *is positive definite.*

Proof. Since

$$u \cdot \nabla = -LF \cdot \nabla = -F \cdot L^T\nabla,$$
$$\nabla \cdot G\nabla = \hbar T\nabla \cdot (L + L^T)\nabla = 2\hbar T\nabla \cdot L^T\nabla,$$

we can write the Markov equation as

$$\frac{d}{dt}\langle f\rangle = \langle(\hbar T\nabla - F) \cdot L^T\nabla f\rangle.$$

□

15.2.2 Remarks. (i) In terms of ρ_{eq} we can write (15.15) as

$$\frac{d}{dt}\langle f\rangle = \hbar T\langle\rho_{eq}^{-1}\nabla \cdot (\rho_{eq}L^T\nabla f)\rangle \tag{15.18}$$

since $\rho_{eq}^{-1}\nabla \cdot (\rho_{eq}g) = e^{\beta\Phi}\nabla(e^{\beta\Phi}g) = e^{\beta\Phi}(e^{-\beta\Phi}\nabla g - \beta(\nabla\Phi)e^{\beta\Phi}g) = (\nabla - \beta F)g$.

This shows directly that ρ_{eq} is a stationary solution.

(ii) For **open** systems, the canonical form extends by adding to F the external force, i.e., we replace (15.16) by

$$F = \nabla\Phi + F_{\text{ext}}. \tag{15.19}$$

(iii) In the zero temperature limit, $T \to 0$, noise can be neglected ($G \to 0$), and the equilibrium state approches (saddle point approximation!) $\rho_{eq} \to \delta(x - x_{eq})$, where x_{eq} is the global minimizer of Φ (assumed unique). The motion becomes deterministic.

We now consider the deterministic approximation. According to Chapter 5 , this is given by the differential equation.

$$\dot{x} = v(x)$$

with the drift

$$v = u + \frac{1}{2}\nabla \cdot G = -LF + \frac{\hbar T}{2}\nabla \cdot (L + L^T).$$

However, because of covariance and the next result, it is more appropriate to use in place of v the covariant drift $u = -LF$. The two are the same when $L + L^T$ is constant, a very common case; in general they differ at low noise ($\hbar T$ small) only in higher order terms.

15.2.3 Theorem. *For the* **covariant deterministic approximation** *of the closed diffusion process* (15.15)*, given by*

$$\dot{x} = -L(x)F(x), \text{ where } F(x) = \nabla\Phi(x), \tag{15.20}$$

the potential $\Phi(x)$ decreases with time ("energy dissipates"):

$$\frac{d}{dt}\Phi(x) = -F(x)^T L(x) F(x) \leq 0. \tag{15.21}$$

If L is definite and Φ is coercive and below then any limit point of $x(t)$ for $t \to \infty$ is a stationary point of the thermodynamic potential, and the only stable equilibria are the local minima of Φ.

Proof. (15.21) holds since $\frac{d}{dt}\Phi(x) = \nabla\Phi(x) \cdot \dot{x}$. If Φ is coercive and bounded below then $\lim_{t\to\infty} \Phi(x)$ exists, $\frac{d}{dt}\Phi(x) \to 0$, whence $F^T L F = 0$ at any limit point. If L is definite, this implies $F = 0$. □

By (15.21), L describes the amount of energy **dissipation**; and since

$$\langle G \rangle = \langle (x - \bar{x})(x - \bar{x})^T \rangle$$

describes the size of **fluctuations**, the relation (15.14) between G and L is called a **fluctuation-dissipation theorem**.

In particular, **conservative** systems have

$$L^T = -L \Leftrightarrow \text{no dissipation} \Leftrightarrow \text{no fluctuation}.$$

In this case, we can transform the system into **symplectic form** :

$$L = MJM^T, \; J = \begin{pmatrix} 0 & I & 0 \\ -I & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$H(z) := \Phi(Mz), \nabla H = M^T \nabla M$$

$$\Rightarrow x = Mz, \; \dot{z} = J\nabla H(z).$$

15.2.4 Remark. Other instances of **fluctuation - dissipation theorems**:

(i) Huang: "susceptibilites" or "response functions" are expressible as covariances (fluctuations); *cf* therm.tex.

$$(7.14) \quad \hbar T^2 C_V = \langle H^2 \rangle_{ph} - \langle H \rangle_{ph}^2$$

$$(7.43) \quad N\hbar T K_T / V = \langle N^2 \rangle_{ph} - \langle N \rangle_{ph}^2$$

$$ch.16(?): \quad \frac{\hbar T}{V} \frac{\partial M}{\partial H_{magn}} = \langle \Gamma(r) \rangle_\Omega = \hbar T \chi$$

where

M = Magnetization = $\langle m(r) \rangle_\Omega$ (extensive, **an order parameter**) (15.275)

H_{magn} = conjugate magnetic field (Hamiltonian $H_0 - H_{magn} M$)

$\Gamma(r) = \langle m(r)m(0)\rangle_{ph} - \langle m(r)\rangle_{ph}\langle m(0)\rangle_{ph}$ = space correlation (measures persistence of memory)

(ii) Reichl p. $545, 554 - 6, 573$ (15.67):

$\chi(\omega)$ is the Fourier transform of $K(\tau)$ (Reichl p. $550/l.1$)

defined by (15.19) **response matrix** (in $1D$ = response function)

for its interpretation see also 15.5. $3 + 4$ (and following lines)

Note that due to (15.56) this is based on the **linear** model.

so we should have to derive this from the general canonical form.

(iii) Kreuzer [Ho Stat Me 96] p.11/12:

$$(1.15) \quad \langle (dU)^2\rangle = \hbar T^2 n C_V$$

$$(1.32) \quad \langle (dT)^2\rangle = \hbar T^2 / n C_V$$

$$\Rightarrow \triangle U \triangle T = \hbar T^2 = \frac{RT^2}{N_A} = O(N_A^{-1})$$

uncertainty relation between time and energy.

(iv) relation between equilibrium covariance and damping term in a linear stochastic differential equation

(v) response matrix (to past forces) $\leftrightarrow$ time correlations; generalize C_V expression?

(vi) The differential equation for the Ornstein-Uhlenbeck process.

15.3 Ornstein-Uhlenbeck processes

The **driven Ornstein-Uhlenbeck process** is defined by the diffusion process

$$\frac{d}{dt}\langle f\rangle = \langle v \cdot \nabla f + \frac{1}{2} G : \nabla^2 f\rangle, \tag{15.22}$$

where

$$v(x) = -L(\Sigma x - F_{ext}(t)) \tag{15.23}$$

$$G = \hbar T(L + L^T) \tag{15.24}$$

and L, Σ are positive semidefinite matrices, Σ symmetric. Usually they are nonsingular 9and hence definite).

The most important feature of these processes is that they preserve Gaussian distributions. In particular, this implies that their statistical behavior is completely determined by the mean

$$\bar{x}(t) := \langle x\rangle_t$$

and the covariance

$$C(t) := \langle (x-\bar{x})(x-\bar{x})^T \rangle_t.$$

From Chapter 5 , we have

$$\frac{d}{dt}\bar{x}(t) = \langle v \rangle = -L(\Sigma\bar{x}(t) - F_{ext}(t)), \tag{15.25}$$

$$\frac{d}{dt}C(t) = \langle G + v(x-\bar{x})^* + (x-\bar{x})v^* \rangle = G - L\Sigma C(t) - C(t)\Sigma L^T, \tag{15.26}$$

and these equations are **exact** consequences of (15.22) - (15.24). [i.e., all approximations made are already in the model formulation.] (15.25) describes a deterministic system of coupled and damped driven harmonic oscillators, while (15.22) is the corresponding stochastic version.

The mean equation (15.25) and the covariance equations (15.26) are decoupled, and can be solved explicitly:

$$\bar{x}(t) = e^{-tL\Sigma}\bar{x}(0) + \int_0^t e^{-(t-\tau)L\Sigma} L F_{ext}(\tau) d\tau, \tag{15.27}$$

$$C(t) = \hbar T \Sigma^{-1} + e^{-tL\Sigma} B (e^{-tL\Sigma})^T, \tag{15.28}$$

where

$$B = C(0) - \hbar T \Sigma^{-1}. \tag{15.29}$$

We now dicuss the solution (15.27), (15.28), assuming that Σ and L are **definite**. The **dissipation matrix**

$$A := -L\Sigma$$

has its spectrum in the negative half plane $\mathbb{C}_-$,

$$Ax = \lambda x, x \neq 0 \quad \Rightarrow \quad \operatorname{Re}\lambda = -\frac{(\Sigma x)^* L(\Sigma x)}{x^* \Sigma x} < 0.$$

Thus the initial state $\bar{x}(0)$ and "old" forces get exponentially damped, and **after long times,** the system behaves ike the special solution

$$\bar{x}(t) = \int_{-\infty}^t e^{-(t-\tau)L\Sigma} L F_{ext}(\tau) d\tau = \int_0^\infty e^{-sL\Sigma} L F_{ext}(t-s) ds. \tag{15.30}$$

The equilibrium of an Ornstein-Uhlenbeck process with positive definite G is unique; since the potential is quadratic, the equilibrium is **Gaussian**, with mean 0 and covariance $C = \hbar T \Sigma^{-1}$. The covariance matrix C is related to the dissipation matrix A and the diffusion matrix G by

$$G = AC + CA^T \tag{15.31}$$

which is another expression of the **fluctuation-dissipation theorem**.

In particular, since (15.31) implies that $C(t) = C$ is a solution of (15.26), uniqueness of the equilibrium implies unique solvability of (15.31) when A and G are given. This is a linear system for C; the solution gives also the transport matrix

$$L = (\hbar T)^{-1} AC.$$

15.4 Linear processes with memory

(15.30) is a special case of a **deterministic dissipative linear process with memory**, defined by

$$\bar{x}(t) := \int_0^\infty R(s)F_{ext}(t-s)ds, \tag{15.32}$$

where the **response function** $R(s)$ decays to 0 exponentially as $s \to \infty$.

In particular, for a harmonic external force

$$F_{ext}(t) = F_0 \cos \omega t = \mathrm{Re}(F_0 e^{-i\omega t}),$$

the response is given by

$$\begin{aligned} \bar{x}(t) = & \ \mathrm{Re} \int_0^\infty R(s)F_0 e^{-i\omega(t-s)}ds = \mathrm{Re}\, e^{-i\omega t}\hat{R}(\omega)F_0 \\ = & \ (\cos(\omega t)\,\mathrm{Re}\,\hat{R}(w) + \sin(\omega t)\,\mathrm{Im}\,\hat{R}(\omega))F_0 \end{aligned} \tag{15.33}$$

with the **transfer matrix**

$$\hat{R}(\omega) = \int_0^\infty e^{i\omega s}R(s)ds = \int_{-\infty}^\infty e^{i\omega s}R(s)ds \tag{15.34}$$

if one extends the response function to $s < 0$ by setting $R(s) = 0$ for $s < 0$. The energy dissipated in a period is

$$E = \int F_{ext}(t) \cdot d\bar{x}(t) = \int_0^{2\pi/\omega} F_{ext}(t) \cdot \dot{\bar{x}}(t)dt = \ldots = \pi F_0^T(\mathrm{Im}\,\hat{R}(\omega))F_0. \tag{15.35}$$

Since $R(t)$ can be recovered form $\mathrm{Im}\,\hat{R}(w)$ as

$$R(t) = \frac{2}{\pi}\int_0^\infty \mathrm{Im}\,\hat{R}(\omega)\sin(\omega t)d\omega$$

(from Fourier inversion formula since R is real), this implies that (the symmetric part of) the response function and the transfer matrix can be obtained very accuratly by measuring the power absorption dE/dt (averaged over N periods of a harmonic driving force with angular frequency ω. This gives $\frac{\omega N}{2\pi}E$; hence (the symmetric part of) $\mathrm{Im}\,\hat{R}(\omega)$ is directly computable from (15.35). Then one can calculate $R(t)$. Finally, $\mathrm{Re}\,\hat{R}(\omega)$ is reconstructed either by Fourier transform of $R(t)$, or by the Kramers-Kronig relations.

The system responds by forced oscillations of the same frequences, but the force is weighted by the transfer matrix. In particular, *resonances* occur at frequencies where $\hat{R}(\omega)$ is large.

For the Ornstein-Uhlenbeck process, (15.3.15.30) shows that the response function is

$$R(s) = \begin{cases} e^{-sL\Sigma}L & \text{if } \ s > 0, \\ 0 & \text{if } \ s < 0. \end{cases} \tag{15.36}$$

The transfer matrix becomes

$$\hat{R}(\omega) = \int_0^\infty e^{-s(L\Sigma - i\omega)} L ds = (L\Sigma - i\omega)^{-1} e^{-s(L\Sigma - i\omega)} L \Big|_0^\infty;$$

hence

$$\hat{R}(\omega) = -(i\omega - L\Sigma)^{-1} L \tag{15.37}$$

is a rational function of ω. The dissipated energy (15.35) involves

$$\begin{aligned} \operatorname{Im} \hat{R}(\omega) = & \operatorname{Im}(i\omega - L\Sigma)^{-1} L = [\omega^2 + (L\Sigma)^2]^{-1} \operatorname{Im}(-i\omega - L\Sigma) L \\ = & [\omega^2 + (L\Sigma)^2]^{-1} \omega L. \end{aligned}$$

In particular, $\hat{R}(\omega)$ will be large when ω is close to the imaginary part of an isolated eigenvalue of $L\Sigma$ with small real part. This is the reason why one defines **resonances** mathematically by the poles of the transfer matrix in the half plane $\omega \in \mathbb{C}_+$ where (15.34) makes sense.

For numerical calculation, we use a Cholesky factorization

$$\Sigma = R^T R$$

and a spectral factorization

$$RLR^T = Q\Lambda Q^{-1}, \qquad \Lambda \text{ diagonal}, \qquad \operatorname{Re} \Lambda \geq 0.$$

The columns of $R^{-1}Q$ are eigenvectors of $L\Sigma$, and we have (for $s > 0$)

$$R(s) = e^{-sL\Sigma} L = R^{-1} Q e^{-s\Lambda} \Lambda Q^{-1} R^{-T} = R^{-1} Q,$$

$$e^{-tL\Sigma} B (e^{-tL\Sigma})^T = R^{-1} Q e^{-s\Lambda} Q^{-1} R B (Q^{-1} R)^* e^{-s\Lambda^*}.$$

For symmetric L, we rather factor

$$L = R^T R$$

and

$$R\Sigma R^T = Q\Lambda Q^T,$$

with orthogonal Q and diagonal $\Lambda \geq 0$. Now the columns of $R^T Z$ are eigenvectors of LZ, and we get

$$e^{-sL\Sigma} L = R^T Q e^{-s\Lambda} Q^T R,$$

$$e^{-tL\Sigma} B (e^{-tL\Sigma})^T = R^T Q E^{-t\Lambda} \bar{B} e^{-t\Lambda} Q^T R,$$

where

$$\bar{B} = Q^T (R^{-1} B R^{-1}) Q.$$

- **spectral density**
- time correlations. why $|t|$? "two kinds of order"

- relation to $B(t)$ = return to equilibrium response after a force switch

  This is another F/D version

- $B(t) = \frac{2}{\pi}\int_0^\infty \operatorname{Im}\hat{R}(\omega)\cos\omega(t)\frac{d\omega}{\omega}$ (B is the fluctuation = time correlation, $\operatorname{Im}\hat{R}$ the dissipation.)

- Quantum version

- The Brownian particle correponds to linearized damped Hamiltonian systems. Force only applies to the second order term.

driven continous-time linear state space model = driven Ornstein-Uhlenbeck process with derived measurable quantities y.

$$\dot{x}(t) = -L(\Sigma x(t) - F_{ext}(t)) \quad + \quad \text{noise},$$

$$y(t) = Yx(t) \quad + \quad \text{noise},$$

$$\bar{x}(t) = \int_0^\infty e^{-sL\Sigma} LF_{ext}(t-s)ds.$$

For a constant pulse of length T,

$$F_{ext}(t) = \begin{cases} F_0 & \text{for } t \in [-T, 0], \\ 0 & \text{otherwise,} \end{cases}$$

the system responds for times $t > 0$ with

$$\begin{aligned} \bar{x}(t) &= \int_{-T}^0 e^{-(t-\tau)L\Sigma} LF_0 d\tau = e^{-tL\Sigma}\Big(\int_{-T}^0 e^{\tau L\Sigma} d\tau\Big) LF_0 \\ &= e^{-tL\Sigma}(1 - e^{-TL\Sigma})(L\Sigma)^{-1} LF_0 = (e^{-tL\Sigma} - e^{-(t+T)L\Sigma})\Sigma^{-1} F_0. \end{aligned}$$

In particular, if $L\Sigma Q = Q\Lambda$ (Λ diagonal) then

$$\bar{y}(t) = YQ(e^{-t\Lambda} - e^{-(t+T)\Lambda})Q^{-1}\Sigma^{-1}F_0 = Qe^{-t\Lambda}(1 - e^{-T\Lambda})Q^{-1}\Sigma^{-1}F_0.$$

So the **pulse response** $y(t)$ is a linear combination of exponentials. More generally, when the spectral factorzation is not possible because of defective $L\Sigma, y(t)$ is still expolynomial.

15.5 Dissipative Hamiltonian Systems

A conservative Hamiltonian system is an energy-conserving process characterized by a **Hamiltonian function** $H(p, q)$ in the position vector q and the conjugate momentum vector p and defined by the differential equations

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}. \tag{15.38}$$

Energy conservation follows since

$$\frac{d}{dt}H(p,q) = H_p\dot{p} + H_q\dot{q} = 0,$$

so that $H(p,q)$ must be constant. But energy conservation for macroscopic systems is an idealization, and more realistic models include energy loss due to **friction**. Friction is energy dissipation caused by random microscopic forces producing **heat**. We use the canonical form to derive an equation for the phase vector

$$x = \begin{pmatrix} q \\ p \end{pmatrix}.$$

Friction is experienced as a restraining force proportional to the velocity $\dot{q}$; in the covariant approximation, Newton's law gives the modified differential equation

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q} - C(q)\dot{q} = -\frac{\partial H}{\partial q} - C(q)\frac{\partial H}{\partial p} \tag{15.39}$$

describing a **dissipative Hamiltonian system**.

With this dynamics, the energy change is

$$\frac{d}{dt}H(p,q) = \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial q}\dot{q} = -\dot{q}^T C(q)\dot{q},$$

and we see that the damping matrix $C(q)$ must be assumed to be **positive definite** (but not necessarily symmetric) in order to have dissipation except at rest.

In terms of the potential (total energy)

$$\Phi(x) = H(p,q),$$

the thermodynamic force becomes

$$F = \begin{pmatrix} \frac{\partial H}{\partial p} \\ \\ \frac{\partial H}{\partial q} \end{pmatrix};$$

and we infer from (15.39) that the covariant drift has the form

$$u = \begin{pmatrix} \frac{\partial H}{\partial p} \\ \\ -\frac{\partial H}{\partial q} - C(q)\frac{\partial H}{\partial p} \end{pmatrix} = -\begin{pmatrix} 0 & -I \\ \\ I & C(q) \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial p} \\ \\ \frac{\partial H}{\partial q} \end{pmatrix} = -LF,$$

where

$$L = \begin{pmatrix} 0 & -I \\ I & C(q) \end{pmatrix}. \tag{15.40}$$

The fluctuation-dissipation theorem now shows that the correct diffusion matrix is

$$G = \hbar T(L + L^T) = \hbar T \begin{pmatrix} 0 & 0 \\ 0 & C(q) + C(q)^T \end{pmatrix} \tag{15.41}$$

Thus we end up with the canonical diffusion process

$$\frac{d}{dt}\langle f(p,q)\rangle = \left\langle \frac{\partial H}{\partial p} \cdot \frac{\partial f}{\partial q} - \left(\frac{\partial H}{\partial q} + C\frac{\partial H}{\partial p}\right) \cdot \frac{\partial f}{\partial p} + \hbar T \frac{\partial}{\partial p} \cdot \left(C \cdot \frac{\partial f}{\partial p}\right)\right\rangle. \tag{15.42}$$

The stationary density turns out to be the **canonical ensemble**

$$\rho_{eq}(p,q) = Z^{-1} e^{-\beta H(p,q)}, \quad Z = \operatorname{tr} e^{-\beta H(p,q)}. \tag{15.43}$$

For constant C we get the associated stochastic differential equation

$$dq = \frac{\partial H}{\partial p} dt, \quad dp = \left(-\frac{\partial H}{\partial q} - C\frac{\partial H}{\partial p}\right) dt + d\varepsilon,$$

$$d\varepsilon \sim N(0, \hbar T(C + C^T)).$$

In the special case of Cartesian coordinates, where

$$H = \frac{1}{2} p^T M^{-1} p + V(q)$$

we can write $q = x,\ p = M\dot{x}$ (from $dq = M^{-1} p dt$) and get

$$M\ddot{x} + C\dot{x} + \nabla V(x) = B\dot{W}(t)$$

where

$$BB^T = \hbar^T (C + C^T)$$

and B, C are constant.

Chapter 16

Collective Processes

16.1 The master equation

In this section we discuss the general set-up of a system in which a large number of individuals interact through private communication in an environment where collective forces govern the frequency of communication events.

Our communication model has the following ingredients.

$(C1)$ there are q **species** $X_j (j = 1, \ldots, q)$ describing **individuals**. The number of individuals of species X_j in a system is written as N_j; these numbers define the **population vector** $N \in \mathbb{Z}^q$; **The density** $\rho_t(N)$ describes the likelihood to have at time t a population number N, and the integral is

$$\int f = \sum_{N \in \mathbb{Z}^q} f(N).$$

$\mathbb{E}$ consists of all geometrically decaying functions of N.

In practice, species may be elementary particles, molecules of fixed chemical composition, biologigal species (of animals or plants), diseases of people, professions of people, spectral classes of stars, etc. We take the number of different species as finite, although everything extends to $q = \infty$, with examples e.g. in polymer physics, where j is the chain length).

$(C2)$ There are r kinds of **events**

$$\sum_{j=1}^{q} \nu_{lj}^{+} X_j \rightleftharpoons \sum_{j=1}^{q} \nu_{lj}^{-} X_j \qquad (l = 1, \ldots, r) \tag{16.1}$$

with nonnegative numbers $\nu_{lj}^{\pm} \quad (l = 1, \ldots, r; j = 1, \ldots, q)$.

Events model the elementary units of communtication; an event consists in the meeting of a collection of ν_{lj}^{+} individuals of kind $X_j (j = 1, \ldots, q)$ changing during the meeting into a collection of kind ν_{lj}^{-} individuals of kind $X_j (j = 1, \ldots, q)$; or reversed. If the reverse process

is impossible we write $\to$ in place of $\rightleftharpoons$. Events are considered as black boxes about which no details are available. Again we assume r to be finite.

Usually $\sum v_{lj}^+$ and $\sum v_{lj}^-$ are very small; typically ≤ 3. We may illustrate an event $A+B \rightleftharpoons C+D$ as follows.

Typical instances are:

$$e^+e^- \rightleftharpoons 2\gamma$$

$$H^+ + OH^- \rightleftharpoons H_2O$$

$$\text{[hungry bird]} + \text{[caterpillar]} \to \text{[satisfied bird]}$$

$$\text{[healtly person]} + \text{[ill person]} \to 2\ \text{[ill person]}$$

$$\begin{cases} \text{[husband]} + \text{[wife]} \to \text{[husband]} + \ \text{[pregnant wife]} \\ \text{[pregnant wife]} \to \text{[wife]} + \text{[child]} \end{cases}$$

$$\text{[buyer\&money]} + \text{[seller\&object]} \rightleftharpoons \text{[buyer\&object]} + \text{[seller\&money]}$$

$(C3)$ There are **transition rates** $u_l^\pm : \mathbb{Z}^n \to \mathbb{R}_+ (l = 1, \ldots, r); u_l^+(N)$ and $u_l^-(N)$ specify the likelihood that event l happens in forward or backward direction in a population described by $N; u_l^- = 0$ specifies an event which only oceurs in the forward direction.

The transiton rates are global, collective, properties of the system; they account for non-local, long range interaction between individuals, and for **limitations of freedom** due to overpopulation, mutual attraction, and mutual repulsion. A very common Ansatz for the transmition rates is that of **combinatorial kinetics**, where

$$u_l^\pm(N) = K_l^\pm \pi_{j=1}^q \binom{N_j}{\nu_{lj}^\pm} = \begin{cases} 0 & \text{if } N_j < \nu_{lj}^\pm \text{ for some } j, \\ k_l^\pm \displaystyle\prod_{j=1}^q \frac{N_j!}{(N_j - v_{lj}^\pm)!} & \text{otherwise,} \end{cases} \tag{16.2}$$

with constants $k_l^\pm = k_l^\pm \prod_j (\nu_{lj}^\pm)!$; one writes $\rightleftharpoons_{k_l-}^{k_l^+}$ (or $\overset{k_l^+}{\to}$ if $k_l^- = 0$). This models the assumption that individuals are completely independent and meet only by chance, so that the transition rates are proportional to the number of ways to assemble the required collection of individuals in a population described by N. Combinatorial kinetics describes correctly the chemistry of ideal gases and ideal solutions; it is also used for most systems in biology, medicine, economy, and social sciences, mainly because of simplicity and lack of more detailed knowledge.

$(C4)$ The **probability current** produced by the event l is defined as

$$j_l(N) := u_l^-(N + \nu_l^-)\rho(N + \nu_l^-) - u_l^+(N + \nu_l^+)\rho(n + \nu_l^+). \tag{16.3}$$

Here N is interpreted as the part of the population **not** involved in the event, and the current consists of a positive contribution due to the outcome of the event and a negative contribution due to the input of the event. If we interpret the probability currents as the rate of change of the density due to single events, and count forward events positively, backward events negatively, we end up with the **master equation**

$$\frac{d}{dt}\rho_t(N) = \sum_{l=1}^{r} \left(j_l(N-\nu_l^+) - j_l(N-\nu_l^-)\right) = \sum_{l=1}^{r} \left([u_l^-\rho_t]_N^{N+\varepsilon_l} + [u_l^+\rho_t]_N^{N-\varepsilon_l}\right) \tag{16.4}$$

with the **jump vectors**

$$\varepsilon_l := \nu_l^- - \nu_l^+. \tag{16.5}$$

The master equation is a system of infinitely many ordinary differential equations.

$(C5)$ Finally we shall assume the restrictions

$$N_j \geq \nu_{lj}^+ \quad \text{for all } j \Rightarrow \varepsilon_l^+(N) > 0 \tag{16.6}$$

and

$$n_j < \nu_{lj}^\pm \quad \text{for some } j \Rightarrow u_l^\pm(N) = 0; \tag{16.7}$$

the latter implies that the dynamics preserves the natural condition

$$\rho_t(N) = 0 \quad \text{if some } N_j < 0 \tag{16.8}$$

at all times if it holds at $t = 0$.

A system satisfying (C1)–(C5) is called a **collective process**.

16.1.1 Theorem. *Any collective process is a Markov process, whose forward derivation D is given by*

$$Df : N \to \sum_l \left(u_l^-(N)(f(N-\varepsilon_l) - f(N)) + u_l^+(N)(f(N+\varepsilon_l) - f(N))\right). \tag{16.9}$$

For $x = N$, the drift vector v and the diffusion matrix G are given by

$$v(N) = \sum_l (u_l^+(N) - u_l^-(N))\varepsilon_l, \tag{16.10}$$

$$G(N) = \sum_l (u_l^+(N) + u_l^-(N))\varepsilon_l\varepsilon_l^*. \tag{16.11}$$

Proof. We first note that the sum over $N \in \mathbb{Z}^q$ is translation invariant. Using the notation

$$[f]_{N_1}^{N_2} = f(N_2) - f(N_1),$$

we find

$$\begin{aligned}\sum_N [g]_N^{N+\varepsilon} f(N) &= \sum_N g(N+\varepsilon)f(N) - \sum_N g(N)f(N) \\ &= \sum_N g(N)f(N-\varepsilon) - \sum_N g(N)f(N) = \sum_N g(N)[f]_N^{N-\varepsilon}.\end{aligned}$$

Hence

$$\begin{aligned}\frac{d}{dt}\langle f\rangle &= \sum_N \frac{d}{dt}\dot\rho_t(N)f(N) = \sum_N\sum_l([u_l^-\rho]_N^{N+\varepsilon_l} + [u_l^+\rho]_N^{N-\varepsilon_l})f(N)\\ &= \sum_N\sum_l(u_l^-(N)\rho(N)_N^{N-\varepsilon_l} + u_l^+(N)\rho(N)[f]_N^{N+\varepsilon_l})\\ &= \sum_N \rho(N)(Df)(N) = \langle Df\rangle,\end{aligned}$$

with D defined by (16.9). Clearly, D is $*$-linear and $D1 = 0$. Now

$$Q(f,g) := D(fg^*) - (Df)g^* - f(Dg^*) \tag{16.12}$$

maps N to

$$\begin{aligned}\sum_\pm\sum_l \quad & u_l^\pm(N)\left\{(f(N\pm\varepsilon_l)g^*(N\pm\varepsilon_l) - f(N)g^*(N))\right.\\ & \left.-(f(N\pm\varepsilon_l)g^*(N) - f(N)g^*(N)) - (f(N)g^*(N\pm\varepsilon - f(N)g^*(N))\right\},\end{aligned}$$

hence

$$Q(f,g)(N) = \sum_\pm\sum_l u_l^\pm(N)(f(N\pm\varepsilon_l) - f(N))(g(N\pm\varepsilon_l) - g(N))^*. \tag{16.13}$$

For $g = f$, this is clearly nonnegative; hence D is a forward derivation and we have a Markov process. For $f(N) = N_j,\ g(N) = N_k$ we find the (j,k)-component of the diffusion matrix (16.11), and the drift vector follows from (16.9) for $f(N) = N_j$. □

16.1.2 Remarks. 1. Higher jump momemts are found similarly, with alternating signs of u_l^-.

2. Any Markov process in $\mathbb{E} = \mathbb{C}^n$ can be brought to this form: Introduce for each unordered pair (j,k) an event $X_j \rightleftharpoons X_k$ and note that $\sum N_j = 1$ (or $= N_{\text{tot}}$, with frequency representation) is conserved.

16.1.3 Examples. (i) (**Poisson process**). The simplest **birth process** (e.g., electrons in β-decay, change of composition of the source due to the decay) is given by a single event for a simple species

$$0 \xrightarrow{\lambda} X.$$

With combinational kinetics, we have $u_0^+(N) = \lambda,\ u_0^-(N) = 0$, hence the master equation

$$\dot\rho_t(N) = \lambda(\rho_t(N-1) - \rho_t(N)). \tag{16.14}$$

With the initial condition $\rho_0(N) = \delta_{N0}$ (no individual at $t = 0$), the solution of (16.14) is

$$\rho_t(N) = \frac{(\lambda t)^N e^{-\lambda t}}{N!}, \tag{16.15}$$

describing a Poisson distribution with

$$\langle N\rangle_t = \lambda t, \quad \mathrm{var}_t(N) = \lambda t. \tag{16.16}$$

(16.16) follows more directly from the moment equations

$$\frac{d}{dt}\langle N\rangle = \langle v\rangle = \langle\lambda\rangle = \lambda,$$

$$\frac{d}{dt}\sigma^2 = \langle G\rangle = \langle\lambda\rangle = \lambda.$$

For $t \to \infty$ the variance diverges; hence no stationary solution exists.

(ii) The simplest **birth and death process** (e.g., fog formation) is given by a single event for a single species

$$0 \underset{\gamma}{\overset{\alpha\gamma}{\rightleftharpoons}} X.$$

with combinational kinetics. We get from $u^+(N) = \alpha\gamma,\ u^-(N) = \gamma N$ the master equation

$$\dot\rho_t(N) = \alpha\gamma(\rho_t(N-1) - \rho_t(N)) + \gamma((N+1)\rho_t(N+1) - N\rho_t(N)). \tag{16.17}$$

This can be solved exactly, with a complicated solution (see e.g., Gardiner [99]). Rather we use the moment equations for mean and variance,

$$\frac{d}{dt}\langle N\rangle = \langle v\rangle = \langle\gamma(N-\alpha\gamma)\rangle = \gamma(\langle N\rangle - \alpha),$$

$$\frac{d}{dt}\sigma^2 = \langle G\rangle = \langle\gamma N + \alpha\gamma\rangle = \gamma(\langle N\rangle + \alpha).$$

With initial condition $N = N_0$ (a number) at $t = 0$, we get the solution

$$\left.\begin{aligned}\langle N\rangle_t &= \alpha(1-e^{-\gamma t}) + N_0 e^{-\gamma t},\\ \sigma_t^2 &= (\alpha + N_0 e^{-\gamma t})(1-e^{-\gamma t}).\end{aligned}\right\} \tag{16.18}$$

The equilibrium solution is, characterized by $\dot\rho(N) = 0$ for all N, can be shown to be given by a Poisson distribution

$$\rho(N) = \frac{\alpha^N e^{-\alpha}}{N!},$$

and indeed, (16.18) converges in the limit $t \to \infty$ to mean and variance of this distribution.

(iii) More generally, systems consisting of solitary individuals, where all events are of the form $X_j \rightleftharpoons X_k$, $X_j \leftrightarrow 0$, $X_j \to$ anything, or $0 \to$ anything, have explicitely solvable master equations and linear, triangular moment equations which can be solved recursively.

More interesting cases can only be solved numerically, using the low noise approximation, a discrete Galerkin method, or Monte Carlo simulations.

We say that the linear combination $a^T N = \sum a_k N_k$ is **conserved** in a collective process if

$$a^T \nu_l^+ = a^T \nu_l^- \quad \text{for } l = 1, \ldots, r. \tag{16.19}$$

The typical reason for such a relation is that there is a family $Y_i (i = 1, \ldots, p)$ of **invariants** (conserved quantities, e.g., charge, lepton number, atoms, functional groups, dollars) which, in every event, are exchanged in full units and don't get lost. If each individual of species X_j contains A_{ij} invariants Y_j then

$$A\nu_l^+ = A\nu_l^- \quad \text{for } l = 1, \ldots, r, \tag{16.20}$$

since the ith component of both sides counts the total number of invariants Y_i involved in event l. Hence, if $a_k = \sum b_j A_{jk}$ with arbitrary constants b_j then $a^T \nu_l^+ = b^T A \nu_l^+ = b^T A \nu_l^- = a^T \nu_l^-$, i.e., $a^T N$ is conserved. We say that the invariants $Y_i (i = 1, \ldots, p)$ form a **full set of invariants** if every conserved linear combination $a^T N$ is a linear combination of the components of AN, i.e. if

$$a^T \nu_l^+ = a^T \nu_l^- (l = 1, \ldots, r) \quad \Rightarrow \quad a^T \equiv b^T A \quad \text{for some } b \in \mathbb{R}^P. \tag{16.21}$$

The matrix A is referred to as the composition matrix of the process with respect to $Y_1, \ldots, Y_p$.

16.1.4 Proposition. *If $\rho_t(N)$ is a solution of a master equation* (16.4) *satisfying* (16.20) *then, for all functions g,*

$$\tilde{\rho}_t(N) := \rho_t(N) g(AN)$$

is also a solution of (16.4).

Proof. (16.20) implies $A\varepsilon_l = 0$, hence $g(A(N \pm \varepsilon_l)) = g(AN)$, where we can cancel in ($\tilde{16.4}$) a common factor $g(AN)$. □

The proposition reflects the fact that **any** initial distribution of AN is fixed by the dynamics. Usually one fixes the distribution by assuming deterministic values for the components of AN (i.e. numbers instead of quantities); this reduces the Euclidean *-algebra and turns $g(AN)$ into a number, which cancels under normalization of $\tilde{\rho}$.

A **component** of collective process is a set N consisty of all population vectors $N \in \mathbb{Z}^q$ which are reachable from some fixed N_0 by a sequence of events. Clearly, (16.20) implies that all $N \in \mathcal{N}$ have the same value of AN, and typically components are characterized by the common value of AN for $N \in \mathcal{N}$. However, there are processes like

$$2X_1 \rightleftharpoons 0,$$

where the parity of N_1 is conserved, too, and there are processes like

$$2X_1 \rightleftharpoons 2X_2 \rightleftharpoons X_1$$

which have no invariant but several components, here $\left\{ \binom{0}{0} \right\}$ and $\{N \mid N_1, N_2 \geq 0\} \setminus \left\{ \binom{0}{0} \right\}$.

Clearly, the dynamics in different components is completely independent; so we may restrict $\mathbb{E}_0$ (and hence the density) to functions of N which vanish outside some fixed component.

16.1.5 Theorem. *If $\mathbb{E}_0$ consists of the functions of N which vanish outside some fixed component of a collective process, the forward derivation of the process is primitive. In particular, if a positive equilibrium state exists, it is unique, and is reached from any initial state as $t \to \infty$.*

Proof. By (16.12) and (16.13), $D(ff^*) = (Df)f^* + f(Df^*) \Rightarrow f(N \pm \varepsilon_l) = f(N)$ whenever $u_l^{\pm}(N) > 0$. Thus f is constant on each component. Since by assumption only one component is nontrivial, D is primitive. □

16.2 Canonical form and thermodynamic limit

A generalization of combinatorial kinetics is given by collective processes in which the transition rates have the form

$$u_l^{\pm}(N) = \omega_l^{\pm} \frac{\rho_\Omega(N - \nu_l^{\pm})}{\rho_\Omega(N)}, \tag{16.22}$$

where $\omega_l^{\pm} \geq 0$ and ρ_Ω is a density which is positive when all $N_j \geq 0$, and vanishes otherwise. We call processes satisfying (16.22) **canonical**. Combinatorial kinetics is special case of (16.22) where ρ_Ω is a **multivariate Poisson distribution**, defined by

$$\rho_\Omega(N) = \prod_{j=1}^{q} \frac{\alpha_j^{N_j} e^{-\alpha_j}}{N_j!}; \tag{16.23}$$

substitution into (16.22) and comparison with (16.1.16.2), shows that the rate constants are related to the $\omega_l^{\pm}$ by the equations

$$k_l^{\pm} = \omega_l^{\pm} \prod_{j=1}^{q} \alpha_j^{-\nu_{lj}^{\pm}} \quad (l = 1, \ldots, r). \tag{16.24}$$

[Apparently all processes considered in applicatons are in canonical form. The reason is unclear to me.]

16.2.1 Theorem. *For a canonical collective process with*

$$\omega_l^{+} = \omega_l^{-} \quad (l = 1, \ldots, r), \tag{16.25}$$

we have:

(i) At equilibrum, all probability currents $j_l(N)$ vanish.

(ii) On each component of the process, $\rho_{eq}(N)$ is a constant multiple of $\rho_\Omega(N)$.

Proof. The density $\rho = \rho_\Omega$ produces the current

$$j_l(N) = (\omega_l^+ - \omega_l^-)\rho_\Omega(N).$$

j_l vanishes when $\omega_l^+ = \omega_l^-$. By the master equation, this implies that ρ_Ω is time invariant, and by Theorem 7.1.4, this shows that ρ_{eq} is a multiple of ρ_Ω. □

If (16.25) holds we say the system satisfies **detailed balance**. Each event then satisfies a separate balance equation $j_l(N) = 0$, whereas in general at equilibrium only the total (signed) sum of currents vanishes. Thus (i) and (ii) characterize **closed systems**.

For a noncanonical system, detailed balance does not say too much, only

$$u_l^\pm(N) = \frac{\omega_l(N - \nu_l^\pm)}{\rho_{eq}(N)}$$

for suitable ω_l. Note that microreversibility only gives detailed balance , but not the canonical form, which is an independent axiom.

To discover the equilibrium of a combinatorial process one can try to solve (16.24) with $\omega_l^+ = \omega_l^-$ for the ω_l and α_j ($2r$ equations for $q + r$ unknowns); if these equatons are consistent, (16.23) provides the equilibrium solution (upto a constant factor which depends on the initial distribution of the conserved quantities). If the equations are inconsistent, the system cannot be closed.

The analogy to the canonical form for diffusion processes is seen by introducing the discrete forward derivations δ_l with

$$\delta_l f : N \to f(N + \nu_l^-) - f(N + \nu_l^+);$$

one easily sees that the adjoint δ_l^* is given by

$$\delta_l^* f : N \to f(N - \nu_l^-) - f(N - \nu_l^+).$$

Thus we can write

$$\begin{aligned} Df : N \to \quad & \sum_l \left(u_l^-(N)(\delta_l f)(N - \nu_l^-) - u_l^+(N)(\delta_l f)(N - \nu_l^+)\right) \\ = \quad & \sum_c \omega_l \rho_{eq}(N)^{-1} \left((-\rho_{eq}\delta_l f)(N - \nu_l^-) + (\rho_{eq}\delta_l f)(N - \nu_l^+)\right) \\ = - \quad & \sum_l \rho_{eq}^{-1}\delta_l^*(\omega_l(\rho_{eq}\delta_l f)). \end{aligned}$$

With the vector $\delta = (\delta_l)_{l=1}^r$ and $\Omega = \mathrm{diag}(\omega_l)$ we get

$$Df = -\rho_{eq}^{-1}\delta^*(\Omega\rho_{eq}\delta f)$$

in close analogy to the diffusion case

$$Df = \rho_{eq}^{-1}\nabla(L\rho_{eq}\nabla f) = -\rho_{eq}^{-1}\nabla^*(L\rho_{eq}\nabla f).$$

The latter formula is obtained if we use the approximations

$$\delta_l f \approx \varepsilon_l \cdot \nabla f, \quad \delta_l^* f \approx -\varepsilon_l \cdot \nabla f$$

and put

$$L := \sum_{\|l\| \le r} \omega_l \varepsilon_l \varepsilon_l^T.$$

In practice, collective processes are often studied when N is very large; then a very useful approximation is the consideration of the so-called **thermodynamic limit** $N \to \infty$. The interesting quantities are the relative sizes of the N_j. Thus we shall write

$$N = \Omega x, \qquad \omega_l^{\pm} = \Omega \kappa_l^{\pm}, \tag{16.26}$$

and for combinatorial kinetics also

$$\alpha_j = \Omega a_j \tag{16.27}$$

with x, κ, a_j of order 1 and a number Ω which becomes very large. Ω could be the total number of individuals, or any other extensive quantity (total volume, total mass, etc.). Our next text theorem justifies **deterministic physics** for **macroscopic objects**.

16.2.2 Theorem. *Suppose the* **thermodynamic potential**

$$\Phi(x) := -kT \lim_{\Omega \to \infty} \frac{\log \rho_\Omega(\Omega x)}{\Omega} \tag{16.28}$$

exists and is continuously differentiable. Then:

(i) Φ is homogeneous of degree one, $\Phi(\lambda x) = \lambda \Phi(x)$, and the **thermodynamic force**

$$F(x) := \nabla \Phi(x) \tag{16.29}$$

is scaling invariant, $F(\lambda x) = F(x)$. Moreover, the **Euler equation**

$$\Phi(x) = F \cdot x \tag{16.30}$$

holds.

(ii) The dynamics becomes deterministic in the thermodynamic limit $\Omega \to \infty$, and is given by the differential equation

$$\dot{x} = u(x) := \sum_l \left(\kappa_l^+ e^{\beta \nu_l^+ \cdot F(x)} - \kappa_l^- e^{\beta \nu_l^- \cdot F(x)} \right) (\nu_l^- - \nu_l^+), \tag{16.31}$$

and for finite Ω we have the relation

$$\frac{d}{dt} \langle f(x) \rangle = \langle u(x) \cdot \nabla f(x) \rangle + O(\Omega^{-1} \|f\|). \tag{16.32}$$

Proof. From the definition (16.28), we find

$$\Phi(\lambda x) = -kT \lim_{\Omega\to\infty} \log \rho_\Omega(\Omega\lambda x/\Omega)\Omega = -\lambda \hbar T \lim_{\lambda\Omega\to\infty} \log \rho_\Omega(\lambda\Omega x)/\lambda\Omega = \lambda\Phi(x),$$

whence Φ is homogeneous. Differentiation with respect to λ yields $\nabla\Phi(x)\cdot x = \Phi(x)$, and for $\lambda = 1$ we obtain the Euler equation (16.30).

To derive (16.31), we assume more specifically that

$$-\hbar T \log \rho_\Omega(\Omega x) = \Omega\Phi(x) + \psi(x) + O(\Omega^{-1}). \tag{16.33}$$

Thus

$$\begin{aligned} \hbar T \log \rho_\Omega(N-\nu) &\underset{(16.33)}{=} -\Omega\Phi(x-\nu/\Omega) - \psi(x-\nu/\Omega) + O(\Omega^{-1}) \\ &\underset{\text{Taylor}}{=} -\Omega\Phi(x) + \nabla\Phi(x)\cdot\nu - \psi(x) + O(\Omega^{-1}), \end{aligned}$$

hence

$$\begin{aligned} \log(\rho_\Omega(N-\nu)/\rho_\Omega(N)) &= \log\rho_\Omega(N-\nu) - \log\rho_\Omega(N) \\ &= \beta\nabla\Phi(x)\cdot\nu + O(\Omega^{-1}) = \beta\nu\cdot F(x) + O(\Omega^{-1}). \end{aligned}$$

The transition rates (16.22) become

$$u_l^\pm(N) = \Omega\kappa_l^\pm e^{\beta\nu_l^\pm\cdot F(x)}(1 + O(\Omega^{-1})).$$

For any function $f(x)$ and $\tilde{f}(N) := f(N/\Omega)$ we obtain the forward derivation

$$\begin{aligned} D\tilde{f}(N) &= \sum_\pm\sum_l u_l^\pm(N)\left(\tilde{f}(N\pm\varepsilon_l) - \tilde{f}(N)\right) \\ &= \sum_\pm\sum_l u_l^\pm(N)\left(f(x\pm\varepsilon_l/\Omega) - f(x)\right) \\ &= \sum\sum \Omega\kappa_l e^{\beta\nu_l^\pm\cdot F(x)}\left(1 + O(\Omega^{-1})\right)\left(\nabla f(x)(\pm\varepsilon_l/\Omega) + O(\Omega^{-2})\right) \\ &= \sum\sum \kappa_l e^{\beta\nu_l^\pm\cdot F(x)}(\pm\varepsilon_l\cdot\nabla f(x) + O(\Omega^{-1})) \\ &= u(x)\cdot\nabla f(x) + O(\Omega^{-1}). \end{aligned}$$

Thus, with $u(x)$ defined by (16.31), we find

$$\frac{d}{dt}\langle f(x\rangle = \frac{d}{dt}\langle\tilde{f}(N)\rangle = \langle u(x)\cdot\nabla f(x)\rangle + O(\Omega^{-1}),$$

which is (16.32). In the thermodynamic limit, we obtain the deterministic dynamics

$$\frac{d}{dt}\langle f(x)\rangle = \langle u(x)\cdot\nabla f(x)\rangle$$

belonging to the ordinary differential equation (16.31). □

We call a deterministic process (16.31) with a thermodynamic force $F = \nabla\Phi$ determined by a homogeneous thermodynamic potential Φ of degree 1 and corresponding a **macroscopic collective process**.

16.2.3 Example. (Combinatorial kinetics) For combinatorial kinetics (16.23), Stirlings formula $\log n! = n \log n - n + o(n)$ gives

$$\log \rho_\Omega = \sum_j (N_j \log \alpha_j - \alpha_j - \log N_j!) = -\sum_j N_j(\log(N_j/\alpha_j) - 1) + o(\sum N_j),$$

and by (16.26) - (16.28) we find

$$\beta\Phi(x) = \sum_j x_j(\log(x_j/a_j) - 1), \tag{16.34}$$

as the negative entropy contribution to an ideal mixture. Noting that in the multivariate Poisson distribution

$$\langle u_l^\pm(N)\rangle_{\text{Poisson}} = k_l^\pm \prod_j \langle N_j\rangle_{\text{Poisson}}^{\nu_{lj}^\pm},$$

it is more appropriate to replace expectation by Poisson expectation (= equilibrium expectation!) and get from

$$\frac{d}{dt}\langle N\rangle = \langle v(N)\rangle \underset{(16.10)}{=} \sum_l \left(\langle u_l^+(N)\rangle - \langle_l^-(N)\rangle\right)\varepsilon_l$$

the **Poisson approximation**

$$\frac{d}{dt}N(t) = \sum_l \left(k_l^+ \prod_j N_j(t)^{\nu_{lj}^+} - k_l^- \prod_j N_j(t)^{\nu_{lj}^-}\right)(\nu_l^- - \nu_l^+)$$

which is precisely the same. In the thermodynamic limit, we find

$$\dot{x} = \sum_l \left(\kappa_l^+ \prod_j \left(\frac{x_j}{a_j}\right)^{\nu_{lj}^+} - \kappa_l^- \prod_j \left(\frac{x_j}{a_j}\right)^{\nu_{lj}^-}\right)(\nu_l^- - \nu_l^+) \tag{16.35}$$

$$= \sum_l (\bar{k}_l^+ \prod x_j^{\nu_{lj}^+} - \bar{k}_l^- \prod x_j^{\nu_{lj}^-})(\nu_l^- - \nu_l^+).$$

For a macroscopic, closed system, we can again prove a dissipation theorem.

16.2.4 Theorem. *For a macroscopic colllective process* (16.29) - (16.32) *in a closed system, the potential* $\Phi(x(t))$ *decreases with time. If* A *is the composition matrix of the process with respect to a full set of invariants then* $Ax(t)$ *is time invariant.*

Moreover, if Φ *is coercive and bounded below then any limit point* x^* *of* $x(t)$ *for* $t \to \infty$ *is a stationary point of* $\Phi(x)$ *on the affine subspace* $Ax = Ax(0)$*, and the only stable equilibria are the local minimizers of* $\Phi(x)$ *on some subspace* $Ax = b$*. Moreover, at equilibrium we have detailed balance:*

$$\nu_l^+ \cdot F = \nu_l^- \cdot F \quad \text{for all } l.$$

Proof. We assume $\kappa_l^+ = \kappa_l^- =: \kappa_l$ and write $f_l^\pm := \nu_l^\pm \cdot F(x)$. Then

$$\begin{array}{rcl} \frac{d}{dt}\Phi(x(t)) & = & \nabla\Phi(x(t)) \cdot \dot{x}(t) \underset{(16.34)}{=} F(x) \cdot U(x) \\ & \underset{(16.35)}{=} & \sum_l \kappa_l (e^{\beta f_l^+} - e^{\beta f_l^-})(f_l^- - f_l^+). \end{array}$$

By the mean value theorem, there are $f_l \in \overline{f_l^+ f_l}$ such that this equals

$$\sum_l \kappa_l \beta e^{\beta f_l}(f_l^+ - f_l^-)(f_l^- - f_l^+).$$

Therefore,

$$\frac{d}{dt}\Phi(x(t)) = -\beta \sum_l \kappa_l e^{\beta f_l}(f_l^+ - f_l^-)^2 \leq 0, \tag{16.36}$$

and $\Phi(x(t)$ decreases.

Since $A\nu_l^+ = A\nu_l^+$, (16.31) implies $A\dot{x} = 0$, so that $Ax(t) = Ax(0)$ for all t. If Φ is coercive and bounded below, then $\lim_{t\to\infty} \Phi(x(t))$ exists, so $\frac{d}{dt}\Phi(x(t)) \to 0$. Therefore (16.36) gives $f_l^+ - f_l^- = 0$ at any limit point x^* of $x(t)$ for $t \to \infty$. By definition of $f_l^\pm$, this implies that $F(x^*) \cdot N$ is conserved, and hence that

$$F(x^*)^T = \lambda^T A \text{ for some } \lambda \in \mathbb{R}^p. \tag{16.37}$$

Now we note that the stationary points x^* of $\Phi(x)$ on the affine subspace $Ax = Ax(0)$ are the stationary points of the Lagrangian

$$L(x) = \Phi(x) - \lambda^T(Ax - Ax(0)),$$

and since $L'(x) = (\nabla\Phi)^T - \lambda^T A = F^T - \lambda^T A$, this is just the condition (16.37). □

16.3 Stirred chemical reactions

Here the X_i are **substances** (molecule species),

$$[X_j] := x_i = N_i/\Omega \textbf{ concentrations,}$$

$$\nu_j := F; \textbf{ chemical potentials,}$$

$$\text{transition rates } =: \textbf{ reaction rates,}$$

$$\text{rate constants } =: \textbf{ reaction constants.}$$

The constants are normalized with respect to so-called **standard states** defined by fixed reference chemical potentials μ_j^0.

The rate constants at standard state are then defined as

$$k_l^\pm := \kappa_l^\pm e^{\beta\nu_l^\pm \cdot \mu^0} \text{ (with } \kappa_l^+ = \kappa_l^- \text{ for closed systems)}, \tag{16.38}$$

and we get

$$\kappa_l^{\pm} e^{\beta\nu_l^{\pm}\cdot F(x)} = f_l^{\pm} e^{\sum_j \beta\nu_{lj}^{\pm}(F_j(x)-\mu_j^0)} = k_l^{\pm} \prod_j z_j(x)^{\nu_{lj}^{\pm}},$$

where

$$z_j(x) := e^{\beta(F_j(x)-\mu_j^0)} \tag{16.39}$$

is the **activity** of the jth species. The **macroscopic** reaction process therefore takes the form of the system of differential equations

$$\dot{x} = u(x) := \sum_{l=1}^{r} \left(k_l + \prod_{j=1}^{q} z_j(x)^{\nu_{lj}^+} - k_l^- \prod_{j=1}^{q} z_j(x)^{\nu_{lj}^-} \right) (\nu_l^- - \nu_l^+). \tag{16.40}$$

This looks like combinatorial kinetics, which is the special case $z_j(x) = x_j = [X_i]$ corresponding to an ideal mixture.

Note: For conservation of nonnegativity we need $z_j(x) = 0$ if some $x_j = 0$; thus F_j must contain a $\log x_j$ term, i.e., ρ_0 is an analytic multiple of the Poisson $-\rho_0$. Thus the $N!$ is perhaps best moved into the trace?

Chemical reactions are most commonly described at constant temperature T and constant pressure P; then the appropriate thermodynamic potential is $\Phi = G$, the **Gibbs potential**. A useful phenomenological form is the so-called **NRTL model** which describes the potential by a correction to the ideal mixture potential,

$$\beta G = \sum_j \beta G_j(x_j) + \sum x_j \log x_j - \left(\sum x_j\right) \log \left(\sum x_j\right) + \sum_j \frac{(Ax)_j x_j}{x_j + (Bx)_j}. \tag{16.41}$$

where A, B are matrices with $A_{jj} = B_{jj} = 0, B_j n \geq 0$. [the $\sum \log \sum$ term vanishes when $\sum x_j = 1$ ($\leq \Omega = \sum N_j$) but preserves the homogeneity of βG in the general case.]

This model has the advantage that the $G_j(x_j)$ can be determind form pure substances, and the coefficients A_{jk}, B_{jk} can be determined from experiments with binary mixtures.

For a closed system, the equilibium is characterized by detailed balance, which says that in (16.40) the contribution of each reaction vanishes separately. This gives the **law of mass action**,

$$k_l^+ \prod_{j=1}^{q} z_j(x)^{\nu_{lj}^+} = k_l^- \prod_{j=1}^{q} z_j(x)^{\nu_{lj}^-}, \tag{16.42}$$

which, in the case of ideal mixing, reduces to the more familiar form

$$k_l^+ \prod_{j=1}^{q} [X_j]^{\nu_{lj}^+} = k_l^- \prod_{j=1}^{q} [X_j]^{\nu_{lj}^-}.$$

In particular, for a binary reaction

$$A + B \underset{\beta}{\overset{\alpha}{\rightleftharpoons}} C + D \qquad\qquad + = \text{ input}$$

we get

$$\alpha[A][B] = \beta[C][D].$$

(Traditionally, this is derived by probabilistic hard sphere arguments.)

However, for practical calculation of nonideal cases if is preferable to solve the constrained optimization problem

$$\begin{aligned} &\min_N G(T,P,N) \\ &\text{s.t. } AN = AN^0, \quad N \geq 0, \end{aligned} \tag{16.43}$$

where N_0 is the initial composition.

If the Helmholtz potential $A(T,V,N)$ is given as the thermodynamic function, then we must also consider variation of volume by considering volume elements as separte species X_{vol}, and specifying the change of volume in each reaction.

The Gibbs potential is now

$$G = PV + A$$

(with V corresponding to N_{Vol}), and the optimization problem becomes

$$\begin{aligned} &\min_{N,V}(PV + A(T,V,N) \\ &\text{s.t. } AN = AN^0, \ N \geq 0. \end{aligned} \tag{16.44}$$

(V does not contribute to conservation laws.)

If the entropy $S(U,V,N)$ is given as thermodynamic function, we must also consider variation of internal energy by considering energy elements as separate species X_{ie} and specifying the change of energy in each reaction. (This is typically expressded in terms of change of enthalpy $H_{\text{ent}} = U + PV$.) The Gibbs potential is now

$$G = PV + U - TS$$

with $U \hat{=} N_{jl}$), and the optimization problem becomes

$$\begin{aligned} &\min_{N,U,V} PV + V - TS(U,V,N) \\ &\text{s.t. } AN = AN^0, \quad N \geq 0. \end{aligned} \tag{16.45}$$

16.4 Linear response theory

We assume a macroscopic situtation (Ω large but not infinite) so that the concept of a time-dependent **external** thermodynamic force $F_{ext}(t)$ makes sense. As can be seen from the thermodynamic limit

$$\dot{x} = \sum_l \left(\kappa_l^+ e^{\beta\nu_i^+ \cdot F(x)} - \kappa_l^- e^{\beta\nu_l^- F(x)}\right)(\nu_l^- - \nu_l^+),$$

changing $F(x)$ to $F(x) - F_{ext}(t)$ amounts the replacement of $\kappa_l^{\pm} = \kappa_l$ for a closed system by time dependent rate constants

$$\kappa_l^{\pm} = \kappa_l e^{-\beta \nu_{\pm l} \cdot F_{ext}(t)} \tag{16.46}$$

for an open system. (16.46) is valid for arbitrary systems.

For small forces $F, F_{ext} = O(\Omega^{-1/2})$ we can use $\omega_l^{\pm} = \Omega \kappa e^{\pm}$ to express drift and diffusion in terms of

$$L := \beta \sum \omega_l \varepsilon_l \varepsilon_l^* \tag{16.47}$$

(of order $O(\Omega)$, symmetric) as

$$v = -L(F(N) - F_{ext}(t)) + O(1),$$

$$G = 2\hbar T L + 0(\Omega^{-1/2}).$$

An analysis similar to that for the thermodynamic limit reveals that higher than second derivatives in Df can be neglected, so that we can approximate the process by a diffusion process. Ignoring also the error terms in drift and diffusion we find the following **canonical form of linear response theory**,

$$\frac{d}{dt}\langle f \rangle = \langle v \cdot \nabla f + \frac{1}{2} G : \nabla^2 f \rangle, \tag{16.48}$$

valid for open macroscopic systems with **small thermodynamic forces**, where

$$v = -L(\nabla \Phi(N) - F_{ext}(t)) \tag{16.49}$$

$$G = 2\hbar T L \tag{16.50}$$

since, by (16.47), the **transport matrix** L is constant and symmetric positive semidefinite.

16.4.1 Remarks. 1. In the absense of external forces, (16.48 - 16.50) describes a diffusion process in canonical form; since L is constant, the covariant drift u agrees with v.

2. The entries of L are called the **transport coefficients**; the symmetry relations $L_{ik} = L_{ki}$ are called the **Onsager relations**.

3. The rate constants ω_l often grow nearly linear with T so that $\beta\omega_l$ and hence L only depends weakly on temperature.

4. Written as stochastic differential equation we have

$$dN = L(-\nabla \Phi(N) + F_{ext}(t))dt + d\varepsilon, \quad d\varepsilon \sim N(0, 2\hbar T L dt). \tag{16.51}$$

5. In the space-dependent case, the Onsager relations must be modified for variables like velocities which are not time-reversal invariant; then L is no longer symmetric (i.e., self-adjoint) and (16.50) reads

$$G = \hbar T(L + L^T). \tag{16.52}$$

Linear response theory is used for an impressively large collection of applications.

A particular case where thermodynamical forces are small is when a system operates **close to equilibrium**. In this case the potential can be expanded in powers of deviations $x := N - N^*$ from a minimizer N^* of $\Phi(N)$, and sufficiently close to equilibrium, a quadratic expansion is sufficient. The Hessian $\Sigma := \Phi''(N^*)$ at the minimizer is symmetric and positive semidefinite, and we get

$$\Phi(N) = \Phi(N^*) + \frac{1}{2}x^T \Sigma x + O(\|x\|^3).$$

Ignoring the error term, the substitution into linear response theory yields the driven Ornstein-Uhlenbeck process discussed in Section 15.3.

16.5 Open system

All interesting phenomena in our world are **alive** in a more or less complex way, and this is due to the fact that the systems involved are not closed but **open**, interacting with the **environment**. **Life is dependent on communication; a closed system is doomed to death**, by the second law of thermodynamics which moves the system to equilibrium where nothing happens anymore. Such a system can be brought back to life only by exerting external influence.

Now it is a very remarkable fact that the same thermodynamic laws which force closed systems towards death operate on open systems in such a way that an enormously rich variety of living structures appear, evolve and change. Indeed, we shall see that the universe is teleological and comprehensible precisely because of dissipation: **Life forces and death forces are identical**.

Modern science has just started to understand some details of this fascinating vision of the world, and like concepts **self-organization, evolution, synergetics, chaos** created new **paradigms** whose further unfolding will enrich and change our scientific understanding of the world.

Mathematically, open systems are characterized by the occurence of (in general time dependent) **external flows or forces** $\lambda = \lambda(t)$. Corresponding to each value λ there is a forward derivation D_λ which specifies the dynamics at constant external conditions. $\lambda = 0$ describes a closed system with detailed balance, but for $\lambda \neq 0$, detailed balance is usually violated. A general open system is described by the forward derivation D defined by

$$Df(\lambda, x) := \frac{\partial f}{\partial \lambda}(\lambda, x)\dot{\lambda} + D_\lambda f(\lambda, x) \tag{16.53}$$

or a time-dependent version of it. When decay to equilibrium is **extremely slow**, on time scales accessible to experiment, the behavior of a system may, for practical purposes, remain different from the steady state; this situation is usually approximated by setting tiny reaction rates κ_l^- to zero and huge concentrations to infinity. The resulting reduced system then accounts for the behavior on **shorter time scales** which are hardly affected by these approximations, but detailed balance is now already lost for $\lambda = 0$.

If λ **is fixed** in (16.53), the corresponding Markov process is **autonomous** (i.e., has a time-independent dynamics) and we expect a unique limit behavior as $t \to \infty$. If λ is small, the system is nearly closed and we expect decay to a steady state near equilibrium. When λ becomes larger one expects a repetitive "mechanical" behavior restricted to a low-dimensional **attractor** parametrized by a few microscopically conserved quantities; depending on the details, the system may be periodic or chaotic. (This is impossible for dissipative systems with detailed balance.)

The fact that attractors are usually of much lower finite-dimensional dimension than the system itself accounts to a large extend for the **comprehensibility of our world**, since our awareness can only process a limited amount of information.

In reality, the external conditions are usually **not constant**. As λ changes slightly the attractor changes its position but "generically" preserves its qualitative (topological) features. However, typically, when λ crosses certain surfaces (points if $\lambda \in \mathbb{R}$, curves if $\lambda \in \mathbb{R}^2$), the topology of the attractor (fixed point, number of independent periods, chaos) changes. This situation is described mathematically as **bifurcation**, physically as **(nonequilibrium) phase transition**, and in general language as **structural change**, **catastrophe**, **self-organization**, or **miracle**, depending on the context of observer and observation (see books on dynamical systems or synergetics).

The term **self-organization is somewhat misleading**, since "self" only refers to the collective response of the system to the **external** stimulus $\lambda(t)$; any life pattern depends in its existence on the presence of the appropriate environment. The external stimulus may be viewed as a **constraint** (canceling internal forces) or as **enticement** (reinforcing internal forces).

The individuals try to **optimize their owns interest** , and this collectively leads — because of dissipation — to a decrease of the free energy of the system. Thus the system remains in a state of **nearly minimal free energy** (subject to the external contraints) and hence preserves ("self-organizes") its structure. At certain thresholds for λ, the system's free energy surface changes its global minimum, and in a **crisis**, a new structure (more alive or more dead) forms. It is clear that both the external stimulus and the physical law (defined by potential and rate constants) are needed to "self-organize" something **new**.

Figure: A crisis of a collection of noninteracting individuals. When (second diagram) the global minimum is not unique, two equilibrium states coexist.

16.6 Some philosophical afterthoughts

Related to the dynamics of open systems is the **teleological** (i.e., goal-directed) nature of our world. In contrast to a widely held view, physical laws have a natural teleological interpretation as **democracy of forces** in collaboration and conflict:

Forces are teleological, their goal is trying to move particles along the field lines, in a way similar to the way we try to earn our livings, make a career, win a game, etc.. The **laws of physics are constraints** which resolve conflicts between competing forces in a democratic way (forces are additive). As in society, if many individual forces are present the **collective behavior is often different from what the individuals hope for**. The analogy to human affairs is close, and indeed one can model sociological systems by the same mathematics as chemical systems, say, though much less accurately.

The **mind-matter problem** is located on this level, and perhaps one is not too far away from modeling mind-matter interaction by open collective processes involving **mind fields** expressing feeling, awareness and will – and on the society level, mass media).

In a **local** perspective, our mind is able to set some external stimuli to the working of our physical body; further external stimuli come through our senses (and perhaps further through inspiration, telepathy, etc.). We all know the lack of self-organization in learning due to wrong circumstances — distracting thoughts (mind stimuli), talking neighbours (physical stimuli), missing information (lack of stimuli), and the phase transitions induced by the presentation of strange new information — after a period of intermittend chaos the formation of understanding: "it dawned upon him, she catched on". Reaching a stable equilibrium corresponds to the death of doubts and questions.

In a **global** perspective, **God's mind** sets the conditions for a world created by Him to serve this purpose. Some people think of God as the mind of the universe, and in this view one might consider the universe as the body of God; but, like with all images of God, this view is only partially appropriate.

Part V

Mechanics and differential geometry

Chapter 17

Fields, forms, and derivatives

Part V introduces the relevant background from differential geometry and applies it to classical Hamiltonian and Lagrangian mechanics, to a symplectic formulation of quantum mechanics, and to Lie groups.

In this chapter we introduce basic material on manifolds, the associated commutative algebra of scalar fields, and the Lie algebra of vector fields. All manifolds used in this book are arbitrarily often differentiable, real manifolds whose dimension need not be finite. However, we are very brief and sometimes incomplete in the technical details that need attention in the infinite-dimensional case; on first reading, the reader may restrict everything to the finite-dimensional case, where these details are not required.

We first recall some basics from differential geometry. Our approach differs from standard introductions to differential geometry since, consistent with the theme of the book, all definitions are given in an algebraic way. As a side benefit, this prepares the reader to noncommutative geometry, only briefly touched in this book, where a manifold structure is no longer available and all geometry enters in an algebraic way. Among other applications, noncommutative geometry gives an interesting geometric perspective to the quantum field theory of the standard model.

Vector fields on a manifold $\mathbb{M}$ are essentially equivalent to derivations on the commutative algebra $C^\infty(\mathbb{M})$ of scalar fields. However, to be able to use the traditional terminology, where vector fields and the corresponding derivations (Lie derivatives) are distinguished, we introduce an abstract set $\mathbb{W} = \operatorname{vect}\mathbb{M}$ of vector fields, whose elements are put into correspondence with derivations by means of a mapping $d : \operatorname{vect}\mathbb{M} \to \operatorname{Der}\mathbb{M}$ which is applied at the right. In this way, the calculus on manifolds can be formulated in a purely algebraic way, without any reference to the manifold.

We therefore formulate everything in terms of an arbitrary topological commutative algebra $\mathbb{E}$ in place of $C^\infty(\mathbb{M})$, and an arbitrary set $\mathbb{W}$ in place of $\operatorname{vect}\mathbb{M}$. However, the main situation that the reader should have in mind is where $\mathbb{E}$ is an algebra of complex-valued, arbitrarily often differentiable functions on a finite-dimensional manifold, for example $C^\infty(\mathbb{R}^n)$. But $\mathbb{E}$ could also be the Schwartz space of arbitrarily often differentiable functions all of whose derivatives decay faster than polynomially at infinity.

As a result, our presentation is completely coordinate-free, except in some examples. For readers accustomed to differential geometry in index notation but not to the coordinate-free Cartan notation, we suggest that they translate the definitions and main results into coordinates to understand their meaning, but to treat proofs as if the concepts introduce new abstract algebraic notions.

17.1 Scalar fields and vector fields

We introduce the objects, operators, and operations needed for presenting the traditional differential calculus in a purely algebraic framework: Lie derivatives applied to multilinear forms, and exterior products and the exterior derivative of alternating forms. As the most important special case, we consider manifolds and associated geometric notions, in particular diffeomorphisms.

Before giving the definitions, we discuss the letter conventions and priority rules used in the formulas.

We typically (i.e., when not forced by conflicts or tradition to do otherwise) use lower case letters from the middle of the alphabet, such as f, g, h, to denote scalar fields, capital letters from the end of the alphabet, such as X, Y, Z to denote vector fields, capital letters from the beginning of the alphabet, such as A, for general multilinear forms, but z, for linear forms, ω for alternating bilinear forms, and η for symmetric bilinear forms.

We use the convention that a Lie derivative acts on the shortest following expression which is syntactically a vector field or a multilinear form. Similarly, the exterior derivative operator d acts from the right on a vector field X, giving Xd, or from the left on the shortest following expression that is syntactically an alternating form ω, giving $d\omega$.

The wedge product $\wedge$ has lower priority than the operations written as juxtaposition, but higher priority than $+$ and $-$.

17.1.1 Definition.
(i) A **differential geometry** consists of a commutative algebra $\mathbb{E}$ containing $\mathbb{C}$, a left $\mathbb{E}$-module $\mathbb{W}$ with an additional Lie product $\angle$, both equipped with a topology such that all operations are continuous, and a continuous mapping d (written on the right), which maps $X \in \mathbb{W}$ to $Xd \in \operatorname{Der} \mathbb{E}$, such that

$$(X+Y)d = Xd + Yd, \quad (fX)d = f(Xd), \quad (X \angle Y)d = [Xd, Yd], \tag{17.1}$$

for all $X, Y \in \mathbb{W}, f \in \mathbb{E}$. The differential geometry is called **(non-)commutative** if the multiplication in $\mathbb{E}$ is (non-)commutative.

(ii) We refer to the elements of $\mathbb{E}$ as **scalar fields**, and to the elements of $\mathbb{W}$ as **vector fields**. The **Lie derivative** of a vector field X is the linear mapping L_X which maps a scalar field f to[1]

$$L_X f := Xd\, f, \tag{17.2}$$

[1]As will become apparent in Section 17.3 (cf. Theorem 17.3.2), we may read the term $Xd\, f$ also as

and a vector field Y to

$$L_X Y \;:=\; X\angle Y \;=\; -\,L_Y X\;. \tag{17.3}$$

The scalar field $L_X f$ (resp. the vector field $L_X Y$) is called the **directional derivative** of the scalar field f (resp. the vector field Y) in the direction of the vector field X.

The following example is responsible for the naming. Interpreting the set $\mathbb{M}$ in the example as the domain of a chart of a finite-dimensional manifold, one can translate everything said here to general finite-dimensional manifolds by a process described in all books on differential geometry. Thus the example gives essentially the full intuition for our constructions, except for the complications that may arise in infinite dimensions.

17.1.2 Example. (Differential geometry of open subsets in $\mathbb{R}^{\times n}$)
Let $\mathbb{R}^{\times n}$ denote the vector space of row vectors[2] $x = (x^1, \ldots, x^n)$ with n real components x^j, let $\mathbb{M}$ be a nonempty, open subset of $\mathbb{R}^{\times n}$, and let $\mathbb{E} = C^\infty(\mathbb{M})$ and $\mathbb{W} = C^\infty(\mathbb{M}, \mathbb{C}^{\times n})$, equipped with the weak topology. Thus scalar fields are real-valued functions, while vector fields are row vector valued functions. In terms of the partial differential operators ∂_j defined by

$$\partial_j f(x) := \partial f(x)/\partial x^j,$$

we define the **gradient** ∂f of a scalar field as the column vector with n entries

$$(\partial f)_j = \partial_j f.$$

It is not difficult to show that an arbitrary derivation δ on t he algebra of scalar fields can be uniquely expressed as a linear partial differential operator of the form

$$\delta = X\partial = \sum_{j=1}^{n} X^j \partial_j,$$

with a vector field X. This derivation then acts on scalar fields f as

$$\delta f = X\partial f = \sum_{j=1}^{n} X^j \partial_j f.$$

Thus the mapping d which maps the vector field X to the differential operator $X\partial$ is a bijection of the type required in the previous example. Thus we have a canonical differential geometry; it is clearly commutative. The reader is invited to check that the Lie derivative takes the form

$$L_X f = X\partial f, \quad L_X Y = X\partial Y - Y\partial X. \tag{17.4}$$

A second, noncanonical differential geometry results by using in the above construction in place of $C^\infty(\mathbb{M})$ the subalgebra $C_0^\infty(\mathbb{M})$ of scalar fields with compact support, and in place of $C^\infty(\mathbb{M}, \mathbb{C}^{\times n})$ the subspace $C_0^\infty(\mathbb{M}, \mathbb{C}^{\times n})$ of vector fields with compact support.

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product of the vector field X with the exact linear form df. Until then, we shall write an explicit space after d to remind the reader of the correct way to group the letters.

[2]The index notation corresponds to standard differential geometric practice when working in a chart of a manifold (which is essentially the situation we are discussing here). The interpretation in terms of rows (row vectors = **rovectors**, indexed by upper indices = **roindices**) and columns (column vectors = **covectors**, indexed by lower indices = **coindices**) makes the transition to standard linear algebra transparent.

17.1.3 Example. (Canonical differential geometries)
Let $\mathbb{E}$ be an arbitrary topological algebra containing $\mathbb{C}$. We may give $\mathbb{E}$ the structure of a differential geometry by picking an arbitrary set $\mathbb{W}$ with the same cardinality as Der $\mathbb{E}$, and choosing an arbitrary bijection d from $\mathbb{W}$ to Der $\mathbb{E}$. $\mathbb{W}$ inherits all properties of Der $\mathbb{E}$ by means of the bijection d: We turn $\mathbb{W}$ into a Lie algebra and a topological $\mathbb{E}$-module by defining

$$X + Y := (Xd + Yd)d^{-1}, \quad fX := (f(Xd))d^{-1},$$

$$X\angle Y := [Xd, Yd]d^{-1}.$$

for $X, Y \in \mathbb{W}$ and $f \in \mathbb{E}$, and by calling a set $S \in \mathbb{W}$ closed if its image under d is closed in the topology of Der $\mathbb{E}$ induced by that of $\mathbb{E}$. The result is a differential geometry. We call differential geometries constructed in this way **canonical**.

17.1.4 Proposition. *The* ***product rule***

$$L_X(fg) = (L_X f)g + f(L_X g), \quad L_X(fY) = (L_X f)Y + f(L_X Y), \tag{17.5}$$

the ***commutation rule***

$$[L_X\,, L_Y] = L_{X\angle Y}, \tag{17.6}$$

and the equations

$$L_{fX}\, g = f L_X\, g, \tag{17.7}$$

$$L_{fX} Y = f L_X Y - XYd\ f \tag{17.8}$$

hold for $f, g \in \mathbb{E}$ and $X, Y \in \mathbb{W}$,

Proof. The first part of (17.5) is trivial since in this case $L_X = Xd$ is a derivation on $\mathbb{E}$. For the second part of (17.5), we note that

$$\begin{aligned}\Big(L_X(fY)\Big)d\ g &= (X\angle fY)d\ g = [Xd\,, fYd\,]g = Xd\Big(f(Yd\ g)\Big) - fYd\,(Xd\ g)\\ &= (Xd\ f)(Yd\ g) + fXd\,(Yd\ g) - fYd\,(Xd\ g)\ .\end{aligned}$$

Also,

$$((L_X f)Y)d\ g = ((Xd\ f)Y)d\ g = (Xd\ f)(Yd\ g)$$

and

$$\begin{aligned}\Big(f(L_X Y)\Big)d\ g &= \Big(f(X\angle Y)\Big)d\ g = f[Xd\,, Yd]g\\ &= f\Big(Xd\,(Yd\ g) - Yd\,(Xd\ g)\Big) = fXd\,(Yd\ g) - fYd\,(Xd\ g)\end{aligned}$$

Putting these three pieces together proves the second part of (17.5).

To prove (17.6), note that $L_Y f = Yd\ f$ is in $\mathbb{E}$, so $L_X L_Y f = L_X(Yd\ f) = Xd\ (Yd\ f)$. Interchanging X, Y we find for the commutator:

$$[L_X, L_Y]f = Xd\,(Yd\ f) - Yd\,(Xd\ f) = [Xd, Yd]f = (X\angle Y)d\ f = L_{X\angle Y}\, f\ .$$

Formula (17.7) is immediate from the definition, and (17.8) follows from the product rule $X\angle fY = (Xd\ f)Y + f(X\angle Y)$ by swapping X and Y, using the anticommutativity of $\angle$. $\square$

In the following, we develop the differential calculus for commutative differential geometries only; thus, with exception of the remarks on noncommutative geometry in Section 17.5, **the algebra $\mathbb{E}$ of scalar fields is always assumed to be commutative.** In this case, we extend the left module structure on vector fields to a bimodule structure by putting

$$Xf := fX$$

for $f \in \mathbb{E}$ and $X \in \mathbb{W}$. Note that some authors treat vector fields as synonymous with derivations and therefore write $X(f)$ for $Xd\ f$. This should not be confused with the present notation Xf for multiplying the vector field X with the scalar field f.

17.2 Multilinear forms

Apart from scalar and vector fields, differential geometry makes heavy use of multilinear forms and tensors, which we define next.

17.2.1 Definitions.
(i) A **linear form** ζ is a continuous, $\mathbb{E}$-linear mapping $\zeta : \mathbb{W} \to \mathbb{E}$ (written on the right[3]) which maps the vector field X to the scalar field $X\zeta$. We write $\mathbb{W}^*$ for the $\mathbb{E}$-module consisting of all linear forms, (sometimes called the "$\mathbb{E}$-dual" of $\mathbb{W}$), with scalar multiplication of $\zeta \in \mathbb{W}$ by $f \in \mathbb{E}$ defined via

$$X(f\zeta) := f(X\zeta).$$

(ii) A **c-linear** form ϕ is a mapping $\phi : \mathbb{W} \times \ldots \times \mathbb{W} \to \mathbb{E}$ (with c factors of $\mathbb{W}$ in the Cartesian product) such that the image[4] $X_1 \ldots X_c\phi$ of $(X_c, \ldots, X_1) \in \mathbb{W} \times \ldots \times \mathbb{W}$ depends $\mathbb{E}$-linearly on each argument X_k, i.e., if, for all $X_j, Y, Z \in \mathbb{W}$ and $f, g \in \mathbb{E}$,

$$X_1 \ldots (fY + gZ) \ldots X_c\phi \ = \ fX_1 \ldots Y \ldots X_c\phi \ + \ gX_1 \ldots Z \ldots X_c\phi \ .$$

[3]Strictly speaking, they should be called $\mathbb{E}$-linear forms, and a similar remark applies later to multilinear forms. Talking about a *form* rather than a mapping implies the assumption of continuity.
The standard notation for $X\zeta$ is $i_X\zeta = \zeta(X)$; the present notation simply replaces i_X by X. This way of writing the mapping generalizes standard matrix calculus if we use the intuition gained from Example 17.1.2 and think of vector fields as row vectors and of linear forms as column vectors, an intuition that extends to matrix fields. Since in the general situation, linear forms are often called **covectors**, we shall occasionally use the analogous word **rovector** to denote a vector field, although, strictly speaking, one should talk about covector fields and rovector fields. The same ambiguity is traditionally maintained for multilinear forms on manifolds, which refer both to the corresponding fields and to their values at a particular point.

[4]The traditional notation for $X_1 \ldots X_c\phi$ is $i_{X_1} \ldots i_{X_c}\phi = \phi(X_c, \ldots, X_1)$; as for linear forms, the present notation simply replaces the i_X by X. Note the reverse order resulting in the arguments written in the traditional way, needed in order that (17.9) together with our definition (17.10) of insertion is consistent with the traditional definition $(i_X\phi)(X_1, \ldots, X_{c-1}) = \phi(X, X_1, \ldots, X_{c-1})$. In our notation this translates into $X_{c-1} \ldots X_1(i_X\phi) = X_{c-1} \ldots X_1 X\phi$.

Here the unindexed argument between the dots replaces the kth argument X_k, for some k in $1, \ldots, c$. In the degenerate case $c = 0$, we consider the 0-linear mappings to be the scalar fields.

(iii) We write[5] $\mathbb{W}_c$ for the $\mathbb{E}$-module of continuous c-linear mappings on $\mathbb{W}$. Scalar multiplication of $\phi \in \mathbb{W}_c$ by $f \in \mathbb{E}$ is defined via

$$X_1 \ldots X_c(f\phi) \;:=\; f(X_1 \ldots X_c\phi) \;.$$

The elements of $\mathbb{W}_c$ are called **multilinear forms** or **c-linear forms**; for $c = 2$ also **bilinear forms**. Note that $\mathbb{W}_0 = \mathbb{E}$ consists of scalar fields (or 0-forms), and $\mathbb{W}_1 = \mathbb{W}^*$ consists of linear forms (or 1-forms).

(iv) The **product** of a vector field $X \in \mathbb{W}$ and a c-linear form $\phi \in \mathbb{W}_c$ is for $c = 0$ the vector field $X\phi$ defined by scalar multiplication with the scalar ϕ, and for $c > 0$ the $(c-1)$-linear form $X\phi$ defined by

$$X_1 \ldots X_{c-1}(X\phi) \;:=\; X_1 \ldots X_{c-1}X\phi \;, \qquad \text{for all } X_1, \ldots, X_{c-1} \in \mathbb{W}. \tag{17.9}$$

The operator i_X defined on multilinear forms ϕ by

$$i_X\phi \;:=\; X\phi \tag{17.10}$$

is traditionally called the **insertion** of $X \in \mathbb{W}$; cf. footnote 17.2.1.

(v) A c-linear form ϕ is called **alternating** (or a **c-form**) if either $c \leq 1$ or $X\phi$ is alternating and $XX\phi = 0$ for all vector fields X. ϕ is called **symmetric** if either $c \leq 1$ or $X\phi$ is symmetric and $XY\phi = YX\phi$ for all vector fields X, Y. We write $\mathbb{A}_c$ and $\mathbb{S}_c$ for the space of alternating and symmetric c-linear forms, respectively. In particular,

$$\mathbb{E}_0 = \mathbb{W}_0 = \mathbb{E}, \quad \mathbb{E}_1 = \mathbb{W}_1, \quad \mathbb{E}_2 \oplus \mathbb{S}_2 = \mathbb{W}_2 \;.$$

(vi) The **transpose** of a bilinear form ϕ is the bilinear form ϕ^T defined by

$$XY\phi^T := YX\phi \tag{17.11}$$

for all vector fields X, Y. In particular, a bilinear form ϕ is symmetric iff $\phi^T = \phi$ and alternating iff $\phi^T = -\phi$. A bilinear form ϕ is called **nondegenerate** if every linear form $\zeta \in \mathbb{W}^*$ can be written as $\zeta = X\phi$ for a unique vector field X; otherwise **degenerate**. A bilinear form ϕ may be considered as a linear mapping from $\mathbb{W}$ to $\mathbb{W}^*$ that maps the vector field X to the linear form $X\phi$. If ϕ is nondegenerate, this mapping is invertible, and the inverse ϕ^{-1} is a linear mapping from $\mathbb{W}^*$ to $\mathbb{W}$, which maps a linear form ζ to the vector field $\zeta\phi^{-1}$ in such a way that

$$\zeta\phi^{-1}\phi = \zeta. \tag{17.12}$$

A nondegenerate bilinear form is called a **symplectic form** if it is alternating, and a **metric** if it is symmetric.

[5]Writing the "c" in $\mathbb{W}_c$ as a subscript serves as a reminder that when an element ϕ of $\mathbb{W}_3$ (say) is written in index notation, it has 3 *lower* indices: "ϕ_{ijk}". Indeed the "c" is intended to be suggestive of "covector". Note that in terms of the direct products of c factors $\mathbb{W}$ or $\mathbb{W}^*$, there is a canonical isomorphism $\mathbb{W}^* \times \ldots \times \mathbb{W}^* \cong (\mathbb{W} \times \ldots \times \mathbb{W})^* = \mathbb{W}_c^*$.

(vii) A $[c,r]$**-tensor field**[6] T is a continuous $\mathbb{E}$-linear mapping $T : \mathbb{W}_r \to \mathbb{W}_c$. The space of $[c,r]$-tensor fields is denoted by[7] $\mathbb{W}[c,r] = \mathbb{W}_c^r = \mathrm{Lin}(\mathbb{W}_r, \mathbb{W}_c)$. A $[1,1]$-tensor field is called a **matrix field**.

17.2.2 Remarks.
(i) Multilinearity implies

$$XY\omega = -YX\omega \quad \text{for alternating } c\text{-forms } \omega \text{ with } c > 1.$$

Thus, for $c \geq 2$,

$$i_X^2 = 0, \quad i_X i_Y = -i_Y i_X \quad \text{on alternating } c\text{-linear forms,} \tag{17.13}$$

whereas

$$i_X i_Y = i_Y i_X \quad \text{on symmetric } c\text{-linear forms.} \tag{17.14}$$

(ii) Note that there is a canonical identification of $\mathbb{W}[c,0]$ with $\mathbb{W}_c$, and a canonical embedding of $\mathbb{W}$ into $\mathbb{W}[0,1]$. In the case of finite-dimensional manifolds, we may also identify $\mathbb{W}[0,1]$ with $\mathbb{W}$.

(iii) The ordinary operator product of a $[c',c]$-tensor and an $[c,r]$-tensor is well-defined, and is a $[c',r]$-tensor: $\mathbb{W}[c',c]\mathbb{W}[c,s] \subseteq \mathbb{W}[c',s]$. In particular, $\mathbb{W}[1,1] = \mathrm{Lin}\,\mathbb{W}_1$ is an algebra of matrix fields.

17.2.3 Theorem. *For every vector field X, the Lie derivative can be extended uniquely to a linear operator L_X mapping*[8] *vector fields to vector fields and c-linear forms to c-linear forms, and satisfying the* ***product rule***

$$L_X(f\phi) = (L_X f)\phi + f(L_X\phi), \quad L_X(Y\phi) = (L_X Y)\phi + Y(L_X\phi). \tag{17.15}$$

for $f \in \mathbb{E}$, $Y \in \mathbb{W}$, and $\phi \in \mathbb{W}$ or $\phi \in \mathbb{W}_c$. The extended Lie derivative satisfies the commutation rules

$$[L_X, L_Y] = L_{X\angle Y}, \tag{17.16}$$

$$[L_X, i_Y] = i_{X\angle Y} \tag{17.17}$$

for $X, Y \in \mathbb{W}$.

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[6]An $[c,r]$-tensor is also called a tensor of $[{}^r_c]$-valence (Penrose & Rindler [215]). With traditional index notation, a c-linear form is written with c lower (co)indices, and a $[c,r]$-tensor is written with r upper (ro)indices and c lower (co)indices. E.g., a $[3,2]$-tensor T is written $T_{ijk}{}^{mn}$, and the image $T\phi$ of a bilinear form is written $(T\phi)_{ijk} = T_{ijk}{}^{mn}\phi_{mn}$, using the traditional **Einstein summation convention** (which deletes the explicit indication of the sum over m and n so as not to unnecessarily inflate the formulas without conveying any more information). In the more modern **abstract index notation** of Penrose & Rindler [215], such repeated indices denote instead an insertion (dual-pairing) *without* any implied connotation of summation over basis-dependent components, and such indices may be used to keep explicit track of the types of complicated objects.

[7]For the differential geometry of open subsets $\mathbb{M}$ of $\mathbb{R}^n$ (Example 17.1.2), $\mathbb{W}[c,r] = \mathbb{W}_c^r$ is, in the traditional terminology, the space of sections of the tensor bundle $T_c^r\mathbb{M}$.

[8]The Lie derivative can also be extended to tensors $T \in \mathbb{W}[c,r]$ by defining

$$(L_X T)B := L_X(TB) - TL_X B \quad \text{for } B \in \mathbb{W}_r.$$

We do not need such an extension for our limited applications; it would be needed, however, in a treatment of general relativity. The reader is invited to verify that $L_X T \in \mathbb{W}[c,r]$ and to formulate and prove the analogues to (17.15) and (17.16).

Proof. We first assume that the product rule holds, and show that this fixes the operation of L_X on all multinear forms. By the product rule (17.15),

$$YL_X\phi = L_X(Y\phi) - (L_XY)\phi, \tag{17.18}$$

This formula shows that L_X is determined on c-linear forms by its action on $(c-1)$-linear forms, and since it is given on scalar fields, it is unique if it exists at all.

Conversely, to show existence of the extension, we define L_X recursively by (17.18), starting with the known action of L_X on scalar fields.

Since $(fY)L_X\phi = L_X(fY\phi) - L_X(fY)\phi = (L_Xf)Y\phi + fL_X(Y\phi) - (L_Xf)Y\phi - f(L_XY)\phi = f(L_X(Y\phi) - f(L_XY)\phi = f(YL_X\phi)$, we see inductively that $YL_X\phi$ is $\mathbb{E}$-linear in Y, so that $L_X\phi$ is indeed a tensor.

The first part of the product rule holds since, by (17.18), the equation $YL_X(f\phi) = L_X(Yf\phi) - (L_XY)(f\phi) = L_X(fY\phi) - (L_XY)(f\phi) = (L_Xf)Y\phi + fL_X(Y\phi) - (L_XY)f)\phi - f(L_XY)\phi = Y(L_Xf)\phi + Yf(L_X\phi)$ holds for all vector fields Y. The second part of the product rule follows directly from (17.18).

To prove (17.16), we first note that by (17.18), we have $ZL_XL_Y\phi = L_X(ZL_Y\phi) - (L_XZ)L_Y\phi = L_X(L_Y(Z\phi) - (L_YZ)\phi) - (L_XZ)L_Y\phi = L_XL_Y(Z\phi) - (L_XL_YZ)\phi - (L_YZ)L_X\phi - (L_XZ)L_Y\phi$. The last two terms are symmetric in X, Y, hence cancel when taking the difference with $ZL_YL_X\phi$ in $Z[L_X, L_Y]\phi = ZL_XL_Y\phi - ZL_YL_X\phi = (L_XL_Y - L_YL_X)(Z\phi) - (L_XL_YZ - L_YL_XZ)\phi = [L_X, L_Y](Z\phi) - ([L_X, L_Y]Z)\phi$. Since (17.16) is already known by (17.6) to hold on vector fields and on scalar fields (0-linear forms), we assume that we know its validity for the action on c-linear forms. Taking for ϕ a $(c+1)$-linear form, we may conclude that $Z[L_X, L_Y]\phi = L_{X\angle Y}(Z\phi) - (L_{X\angle Y}Z)\phi = ZL_{X\angle Y}\phi$ by (17.18). Since Z was arbitrary, we conclude that $[L_X, L_Y]\phi = L_{X\angle Y}\phi$ for $(c+1)$-linear forms ϕ. By induction, (17.16) holds in general.

(17.17) follows from the product rule (17.15) since

$$[L_X, i_Y]\phi = L_X(Y\phi) - Y(L_X\phi) = (L_XY)\phi = (X\angle Y)\phi = i_{X\angle Y}\phi.$$

□

The reader may wish to prove inductively that, for c'-linear forms ϕ with $c' \geq c$,

$$X_1 \dots X_c L_X\phi = L_X(X_1 \dots X_c\phi) - \sum_{k=1}^{c} X_1 \dots X\angle X_k \dots X_c\phi.$$

17.2.4 Proposition. *The Lie derivative of an alternating c-form is again an alternating c-form.*

Proof. Indeed, for any alternating form ω,

$$\begin{aligned} YYL_X\omega &= Y(L_X(Y\omega) - (L_XY)\omega) = YL_X(Y\omega) - Y(L_XY)\omega \\ &= YL_X(Y\omega) + (L_XY)Y\omega = L_X(YY\omega) = 0\ . \end{aligned}$$

□

17.3 Exterior calculus

In the case of differential geometry in $\mathbb{R}^{\times n}$ (Example 17.1.2), the gradient operator $d = \partial$ behaves symbolically similarly to a covector, except for the nontrivial behavior implied by the Leibniz product rule. However, the gradient operator d, defined there on scalar fields only, cannot be extended to a gradient operator that associates with a general c-linear form ϕ a $(c+1)$-linear form $d\phi$ such that $L_X\phi = Xd\phi$ for all vector fields X. The existence of such an extension would imply that $L_{fX}\phi = fL_X\phi$. While this holds by (17.7) when ϕ is a scalar field, it fails already when ϕ is a linear form. For a linear form ζ, we have instead

$$L_{fX}\zeta = fL_X\zeta + df X\zeta,$$

which follows as a special case of (17.21) below, or from

$$L_X\zeta = X(\partial\zeta)^T + \partial X\zeta$$

by substituting fX for X. However, the gradient can be generalized in a different way to alternating forms, leading to the exterior derivative.

The generalization is valid not only for Example 17.1.2, but in full generality. To define the exterior derivative we need some preparations.

17.3.1 Theorem. *For every linear form ζ, there is a unique $\mathbb{E}$-linear mapping $\zeta\wedge$ mapping alternating c-forms to alternating $(c+1)$-forms for $c = 0, 1, 2, \ldots$, and vector fields to zero, such that*

$$(X\zeta)\omega = X(\zeta \wedge \omega) + \zeta \wedge X\omega \tag{17.19}$$

for all vector fields X and all alternating c-forms ω. $\zeta \wedge \omega$ is called the ***exterior product*** *or* ***wedge product***[9] *of ζ and ω. The exterior product satisfies the rules*

$$\zeta \wedge \zeta' = -\zeta' \wedge \zeta, \tag{17.20}$$

$$L_X(\zeta \wedge \omega) = L_X\zeta \wedge \omega + \zeta \wedge L_X\omega \tag{17.21}$$

for alternating c-forms ω, linear forms ζ, ζ', and vector fields X.

Proof. A necessary and sufficient condition for (17.19) to hold is that

$$X(\zeta \wedge \omega) = (X\zeta)\omega - \zeta \wedge X\omega; \tag{17.22}$$

in particular,

$$\zeta \wedge \omega = \zeta\omega \quad \text{for a 0-form } \omega, \tag{17.23}$$

This completely specifies the exterior product of a linear form ζ and an alternating $(c+1)$-form ω, given the exterior product with an alternating c-form. Therefore, if the exterior product exists, it is unique.

To prove the existence of the exterior product, we have to define the exterior product of a linear form ζ and an alternating c-form ω to be the expression $\zeta \wedge \omega$ defined for $c = 0$

[9] One can define an exterior product $\omega' \wedge \omega$ for arbitrary alternating forms ω, ω', but we do not need it.

by (17.23) and for $c > 0$ recursively by (17.22). To show that we really get an alternating $(c+1)$-form, we need to show that $X(\zeta \wedge \omega)$ is alternating for $c > 0$ and any vector field X, and verify

$$(fX)(\zeta \wedge \omega) = f(X(\zeta \wedge \omega)) \tag{17.24}$$

and

$$XX(\zeta \wedge \omega) = 0. \tag{17.25}$$

□

17.3.2 Theorem. *There is a unique linear mapping d mapping vector fields to zero and alternating c-forms to alternating $(c+1)$-forms (for $c = 0, 1, 2, \ldots$) such that*[10]

$$L_X\omega = Xd\omega + d(X\omega) \tag{17.26}$$

for all alternating c-forms ω and vector fields X. The alternating form $d\omega$ is called the ***exterior derivative*** *of ω, and satisfies the* ***exactness relation***

$$dd\omega = 0 \tag{17.27}$$

and the ***product rules***

$$d(f\omega) = fd\omega + df \wedge \omega, \tag{17.28}$$

$$d(\zeta \wedge \omega) = d\zeta \wedge \omega - \zeta \wedge d\omega, \tag{17.29}$$

$$L_{fX}\omega = fL_X\omega + df \wedge X\omega, \tag{17.30}$$

for all alternating froms ω, scalar fields f, linear forms ζ and vector fields X. Note the minus sign in (17.29)*!*

Proof. A necessary and sufficient condition for (17.26) to hold is that

$$X(d\omega) = L_X\omega - d(X\omega); \tag{17.31}$$

in particular,

$$X(d\omega) = Xd\,\omega = L_X\omega \quad \text{for a 0-form } \omega. \tag{17.32}$$

This completely specifies the exterior derivative of an alternating c-form. Therefore, if the exterior derivative exists, it is unique. To prove the existence of the exterior derivative, we have to define the exterior derivative of an alternating c-form ω to be the expression $d\omega$ determined for $c = 0$ by (17.32) and for $c > 0$ recursively by (17.31).

To show that we really get an alternating $(c+1)$-form, we need to show that $X(d\omega)$ is alternating for $c > 0$ and any vector field X, and verify

$$(fX)d\omega = f(Xd\omega) \tag{17.33}$$

[10] In particular, the relation $L_X = Xd$ valid on scalar fields fails to hold for the extension of L_X and d to alternating forms.

which shows that $Xd\omega$ is $\mathbb{E}$-linear in X, so that $d\omega$ is a $(c+1)$-linear form, and

$$XXd\omega = 0 \tag{17.34}$$

which proves antisymmetry. The proof of (17.33) is based on (17.30). To prove (17.30), we get inductively $Y(L_{fX}\omega - fL_X\omega - df \wedge X\omega) = YL_{fX}\omega - fYL_X\omega - Ydf \wedge X\omega = L_{fX}(Y\omega) - (L_{fx}Y)\omega - f(L_X(Y\omega) - (L_XY)\omega) - ((Ydf)X\omega - df \wedge YX\omega)$. Using the induction hypothesis on the first term and (17.28) on the second term, one finds that all terms cancel. From (17.30) one obtains $(fX)d\omega = L_{fX}\omega - d(fX\omega) = fL_X\omega + df \wedge X\omega - (fd(X\omega) + df \wedge X\omega) = f(L_X\omega - d(X\omega) = f(Xd\omega)$, showing that (17.33) holds. (17.34) follows inductively from

$$XXd\omega = XL_X\omega - Xd(X\omega) = XL_X\omega - L_X(X\omega) - d(XX\omega) = -(L_XX)\omega - d(XX\omega) = 0 - 0 = 0.$$

To prove the product rule (17.28), we , and then inductively $Xd(f\omega) = L_X(f\omega) - d(fX\omega) = (L_Xf)\omega + fL_X\omega - (fd(X\omega) + df \wedge X\omega) = f(L_X\omega - d(X\omega)) + (Xdf)\omega - df \wedge X\omega = fXd\omega + X(df \wedge \omega) = X(fd\omega + df \wedge \omega)$, completing the induction.

To prove the exactness relation (17.27), we need the formula

$$d(L_X\omega) = L_X(d\omega). \tag{17.35}$$

Indeed, $Yd(L_X\omega) = L_Y(L_X\omega) - d(YL_X\omega) = LYL_X\omega - d(L_X(Y\omega) - (L_XY)\omega)$, whereas $YL_X(d\omega) = L_X(Yd\omega) - (L_XY)d\omega = L_X(L_Y\omega - d(Y\omega)) - (L_{L_XY}\omega - d(L_XY)\omega) = L_YL_X\omega + d((L_XY)\omega) - L_Xd(Y\omega)$ since $L_{X\angle Y} = L_{X\angle Y} = [L_X, L_Y] = L_XL_Y - L_YL_X$. Comparing the two expressions, one finds that $Yd(L_X\omega) - YL_X(d\omega) = d(L_X(Y\omega) - L_Xd(Y\omega)$, which vanishes inductively.

Now (17.27) follows inductively from the relation $Xd(d\omega) = L_Xd\omega - d(Xd\omega) = L_Xd_\omega - d(L_X\omega - d(X\omega)) = L_Xd\omega - d(L_X\omega) + dd(X\omega) = -dd(X\omega)$, obtained by using (17.35). (For 0-forms, the dd-term is absent, which starts the induction.)

□

In particular, the exterior derivative of the linear form ζ is the alternating bilinear form $d\zeta$ with

$$YXd\zeta = YL_X\zeta - XL_Y\zeta + (X\angle Y)\zeta,$$

since $YXd\zeta = Y(L_X\zeta - d(X\zeta)) = YL_X\zeta - L_Y(X\zeta) = YL_X\zeta - ((L_YX)\zeta + XL_Y\zeta) = YL_X\zeta - XL_Y\zeta - (Y\angle X)\zeta$.

An alternating c-form ω is called **closed** if $d\omega = 0$, and **exact** if it can be written in the form $\omega = d\theta$ for some $(c-1)$-form θ. In particular, a linear form ζ is exact if it has the form $\zeta = df$ for some scalar field f.

By (17.27), every exact c-form is closed. The converse is not generally valid but holds in simple cases, e.g., by the **Poincaré Lemma**, when $\mathbb{E} = C^\infty(\mathbb{M})$, where $\mathbb{M}$ is a nonempty, open and convex subset of $\mathbb{R}^n$).

17.4 Manifolds as differential geometries

A central notion for analysis on infinite-dimensional spaces is that of a convenient vector space. This notion is discussed in detail in Kriegl & Michor [159], and refines the notion of a Hausdorff vector space, which is a vector space with the minimal amount of topological structure to allow the definition of a meaningful limit. A convenient vector space has in addition a meaningful notion of differentiability of paths, a property essential for differential geometry on manifolds. (For more details on basic notions from topology and functional analysis; see, for example, Rudin [242].)

17.4.1 Definition. A vector space $\mathbb{F}$ over $\mathbb{R}$ is called **locally convex** if there is a family S of **seminorms**, i.e., mappings $s : \mathbb{F} \to \mathbb{R}$ such that

$$s(\alpha x + \beta y) \leq |\alpha| s(x) + |\beta| s(y)$$

for all $x, y \in \mathbb{F}$ and all $\alpha, \beta \in \mathbb{R}$, with the property that

$$s(x) = 0 \text{ for all } s \in S \quad \Rightarrow \quad x = 0.$$

A locally convex vector space becomes a Hausdorff space by defining a **neighborhood** of $x \in \mathbb{F}$ to be a set containing for each $s \in S$ some set of the form $\{y \in \mathbb{F} \mid s(y - x) < r\}$ for some real number $r > 0$. Thus a sequence x_l $(l = 0, 1, 2, \ldots)$ in $\mathbb{F}$ converges to $x \in \mathbb{F}$ iff $s(x_l - x) \to 0$ for all $s \in S$. A path π, i.e., a continuous mapping $\pi : \mathbb{R} \to \mathbb{F}$, is called **smooth** or **arbitrarily often differentiable** if there are paths $\pi^{(k)} : \mathbb{R} \to \mathbb{F}$ $(k = 0, 1, 2, \ldots)$ such that

$$\pi(t + h) = \sum_{k=0}^{n} \frac{h^k}{k!} \pi^{(k)}(t) + O(h^{k+1})$$

for all $t, h \in \mathbb{R}$ and all natural numbers n. Clearly, $\pi^{(0)} = \pi$, and we write $\dot{\pi} := \pi^{()}$.

The reader should verify that, for any seminorm s and $\alpha \in \mathbb{R}$, $x \in \mathbb{F}$,

$$s(0) = 0, \quad s(\alpha x) = |\alpha| s(x) \geq 0,$$

that in any locally convex vector space, addition and scalar multiplication are continuous, and that differentiation satisfies the traditional rules.

17.4.2 Definition. A **convenient vector space** is a locally convex vector space $\mathbb{F}$ over $\mathbb{R}$ such that every smooth path in $\mathbb{F}$ is the derivative of another path in $\mathbb{F}$. A complex-valued function f on a nonempty and open subset $\mathbb{M}$ of $\mathbb{F}$ is called **smooth** or **arbitrarily often differentiable** if the complex-valued function $f \circ \pi$ is smooth for every smooth path $\pi : \mathbb{R} \to \mathbb{F}$. The space of smooth functions f from $\mathbb{M}$ to a topological vector space $\mathbb{V}$ is denoted by $C^\infty(\mathbb{M}, \mathbb{V})$, and the space of smooth functions $f : \mathbb{M} \to \mathbb{C}$ is denoted by $C^\infty(\mathbb{M})$.

The reader should verify that in a convenient vector space there is a mapping $\partial \in \mathrm{Lin}(C^\infty(\mathbb{M}), C^\infty$ called the **gradient** such that

$$\frac{d}{dt} f(\pi(t)) = \dot{\pi}(t) \partial f(\pi(t))$$

for all $f \in: C^\infty(\mathbb{M})$, all arbitrarily often differentiable paths $\pi : \mathbb{R} \to \mathbb{M}$ and all $t \in \mathbb{R}$.

17.4.3 Example. The space $\mathbb{F} = \mathbb{R}^n$ is convenient, with S consisting of the Euclidean norm only. Other examples of convenient vector spaces are Hilbert spaces and Schwartz spaces; see Kriegl & Michor [160].

17.4.4 Definition. Let $\mathbb{E}$ be a differential geometry with Lie algebra $\mathbb{W}$ of vector fields.

(i) A **point** is a algebra homomorphism from $\mathbb{E}$ to $\mathbb{C}$ which maps 1 to 1. We write $\mathbb{M}(\mathbb{E})$ for the set of points, and say that the point ξ maps the scalar field f to the **value** $f(\xi)$ of f at ξ.

(ii) If $\mathbb{F}$ is a convenient vector space, an **$\mathbb{F}$-chart** is a homomorphism C from $\mathbb{E}$ to $C^\infty(U(C), \mathbb{C})$ for some nonempty, open subset $U(C)$ of $\mathbb{F}$.

(iii) An **$\mathbb{F}$-manifold** is a differential geometry satisfying the axioms

(M1) If $f(\xi) = 0$ for all $\xi \in \mathbb{M}(\mathbb{E})$ then $f = 0$.

(M2) For all charts C and all $x \in U(C)$, there is a unique $\xi = \xi_C(x) \in \mathbb{M}(\mathbb{E})$ such that

$$f(\xi_C(x)) = (Cf)(x) \quad \text{for all } f \in \mathbb{E}.$$

(M3) For all charts C and all $\delta \in \operatorname{Der} C_0^\infty(U(C))$, there is a unique $\widehat{\delta} \in \operatorname{Der} \mathbb{E}$ such that

$$(\widehat{\delta} f)(\xi) = 0 \quad \text{for all } \xi \notin \xi_C(U),$$

$$(\widehat{\delta} f)(\xi_C(x)) = (\delta C f)(x) \quad \text{for all } x \in U.$$

Informally, property (M1) says that there are sufficiently many points to separate scalar fields. It implies not only that $\mathbb{E}$ is commutative, since $(fg - gf)(x) = f(x)g(x) - g(x)f(x) = 0$ for all points x, but also excludes many other commutative algebras, such as nontrivial quotients of the algebra of polynomials in a single variable.

(M2) expresses that charts are sufficiently large to represent scalar fields locally, and (M3) says that there are sufficiently many derivations to reduce differentiation locally to charts.

17.5 Manifolds as topological spaces

17.5.1 Definition.
(i) Let $\mathbb{F}$ be a convenient vector space. A **manifold** modeled on $\mathbb{F}$ (short **$\mathbb{F}$-manifold** or simply **manifold**[11] if $\mathbb{F}$ is apparent from the context) is a set $\mathbb{M}$ whose elements are called **points** together with a family $\mathcal{C}$ of maps $\xi : U \to \mathbb{M}$ from a (ξ-dependent) nonempty open subset U of $\mathbb{F}$ to $\mathbb{M}$ called **charts**, with the properties

(SM1) Every point of $\mathbb{M}$ is in the **range** $\xi[U]$ of some chart $\xi : U \to \mathbb{M}$;

[11] More precisely, this defines arbitrarily often differentiable, real manifolds whose dimension need not be finite. There are a number of other notions of a manifold which make somewhat different assumptions.

(SM2) A map $\xi : U \to \mathbb{M}$ is in $\mathcal{C}$ if and only if ξ is injective and, for every nonempty open subset V of U and every chart $\xi' : U' \to \mathbb{M}$ in $\mathcal{C}$ with $\xi[V] \subseteq \xi'[U']$,

$$\xi'^{-1}\xi|_V \in C^\infty(V, \mathbb{F}).$$

The manifold is canonically a topological space by declaring as open sets arbitrary unions of finite intersections of ranges of charts.

(ii) The inverse of a chart is called a **local coordinate system**. An **atlas** is a family of charts whose ranges cover $\mathbb{M}$; the family $\mathcal{C}$ of all charts is the **universal atlas**.

(iii) The dimension of $\mathbb{F}$ is called the **dimension** of $\mathbb{M}$. In particular, $\mathbb{M}$ is called **finite-dimensional (d-dimensional)** if $\dim \mathbb{F} < \infty$ (resp. $\dim \mathbb{F} = d$).

(iv) A mapping F from $\mathbb{M}$ to convenient some vector space $\mathbb{U}$ is called **smooth** (or **infinitely differentiable**) if $F(\xi) \in C^\infty(U, \mathbb{U})$ for every chart $\xi : U \to \mathbb{M}$. A **scalar field** on $\mathbb{M}$ is a smooth complex-valued function on $\mathbb{M}$; the algebra of all scalar fields on $\mathbb{M}$ with pointwise operations is denoted by $C^\infty(\mathbb{M})$. A **derivation** on $\mathbb{M}$ is a mapping $\delta \in \operatorname{Lin} C^\infty(\mathbb{M})$ satisfying

$$\delta(fg) = (\delta f)g + f(\delta g) \quad \text{for all } f, g \in C^\infty(\mathbb{M}).$$

Thus a derivation on $\mathbb{M}$ is an element of $\operatorname{Der} C^\infty(\mathbb{M})$, which we also denote by $\operatorname{Der} \mathbb{M}$.

(v) A canonical differential geometry whose scalar fields form the algebra $\mathbb{E} = C^\infty(\mathbb{M})$ of a manifold $\mathbb{M}$ is called a **differential geometry** of $\mathbb{M}$.

Note that a chart ξ is injective, hence its inverse ξ^{-1}, the corresponding local coordinate system is well-defined on the range of the chart, and maps a nonempty, open subset of $\mathbb{M}$ to an open subset of $\mathbb{F}$. In many treatments of differential geometry, the local coordinate system ξ^{-1} rather than ξ is called the chart.

17.5.2 Proposition.
(i) The set $C^\infty(\mathbb{M})$ of all scalar fields on $\mathbb{M}$ is a commutative $*$-algebra under pointwise multiplication.

(ii) The set $\operatorname{Lie} \mathbb{M} := \operatorname{Der} C^\infty(\mathbb{M})$ of all derivations on $\mathbb{M}$ with the commutator of derivations as Lie product is a Lie algebra.

Proof. This is left to the reader as a straightforward exercise. □

17.5.3 Theorem. *$\mathbb{F}$-Manifolds in the sense of Definition 17.4.4(iii) and $\mathbb{F}$-manifolds in the sense of Definition 17.5.1(i) are equivalent concepts.*

Proof. □

The motivating example defining the terminology is the surface of the earth, the **globe**, which may be regarded as a 2-dimensional manifold $\mathbb{M}$ with $\mathbb{F} = \mathbb{R}^{1\times 2}$, the vector space

of 2-dimensional row vectors[12]. Here the domain U of a chart $\xi : U \to \mathbb{M}$ may be viewed as the paper on which the chart (a road map, say) is printed. The important points $q = (x, y) \in U$ correspond to Cartesian coordinates of marks on the road map labeled by towns. $\xi(q)$ denotes the location of the corresponding town on the globe. Note that our charts may have domains which are not neatly cut and may be disconnected or unbounded.

The simplest examples of manifolds are open, nonempty subsets of $\mathbb{R}^n$.

17.5.4 Example. We consider the concrete case where smooth manifolds modeled on the vector spaces $\mathbb{R}^d$ for some $d \in \mathbb{N}$ are embedded into a bigger vector space $\mathbb{R}^n$, and where membership in the manifold is characterized by m equations $F_k(x) = 0$ $(k = 1, \ldots, m)$. For example, a d**-sphere** is the set of points $x \in \mathbb{R}^{d+1}$ satisfying the single $(m = 1)$ equation $F(x) := x^T x - 1 = 0$, where the superscript T denotes the transpose.

Let $\mathbb{M}_0$ be an open subset of $\mathbb{R}^n$ and let $F \in C^\infty(\mathbb{M}_0, \mathbb{R}^m)$. The **gradient** at x of F is given by

$$dF(x) = F'(x)^T \in \mathbb{R}^{n\times m} .$$

This generalizes the traditional terminology for the case where $m = 1$. The implicit function theorem implies that if the gradient has constant rank m, i.e., $\operatorname{rk} dF(x) = m$ for all $x \in \mathbb{M}_0$, then the set $\mathbb{M}$ given by

$$\mathbb{M} = \{x \in \mathbb{M}_0 \mid F(x) = 0\} ,$$

is a d-dimensional manifold with $d = n - m$. If $\mathbb{M}$ defines a d-dimensional manifold given by an equation $F(x) = 0$, then the tangent space at a point $x \in \mathbb{M}$ is given by

$$T_x\mathbb{M} = \left\{X \in \mathbb{R}^{1\times n} \mid X \cdot dF(x) = 0\right\} .$$

Thus the tangent space consists of those vectors perpendicular to the gradient, that is, the tangent vectors at x are tangent to $\mathbb{M}$ at x. Hence the name tangent space. The vector fields of $\mathbb{M}$ are similarly given by

$$\operatorname{vect}\mathbb{M} = \left\{X \in C^\infty(\mathbb{M}, \mathbb{R}^{1\times n}) \mid X(x) \cdot dF(x) = 0, \quad \text{for all } x \in \mathbb{M}\right\} .$$

Given an $\mathbb{F}$-manifold $\mathbb{M}$ and an $\mathbb{F}'$-manifold $\mathbb{N}$, we define $C^\infty(\mathbb{M}, \mathbb{N})$ as the set of maps $A : \mathbb{M} \to \mathbb{N}$ such that if $\xi : U \to \mathbb{M}$ is a chart on $\mathbb{M}$ and $\xi' : V \to \mathbb{N}$ is a chart on $\mathbb{N}$ such that $A(\xi(U)) \subseteq \xi'(V)$ implies $(\xi')^{-1} \circ A \circ \xi \in C^\infty(U, V)$. A **diffeomorphism** of $\mathbb{M}$ is an invertible mapping in $C^\infty(\mathbb{M}, \mathbb{M})$ with an inverse in $C^\infty(\mathbb{M}, \mathbb{M})$; we write Ax for the image of a point $x \in \mathbb{M}$ under a diffeomorphism A.

We assume that the identity map on $\mathbb{M}$ is in $C^\infty(\mathbb{M}, \mathbb{M})$ and that the composition of $f \in C^\infty(\mathbb{M}, \mathbb{N})$ and $g \in C^\infty(\mathbb{N}, \mathbb{N}')$ is in $C^\infty(\mathbb{M}, \mathbb{N}')$, a condition[13] automatically satisfied in

[12]It is convenient to think of points as row vectors; then tangent vectors are row vectors, too, and gradients of scalar fields are naturally column vectors. Thus later expressions like the directional derivative Xdf of a scalar field f in the direction of a vector field X have a natural interpretation as "scalar = row times colums" in terms of ordinary matrix algebra.

[13]In technical terms this says that the modeling vector spaces should admit a category of smooth manifolds.

finite dimensions. Then the set $\operatorname{Diff}\mathbb{M}$ of all diffeomorphisms is a group under composition of maps. Additional conditions are needed to ensure that $\operatorname{Diff}\mathbb{M}$ is a $\operatorname{vect}\mathbb{M}$-manifold and hence (in the terminology of Section 17.7 below) a Lie group; see, e.g., Neeb [200], where one can find a detailed discussion of pathologies that can arise in infinite-dimensional Lie groups.

We define a **motion** on $\mathbb{M}$ as a mapping $A \in C^\infty([0,1], \operatorname{Diff}(\mathbb{M}))$ such that $A(0) = 1$ is the identity. The intuition is that the points $x = A(0)x$ of an object (subset of $\mathbb{M}$) at time $t = 0$, the start of the motion, is moved by the motion to the point $A(t)x$ at time $t \in [0,1]$, ending up in $A(1)x$ at the end of the motion. For every motion A and for all $t \in [0,1]$ we define a vector field $\dot{A}(t)$ on $\mathbb{M}$ by

$$\dot{A}(t)df : x \to \frac{d}{ds} f(A(s)A(t)^{-1}x)\Big|_{s=t}$$

for all scalar fields f and all $x \in \mathbb{M}$. Since the product rule holds for smooth functions in $C^\infty(\mathbb{M})$, the object $\dot{A}(t)d$ is indeed a derivation on $\mathbb{M}$, and hence $\dot{A}(t)$ is a vector field. From the definition of $\dot{A}(t)$ we get the **chain rule**:

$$\frac{d}{dt} f(A(t)x) = \dot{A}(t)df(A(t)x)\,.$$

If we are only interested in what happens in an infinitesimal neighborhood of a point $x \in \mathbb{M}$, the vector fields in

$$N(x) := \{X_0 \in \operatorname{vect}\mathbb{M} \mid X_0 df(x) = 0 \quad \text{for all } f \in C^\infty(\mathbb{M})\}$$

have no effect at x. Since $N(x)$ is a vector space, we can form the quotient space

$$T_x\mathbb{M} = \operatorname{vect}\mathbb{M}/N(x)\,,$$

called the **tangent space** or **tangent (hyper-)plane** at x. We denote with

$$X(x) := X + N(x),$$

the equivalence class of X with respect to the equivalence relation $X \sim Y \Leftrightarrow X - Y \in N(x)$. We call the equivalence class that contains the vector field X the **tangent vector** of X at the point x.

The union $T\mathbb{M}$ of all $T_x\mathbb{M}$ is naturally a manifold called the **tangent bundle** of $\mathbb{M}$.

The Lie derivative in the traditional approach. In the special case where $\mathbb{E} = C^\infty(\mathbb{M})$ for some finite-dimensional manifold $\mathbb{M}$, there is an alternative, traditional route to the calculus on manifolds, using the following traditional definition of the Lie derivative.

For any vector field X, the initial value problem

$$\xi(0) = x, \quad \frac{d}{d\tau}\xi(\tau) = X(\xi(\tau)) \tag{17.36}$$

is solvable for every $x \in \mathbb{M}$, for τ in some x-dependent neighborhood of zero. This follows from the standard theory of ordinary differential equations, since differentiable vector fields are locally Lipschitz.

We denote by $e^{\tau X}$ the local diffeomorphism which maps x into the value $\xi(\tau)$ of the solution ξ of (17.36). Clearly, $e^0 = 1$ is the identity, but for fixed τ, the map $e^{\tau X}$ need not be defined everywhere. The latter is the case only when (17.36) is solvable for all $\tau \in \mathbb{R}$; in this case, the vector field is called **complete**, and the $e^{\tau X}$ form a 1-parameter group of diffeomorphisms. In general, we have, on the domain of definition,

$$e^{\tau X} e^{\tau' X} = e^{(\tau+\tau')X},$$

$$\frac{d}{d\tau} e^{\tau X} x = X(e^{\tau X} x).$$

We define the **directional derivative** $L_X \phi$ of a tensor field ϕ with respect to the complete vector field X by

$$(L_X \phi)(x) := \frac{d}{d\tau} \phi(e^{\tau X} x)\Big|_{\tau=0}.$$

This defines a linear differential operator L_X mapping tensor fields to tensor fields of the same type $[c, r]$, called the **Lie derivative** of X. Clearly,

$$(e^{\tau L_X} \phi)(x) = \phi(e^{\tau X} x).$$

It is not difficult to show the **chain rule**

$$\frac{d}{d\tau} \xi(\tau) = X(\tau)\xi(\tau) \quad \Rightarrow \quad \frac{d}{d\tau} \phi(\xi(\tau)) = L_{X(\tau)} \phi(\xi(\tau))$$

for every smooth path $x : [0, 1] \to \mathbb{M}$. Here $\dot{\xi}(\tau)$ is the tangent vector of the path at $\xi(\tau)$. The chain rule implies the product rule (17.15) for the Lie derivative. Therefore Theorem 17.2.3 implies that the traditional concept coincides with our algebraic concept when $\mathbb{E}$ is the algebra of scalar fields of a finite-dimensional manifold.

In the infinite-dimensional case, this approach can also be carried through, although it requires considerable technicalities to account for the fact that initial-value problems for differential equations in infinite-dimensional spaces are not always solvable. For details, see Kriegl & Michor [159].

17.6 Noncommutative geometry

In this short section, we indicate how things generalize to noncommutative geometry, without giving details; the reader not familiar with the notions used may simply skip the section.

In noncommutative geometry, position measurements are limited by uncertainty relations. The notion of a point therefore loses its meaning, and the evaluation of functions and vectors at a point is no longer well-defined. Thus, in noncommutative geometry, a manifold of points

no longer exists, but in place of $C^\infty(\mathbb{M})$ one has a noncommutative algebra $\mathbb{E}$ whose elements behave in a way analogous to scalar fields. All constructions based only on this algebra rather than a manifold generalize in an appropriate way to the noncommutative situation. Thus most geometric notions extend formally, but they can be matched with true geometric concepts only in certain commutative subalgebras. The basic observation is that a point evaluation is a $*$-homomorphism of $C^\infty(\mathbb{M})$ to $\mathbb{C}$, and conversely, all such homomorphisms of $C^\infty(\mathbb{M})$ are obtained as point evaluations. Now, if $\mathbb{E}_0$ is a commutative normed $*$-subalgebra of $\mathbb{E}$ whose completion is a B^***-algebra** (a term we shall not further use, and hence not introduce formally) then one can reconstruct on $\mathbb{E}_0$ a topological space $\mathbb{M}_0$ by calling the characters of $\mathbb{E}_0$ points; the B^*-algebra is then canonically isomorphic to the algebra of bounded continuous functions on $\mathbb{M}_0$. If $\mathbb{E}_0$ admits sufficiently many derivations then $\mathbb{M}_0$ is a (smooth) manifold. When $\mathbb{E}_1$ and $\mathbb{E}_2$ are two such commutative subalgebras that do not commute, then, in contrast to the commutative situation, the corresponding manifolds $\mathbb{M}_1$ and $\mathbb{M}_2$ are not naturally embedded into a bigger manifold. Thus there may be many maximal manifolds embedded in a single noncommutative geometry.

17.7 Lie groups as manifolds

This section defines Lie groups in full generality. Differential equations defining the flow along a vector field naturally produce Lie groups and the exponential map, which relates Lie groups and Lie algebras.

17.7.1 Definition.
(i) A **Lie group** is a group $\mathbb{G}$ which is at the same time a manifold, such that multiplication and inversion are arbitrarily often differentiable. A Lie group is both a manifold and a group and the two structures are compatible. The identity element in a Lie group will always be written as 1.

(ii) We canonically embed $\mathbb{G}$ into $\mathrm{Diff}(\mathbb{G})$ by associating to $A \in \mathbb{G}$ the map $B \to AB$, which is a diffeomorphism. For the definition of the Lie algebra associated with a Lie group, it is important to know that the group $\mathbb{G}$ acts on $C^\infty(\mathbb{G})$ by right multiplication, that is, to every $A \in \mathbb{G}$ we associate the map $R_A : C^\infty(\mathbb{G}) \to C^\infty(\mathbb{G})$ given by

$$(R_A\varphi)(B) := \varphi(BA)$$

for all $B \in \mathbb{G}$, $\varphi \in C^\infty(\mathbb{G})$. Of course, the group also acts by left-multiplication on $C^\infty(\mathbb{G})$ but this action is not directly related to the Lie algebra.

(iii) The Lie algebra $\mathrm{vect}\,\mathbb{G}$ contains the set

$$\log \mathbb{G} = \{X \in \mathrm{vect}\,\mathbb{G} \mid R_B \angle X d = 0 \quad \text{for all } B \in \mathbb{G}\}$$

of **invariant vector fields**.

It is not difficult to show that every Lie group in the above sense is a Lie group in the sense of Definition 11.3.2, since $\mathbb{G}$ is canonically embedded into $\mathrm{Lin}\, C^\infty(\mathbb{G})$. The converse is also valid but a bit more difficult to establish.

17.7.2 Proposition. *The invariant vector fields* $\log \mathbb{G}$ *form a Lie algebra.*

Proof. To check the statement, we only need to show that the Lie product $X \angle Y$ of two invariant vector fields X and Y is invariant. But this follows from Proposition 11.2.4 since the invariant vector fields form the centralizer of the set $\{R_A \mid A \in \mathbb{G}\}$. □

17.7.3 Proposition. *For any smooth motion* $A \in C^\infty([0,1], \mathbb{G})$*, where* $\mathbb{G}$ *is identified with a subset of* $\mathrm{Diff}(\mathbb{G})$*, the vector field* $\dot{A}(t)$ *is an invariant vector field.*

Proof. We know that $\dot{A}(t)$ is a vector field. Hence we need to check that $\dot{A}(t)$ Lie commutes with R_B for all $B \in \mathbb{G}$. For arbitrary $B \in \mathbb{G}$ and $\varphi \in C^\infty(\mathbb{G})$ we have

$$\begin{aligned}
(R_B \angle \dot{A}(t) d)\varphi(A(t)\zeta) &= R_B(\dot{A}(t) d\varphi)(A(t)\zeta) - \dot{A}(t) d(R_B\varphi)(A(t)\zeta) \\
&= \dot{A}(t) d\varphi(A(t)\zeta B) - \frac{d}{dt}(R_B\varphi)(A(t)\zeta) \\
&= \frac{d}{dt}\varphi(A(t)\zeta B) - \frac{d}{dt}\varphi(A(t)\zeta B) = 0\,.
\end{aligned}$$

□

17.7.4 Remarks. Note that an essential ingredient in the above proof is that the action of $\mathbb{G}$ on $C^\infty(\mathbb{G})$ is defined from the right and the action of the vector field $\dot{A}(t)$ from the left.

17.7.5 Definition. A motion $A(t)$ is called a **uniform motion** if there exists a unique $f \in \log \mathbb{G}$ such that

$$\dot{A}(t) = fA(t) \quad \text{for all } t \in [0,1]. \tag{17.37}$$

In this case we write e^f for the group element $A(1)$ and call it the **exponential** of f. Conversely, f is called the **infinitesimal generator** of the motion.

Formula (17.37) is a linear differential equation with constant coefficients; the initial condition $A(0) = 1$ is already part of the definition of a motion. In finite dimensions, such initial value problems are uniquely solvable; in infinite dimensions, unique solvability depends on additional conditions. It is easy to check that a uniform motion with infinitesimal generator $f \in \log \mathbb{G}$ is given by $A(t) = e^{tf}$.

17.7.6 Example. In any associative algebra, the set of invertible elements is a group. In many cases, the group of invertible elements is a Lie group. In particular, the group $GL(n, \mathbb{K})$ of all invertible $n \times n$-matrices over $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$ is a Lie group, since it is the open set of points in $\mathbb{K}^{n\times n}$ where the determinant does not vanish, so that any point has an open neighborhood on which the identity is a chart. We can choose coordinates x_{ij} for $1 \le i, j \le n$ and then $GL(n, \mathbb{K})$ is the open set where $\det(x_{ij}) \neq 0$. Any derivation is of the form

$$(Xf)(x_{ij}) = \sum_{1\le i,j\le n} X^{ij} \frac{\partial}{\partial x_{ij}} f(x_{ij})\,,$$

for all $f \in C^\infty(GL(n, \mathbb{K}))$ and for some $X^{ij} \in \mathbb{K}$. One finds that $\log GL(n, \mathbb{K}) = gl(n, \mathbb{K})$ is the Lie algebra of all $n \times n$-matrices over $\mathbb{K}$. It is easy to verify these properties by describing everything with matrices. The subgroup of $GL(n, \mathbb{L})$ consisting of the matrices with unit determinant is denoted by $SL(n, \mathbb{K})$. In other words, $SL(n, \mathbb{K})$ is the kernel of the map $\det : GL(n, \mathbb{K}) \to \mathbb{K}^*$, where $\mathbb{K}^*$ is the group of invertible elements in $\mathbb{K}$. The Lie algebra of $SL(n, \mathbb{K})$ is denoted by $sl(n, \mathbb{K})$ and consists of the traceless $n \times n$ matrices with entries in $\mathbb{K}$.

Chapter 18

Conservative mechanics on manifolds

We consider closed 2-forms in manifolds and their associated Poisson algebras. This naturally leads to symplectic geometry and a symplectic formulation of the dynamics of quantum mechanics. It also leads to classical Hamiltonian and Lagrangian mechanics, including constraints.

18.1 Poisson algebras from closed 2-forms

In general, a classical, conservative dynamical system is described in terms of motion on a manifold $\mathbb{M}$, called the **phase space**, such that some algebra of functions on it has a Poisson algebra structure; more precisely, $C^\infty(\mathbb{M})$ is equipped with a Lie product $\angle$ that is antisymmetric and satisfies the Jacobi identity and the Leibniz identity. Such a manifold is called a **Poisson manifold**; see, e.g., Vaisman [275] or da Silva & Weinstein [70] Poisson manifolds provide a general setting for the study of the dynamics of classical conservative mechanical systems by differential geometric methods; for a more comprehensive discussion of different aspects see Marsden & Ratiu [184], Ratiu [227] and Morrison [195].

Every symplectic manifold is a Poisson manifold since the symplectic structure gives rise to a natural Poisson bracket. In the symplectic case, a Hamiltonian is a function of some coordinates q_i and the conjugated momenta p_i. In such cases, the phase space is even-dimensional. In more general cases described, e.g., by Lie-Poisson algebras, the phase space need not be a symplectic manifold. Indeed, symplectic manifolds are always even-dimensional while the manifold $SO(3)$ of the spinning rigid body (see Section 12.2) has dimension 3.

Many Poisson algebras of relevance in classical mechanics may be constructed via a uniform construction based on a closed 2-form characterizing the kinematics of the system of interest. The description is then completed by specifying the dynamics through a Hamiltonian in

the resulting Poisson algebra, and by selecting an initial state describing the preparation of the system. In this section, we discuss the general construction principle.

Let ω be a closed 2-form on a differential geometry $\mathbb{E}$. We call a scalar field $f \in \mathbb{E}$ **compatible** with ω if there is a vector field X_f such that

$$df \;=\; X_f\,\omega\;; \tag{18.1}$$

any such X_f is called a **Hamiltonian vector field** associated with f. We write $\mathbb{E}(\omega)$ for the set of all scalar fields $f \in \mathbb{E}$ which are compatible with ω. In general, X_f need not exist for all f, and if it exists, it need not be unique. Thus $\mathbb{E}(\omega)$ may be a proper subspace of $\mathbb{E}$; this situation is typical for examples arising from constrained Hamiltonian mechanics.

18.1.1 Proposition. *Let ω be a symplectic form. Then every scalar field f is compatible with ω,*

$$X_f = df\omega^{-1}, \tag{18.2}$$

and $\mathbb{E}(\omega) = \mathbb{E}$.

Proof. Since ω is a symplectic form, ω is nondegenerate and has an inverse satisfying (17.12). The defining condition for X_f can therefore be solved uniquely for X_f, for all $f \in \mathbb{E}$, resulting in (18.2). □

A vector field X is called **locally Hamiltonian** (with respect to ω) if the linear form $X\omega$ is closed, and **Hamiltonian** (with respect to ω) if $X\omega$ is exact (and hence closed). Thus, for any $f \in \mathbb{E}(\omega)$, the vector field X_f is Hamiltonian with respect to ω,

18.1.2 Proposition. *If X, Y are locally Hamiltonian vector fields with respect to the closed 2-form ω then $X\angle Y$ is Hamiltonian, and*

$$(X\angle Y)\omega = d(XY\omega). \tag{18.3}$$

In particular, the locally Hamiltonian vector fields and the Hamiltonian vector fields form Lie subalgebras of $\mathbb{W}$.

Proof. Since ω and $X\omega$ are closed, (17.26) implies that $L_X\omega = Xd\omega + d(X\omega) = 0$. Again by (17.26), $d(XY\omega) = L_X(Y\omega) - Xd(Y\omega) = L_X(Y\omega) = (L_XY)\omega + YL_X\omega = (L_XY)\omega = (X\angle Y)\omega$, using the closedness of $Y\omega$ and the product rule (17.15). This proves (18.3). The concluding statement is an immediate consequence. □

18.1.3 Theorem. *For every closed 2-form ω over the manifold $\mathbb{M}$, the set $\mathbb{E}(\omega)$ is a Poisson algebra, with Lie product given by*

$$f\angle g := X_f dg = X_f X_g\omega = -X_g X_f\omega = -X_g df. \tag{18.4}$$

A Hamiltonian vector field associated with $f\angle g$ is given by

$$X_{f\angle g} := X_f\angle X_g. \tag{18.5}$$

In particular, if ω is a symplectic form then

$$f\angle g = df\omega^{-1}dg. \tag{18.6}$$

Proof. We first show that $\mathbb{E}(\omega)$ is a subalgebra of the algebra $\mathbb{E}$. If $f, g \in \mathbb{E}(\omega)$ and $\lambda \in \mathbb{C}$ then $\lambda f, f \pm g, fg \in \mathbb{E}(\omega)$ since we may take

$$X_{\lambda f} = \lambda X_f, \quad X_{f\pm g} = X_f \pm X_g, \quad X_{fg} = fX_g + gX_f.$$

We next show that $f\angle g$ is well-defined. Indeed, if X_f, X'_f are two Hamiltonian vector fields associated with f then $\omega(X'_f - X_f, Y) = 0$, hence $f\angle g$ does not depend on the choice of the Hamiltonian vector fields associated with f and g.

Proposition 18.1.2 implies that (18.5) is a Hamiltonian vector field for $f\angle g$; therefore $f\angle g \in \mathbb{E}(\omega)$.

The operation $\angle$ defined by (18.4) is bilinear, antisymmetric, and satisfies the Leibniz identity. To conclude that $\mathbb{E}(\omega)$ is a Poisson algebra it therefore suffices to show that the Jacobi identity holds. This follows since, with $X := X_f, Y := X_g$,

$$\begin{aligned}
(f\angle g)\angle h &= X_{f\angle g}dh = (X_f\angle X_g)dh = (X\angle Y)dh = L_{X\angle Y}h \\
&= [L_X, L_Y]h = L_XL_Yh - L_YL_Xh = X_fd(X_gdh) - X_gd(X_fdh) \\
&= f\angle(g\angle h) - g\angle(f\angle h) = (f\angle h)\angle g + f\angle(g\angle h).
\end{aligned}$$

Finally, if ω is a symplectic form, (18.2) implies that the Lie product (18.4) can be rewritten in the form (18.6). □

Note that the Lie product can be extended to the case where one argument is in $\mathbb{E}(\omega)$ and the other may be an arbitrary quantity from $\mathbb{E}$:

$$f\angle g = X_f dg \quad \text{for } f \in \mathbb{E}(\omega),\ g \in \mathbb{E},$$

$$f\angle g = -X_g df \quad \text{for } f \in \mathbb{E},\ g \in \mathbb{E}(\omega).$$

Thus if f is compatible with ω, the Lie product is defined even when g is not compatible with ω.

In the manifold case, the above theorem defines, for each closed 2-form ω on an $\mathbb{F}$-manifold $\mathbb{M}$, a Poisson algebra $\mathbb{E}(\omega)$ which is the set of functions $f \in \mathbb{E} = C^\infty(\mathbb{M})$ which are compatible with ω. In the special case where ω is symplectic, we have seen that $\mathbb{E}(\omega) = \mathbb{E}$; thus we may define the **Poisson bracket**

$$\{f, g\} := g\angle f = dg\omega^{-1}df \tag{18.7}$$

of $f, g \in \mathbb{E}$. This is the traditional Poisson bracket associated with the **symplectic space** $(\mathbb{M}, \omega)$.

The affine functions, which map $\xi \in \mathbb{M}$ to $\xi u + \gamma$ for some $u \in \mathbb{F}$ and some $\gamma \in \mathbb{C}$, satisfy

$$(\xi u + \gamma)\angle(\xi v + \gamma') = u\omega{-}1v \in \mathbb{C},$$

hence form a Lie subalgebra, which is a Heisenberg algebra. This provides a faithful classical Poisson representation of general Heisenberg algebras.

18.1.4 Example. We continue the discussion of Example 17.1.2, where scalar fields (resp. vector fields) are the smooth complex-valued (resp. row vector valued) functions on a nonempty, open subset $\mathbb{M}$ of the space $\mathbb{R}^{\times n}$ of rovectors of length n. In this case, it is natural to identify $\mathbb{W}^*$ with the vector space $C^\infty(\mathbb{M}, \mathbb{C}^n)$ of covector-valued fields via

$$(X\zeta)(x) = X(x)\zeta(x)$$

for $X \in \mathbb{W} = C^\infty(\mathbb{M}, \mathbb{C}^{\times n})$ and $\zeta \in \mathbb{W}^* = C^\infty(\mathbb{M}, \mathbb{C}^n)$. In particular, the gradient $df = \partial f$ appears naturally as an element of $\mathbb{W}^*$, consistent with our abstract development.

Now let θ be a distinguished linear form. Then we can define its **Jacobian**, the x-dependent square array $\partial\theta$ whose entries are the partial derivatives

$$\partial_j \theta_k(x) \;=\; \frac{\partial \theta_k(x)}{\partial x^j}\;.$$

We now consider the exact 2-form $\omega = -d\theta$ (the minus sign is traditional). We have

$$YX\omega = Yd(X\theta) - Xd(Y\theta) + (X\angle Y)\theta \quad \text{for } \omega = -d\theta \tag{18.8}$$

since $YX\omega = -YXd\theta = -Y(L_X\theta - d(X\theta)) = -YL_X\theta + Yd(X\theta) = -L_X(Y\theta) + (L_XY)\theta + Yd(X\theta)$ by (17.31) and (17.18). It is not difficult to show that now

$$(X\omega)(x) = \sum X^j(x)\omega_{jk}(x), \tag{18.9}$$

where

$$\omega_{jk}(x) = \partial_k\theta_j(x) - \partial_j\theta_k(x) \tag{18.10}$$

are the components of the antisymmetric expression $(\partial\theta)^T - \partial\theta$ in the Jacobian of θ.

As a consequence, $\omega = -d\theta$ is nondegenerate precisely when $(\partial\theta)^T - \partial\theta$ is nonsingular. If this holds, ω is a symplectic form, and all our results apply. This matches the present development with that found in standard treatises such as Marsden & Ratiu [185].

18.2 Conservative Hamiltonian dynamics

We now apply the results of Section 18.1 to classical Hamiltonian mechanics of conservative systems. The phase space of a classical system is the set of all states that may be attained in some realization of the system. We begin with the unconstrained case, where the phase space is a cotangent bundle over a manifold $\mathbb{M}$, and then extend the discussion to the constrained case, where the phase space has a more complicated structure.

To avoid technicalities, we only treat the case where the manifold can be described by a single chart, so that it can be treated as an open subset of some topological vector space. However, using standard techniques from differential geometry, it is not difficult to lift the discussion to arbitrary manifolds. Thus, in the following, the **configuration space** $\mathbb{M}_c$ is a nonempty, open subset of a convenient vector space $\mathbb{F}$ over $\mathbb{R}$. Thinking of $\mathbb{M}_c$ as a chart of a general manifold, everything we say here extends in a standard way to arbitrary $\mathbb{F}$-manifolds in place of $\mathbb{M}_c$.

We write the bilinear pairing between elements q from $\mathbb{F}$ and elements p from the dual space $\mathbb{F}^*$ as product $p \cdot q = q \cdot p$. We extend this product linearly to the compexifications $\mathbb{CF}$ of $\mathbb{F}$ and $\mathbb{CF}^*$ of $\mathbb{F}^*$, and extend it further pointwise to $\mathbb{CF}$-valued or $\mathbb{CF}^*$-valued functions.

In this section, we consider the case of unconstrained dynamics Here $\mathbb{E} = C^\infty(\mathbb{M})$ and $\mathbb{W} = C^\infty(\mathbb{M}, \mathbb{CF} \times \mathbb{CF}^*)$ are the spaces of scalar fields and vector fields, respectively, on the **cotangent bundle** $\mathbb{M} = T^*\mathbb{M}_c := \mathbb{M}_c \times \mathbb{F}^*$ of $\mathbb{M}_c$.

The reader may think of the Euclidean space $\mathbb{F} = \mathbb{F}^* = \mathbb{R}^n$ of vectors with n real components and bilinear pairing $p \cdot q = \sum_k p_k q_k$. As discussed in Section 5.2, this accounts for the mechanics of point particles. For field theories, $\mathbb{F}$ is an infinite-dimensional function space.

A classical, conservative, **unconstrained mechanical system** is defined by a **Hamiltonian** $H \in \mathbb{E}$ and considering the full cotangent bundle $\mathbb{M}$ as the **phase space** of the system. The point $x = (q, p) \in \mathbb{M}$ is called the **state** with **position** $q \in \mathbb{M}_c$ and **momentum** $p \in \mathbb{F}^*$. The **energy** of the system in the state (q, p) is the value $H(q, p)$ of the Hamiltonian at (q, p).

The state of the system varies with **time** t, which we consider to be a number in the interval $[\underline{t}, \overline{t}]$, where $\underline{t}$ is the **initial time** and $\overline{t} > \underline{t}$ is the **final time** for which the system is considered. The time dependence is modeled by a **trajectory**, a state-valued, arbitrarily often differentiable function of time, mapping $t \in [\underline{t}, \overline{t}]$ to $(p(t), q(t)) \in \mathbb{M}$. The position $q(t)$ and the momentum $p(t)$ at time t are constrained by the **Hamilton equations** in **state form**,

$$\dot{q} = \frac{dq}{dt} = \partial_p H, \quad \dot{p} = \frac{dp}{dt} = -\partial_q H. \tag{18.11}$$

Here $\partial_p = \partial/\partial p$ and $\partial_q = \partial/\partial q$ denote the gradient with respect to momentum p and position q, respectively. Note that if f is a scalar field then $\partial_p f(q, p) \in \mathbb{CF}$ and $\partial_q f(q, p) \in \mathbb{CF}^*$.

The Hamiltonian equations automatically imply the **conservation of energy**: $\frac{d}{dt} H(q, p) = \partial_q H \cdot \dot{q} + \partial_p H \cdot \dot{p} = 0$.

The Hamiltonian equations may be derived from a **variational principle**. We define the **action** as the functional on smooth paths in $\mathbb{M}$ defined by

$$I(q, p) := \int_{\underline{t}}^{\overline{t}} dt \, \Big(p(t) \cdot \dot{q}(t) - H(q(t), p(t)) \Big), \tag{18.12}$$

and consider small variations δq and δp of the arguments q and p, respectively. Since we do not make further use of the principle, we assume without the discussion that the integral

can be manipulated as accustomed from the finite-dimensional case, where $\mathbb{F} = \mathbb{R}^n$. For variations vanishing at $t = \underline{t}$ and $t = \overline{t}$, we have, up to higher order terms,

$$\begin{aligned} I(q+\delta q,p) - I(q,p) &\approx \int_{\underline{t}}^{\overline{t}} dt \, \Big(p(t)\cdot \delta\dot{q}(t) - \partial_q H(q(t),p(t))\cdot \delta q \Big) \\ &= \int_{\underline{t}}^{\overline{t}} dt \, \Big(-\dot{p}(t)\cdot \delta q(t) - \partial_q H(q(t),p(t))\cdot \delta q \Big), \end{aligned}$$

$$I(q,p+\delta p) - I(q,p) \approx \int_{\underline{t}}^{\overline{t}} dt \, \Big(\delta p(t)\cdot \dot{q}(t) - \partial_p H(q(t),p(t))\cdot \delta p \Big),$$

so that the path (q,p) is a stationary point of the action if and only if the extended Hamiltonian equations (18.11) hold.

A vector field $X \in \mathbb{W}$ is a pair of functions $X = (X^q, X^p) \in C^\infty(\mathbb{M}, \mathbb{CF}) \times C^\infty(\mathbb{M}, \mathbb{CF}^*)$; its value at the state (q,p) is $X(q,p) = (X^q(q,p), X^p(q,p))$. Associated with each vector field X is the derivation Xd defined by

$$Xdf := X^q \cdot \partial_q f + X^p \cdot \partial_p f.$$

Using the mapping d defined in this way, it is easily checked that we have a commutative differential geometry. In particular, a general linear form ζ is described by a pair of functions $(\zeta_q, \zeta_p) \in C^\infty(\mathbb{M}, \mathbb{CF}^*) \times C^\infty(\mathbb{M}, \mathbb{CF})$ such that

$$X\zeta = X^q \cdot \zeta_q + X^p \cdot \zeta_p. \tag{18.13}$$

18.2.1 Theorem. *Let $\theta = (p, 0)$ be the linear form defined by*

$$(X\theta)(q,p) := X^q(q,p) \cdot p \ . \tag{18.14}$$

Then $\omega = -d\theta = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ is an exact symplectic form satisfying

$$(YX\omega)(q,p) := X^q(q,p) \cdot Y^p(q,p) - Y^q(q,p) \cdot X^p(q,p) \tag{18.15}$$

for arbitrary vector fields X, Y. Its inverse satisfies

$$X = \zeta\omega^{-1} \quad \Leftrightarrow \quad X^q = \zeta_p, \quad X^p = -\zeta_q. \tag{18.16}$$

for arbitrary linear forms ζ. With the Lie product

$$f\angle g := df\omega^{-1}dg = \partial_p f \cdot \partial_q g - \partial_p g \cdot \partial_q f, \tag{18.17}$$

the algebra $\mathbb{E} = C^\infty(\mathbb{M})$ of scalar fields on phase space $\mathbb{M}$ is a Poisson algebra. $\angle$, ω, and θ are called the ***canonical Lie product****, the* ***canonical symplectic form****, and the* ***canonical linear form***[1] *on phase space $\mathbb{M}$.*

[1] In the notation using components and the Einstein summation convention, we have $\theta = p_j dq^j$ and $\omega = dq^j \wedge dp_j$. Here the linear forms dq^j and dp_j, given by $Xdq^j := (X^q)^j$ and $Xdp_j := (X^p)_j$, are the gradients of the functions q^j and p_j mapping a general state (q,p) to the indicated components.

Proof. ω is an exact 2-form since $\omega = d(-\theta)$. To prove (18.15), we use (18.8) to work out $(YX\omega)(q,p) = Yd(X\theta) - Xd(Y\theta) + (X\angle Y)\theta = Yd(X^q p) - Xd(Y^q p) + (X\angle Y)^q p = Y^q\partial_q(X^q p) + Y^p\partial_p(X^q p) - X^q\partial_q(Y^q p) - X^p\partial_p(Y^q p) + (X\angle Y)^q p$. Using $(X\angle Y)^q = X\partial Y^q - Y\partial X^q = X_q\partial_q Y^q + X_p\partial_p Y^q - Y_q\partial_q X^q - Y_p\partial_p X^q$, which follows from (17.4), the product rule, and $\partial_p p = 1$, everything cancels except for $Y^p X^q - X^p Y^q$. This proves (18.15). By comparing (18.13) with (18.15), we see that

$$\zeta = X\omega \quad \Leftrightarrow \quad \zeta_q = -X^p, \;\; \zeta_p = X^q. \tag{18.18}$$

Thus ω maps $X = (X^q, X^p)$ to $(-X^p, X^q)$, corresponding to right multiplication by the matrix $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. Since the equations (18.18) are uniquely solvable for X by (18.16), we conclude that ω is nondegenerate, hence symplectic.

Since every exact 2-form is closed, Theorem 18.1.3 applies and gives the final assertion. □

Using the chain rule, the dynamics (18.11) is easily seen to be equivalent to the **Hamilton equations** in **general form**,

$$\dot f = \frac{df}{dt} = H\angle f; \tag{18.19}$$

cf. Chapter 5.2.

18.3 Constrained Hamiltonian dynamics

In the constrained case, additional parameters (e.g., Lagrange multipliers) are needed to describe the possible states of the system. Therefore we take $\mathbb{E} = C^\infty(\mathbb{M}\times\mathbb{U})$ and $\mathbb{W} = C^\infty(\mathbb{M}\times\mathbb{U}, \mathbb{CF}\times\mathbb{CF}^*\times\mathbb{CU})$, the spaces of scalar fields and vector fields, respectively, on an **augmented cotangent bundle** $\mathbb{M}\times\mathbb{U}$ of $\mathbb{M}_c$, where, as before, the phase space is $\mathbb{M} = \mathbb{M}_c\times\mathbb{F}$, and $\mathbb{U}$ is a convenient vector space.

A classical, conservative, **constrained mechanical system** is again defined by a **Hamiltonian** $H\in\mathbb{E}$. The point $x = (q,p,u)\in\mathbb{M}\times\mathbb{U}$ is called the **state** with **position** $q\in\mathbb{M}_c$, **momentum** $p\in\mathbb{F}$, and **parameter** $u\in\mathbb{U}$; however, due to the constraints derived below from H, not all points in $\mathbb{M}\times\mathbb{U}$ are physical. As we shall see, the accessible phase space may also be smaller than $\mathbb{M}$. The **energy** of the system in the state (q,p,u) is the value $H(q,p,u)$ of the Hamiltonian at (q,p,u).

The state of the system again varies with time $t\in[\underline{t},\overline{t}]$. The time dependence is modeled by a **trajectory**, a state-valued, arbitrarily often differentiable function of time, now defining position $q(t)$, momentum $p(t)$, and parameter $u(t)$ at time t. These are constrained by the **extended Hamiltonian equations**,

$$\dot q = \frac{dq}{dt} = \partial_p H, \quad \dot p = \frac{dp}{dt} = -\partial_q H, \quad 0 = \partial_u H. \tag{18.20}$$

Here $\partial_u = \partial/\partial u$ denotes the gradient operator with respect to the parameter u. Thus, in place of a system of ordinary differential equations in the unconstrained case we now have a system of **differential-algebraic equations** (**DAE**) involving the **holonomic constraints**

$$0 = \partial_u H(q, p, u). \tag{18.21}$$

Again the extended Hamiltonian equations automatically imply the **conservation of energy**: $\frac{d}{dt}H(q, p, u) = \partial_q H \cdot \dot{q} + \partial_p H \cdot \dot{p} + \partial_u H \cdot \dot{u} = 0$.

The case where the symmetric **Hessian matrix**

$$G := \partial_u^2 H(q, p, u)$$

is invertible is referred to as the **regular** case. Then, by the implicit function theorem, (18.21) can be solved locally uniquely for $u = u(q, p)$, which implies that (18.20) may be viewed as an ordinary differential equation in q and p alone. In the **singular** case where the Hessian G is not invertible, the constraints imply restrictions on p. Thus, not the whole phase space is dynamically accessible, and the analysis of solvability of the DAE is more involved. The details depend on the so-called **index** of a DAE, index 1 corresponding to the regular case, index > 1 to the singular case, and are beyond our treatment.

18.3.1 Example. We consider the constrained Hamiltonian system with $\mathbb{F} = \mathbb{R}^3$ and $\mathbb{U} = \mathbb{R}$, defined by the Hamiltonian

$$H(\mathbf{q}, \mathbf{p}, u) := \frac{1}{2}\mathbf{p}^2 + V(\mathbf{k} \times \mathbf{q}) - (\mathbf{k} \cdot \mathbf{p})u,$$

where $V(\mathbf{E})$ is a potential energy function. The special case $V(\mathbf{E}) := \frac{1}{2}\mathbf{E}^2$, describes the dynamics of a single Fourier mode with wave vector $\mathbf{k}$ of the free electromagnetic field. A straightforward calculation gives the dynamics

$$\dot{\mathbf{q}} = \mathbf{p} - \mathbf{k}u, \quad \dot{\mathbf{p}} = \mathbf{k} \times \nabla V(\mathbf{k} \times \mathbf{q}), \quad 0 = \mathbf{k} \cdot \mathbf{p}.$$

Since $G = \partial_u^2 H = 0$, this is a singular case. Indeed, the dynamically relevant part of the phase space is characterized by the **transversality condition** $0 = \mathbf{k} \cdot \mathbf{p}$, whereas the multiplier u is completely undetermined by the dynamics. This implies that the dynamics of q is determined only up to an arbitrary multiple of $\mathbf{k}$; in other words, only $\mathbf{k} \times \mathbf{q}$ is determined at all times by the initial conditions.

Note that $H \angle \mathbf{k} \cdot \mathbf{p} = \mathbf{k} \cdot (H \angle \mathbf{p}) = \mathbf{k} \cdot \mathbf{p} = 0$, hence the constraint $0 = \mathbf{k} \cdot \mathbf{p}$ is automatically satisfied at all times if it is satisfied at some time. Thus, in the terminology of constrained mechanics, it is called a **first class constraint**, and gives rise to **gauge symmetries**. A **gauge transform** replaces $\mathbf{q}$ by $\mathbf{q} + \mathbf{k}s(\mathbf{q})$ with an arbitrary scalar field $s(\mathbf{q})$, and leaves everything of dynamical interest invariant. The **gauge invariant** quantities are those in the centralizer $C(\mathbf{k} \cdot \mathbf{p})$ of the constraint. f belongs to the centralizer iff it Lie commutes with $\mathbf{k} \cdot \mathbf{p}$, which is the case iff $\mathbf{k} \cdot \partial_q f = 0$, hence iff f depends only on p and $\mathbf{k} \times \mathbf{q}$. Thus, the centralizer consists of all smooth functions of

$$\mathbf{B} := \mathbf{k} \times \mathbf{q}, \quad \mathbf{E} := -\mathbf{p},$$

and the dynamics of the gauge invariant quantities is determined by

$$\dot{\mathbf{B}} = -\mathbf{k} \times \mathbf{E}, \quad \dot{\mathbf{E}} = \mathbf{k} \times \nabla V(\mathbf{B}), \quad 0 = \mathbf{k} \cdot \mathbf{E}. \tag{18.22}$$

The extended Hamiltonian equations may also be derived from a variational principle. Now the **action** is defined on smooth paths in $\mathbb{M} \times \mathbb{U}$,

$$I(q,p,u) := \int_{\underline{t}}^{\overline{t}} dt \, \Big(p(t) \cdot \dot{q}(t) - H(q(t),p(t),u(t)) \Big). \tag{18.23}$$

Variations of the arguments show as before that the path (q,p,u) is a stationary point of the action if and only if the extended Hamiltonian equations (18.20) hold; the constraint equations derive from

$$I(q,p,u+\delta u) - I(q,p,u) \approx \int_{\underline{t}}^{\overline{t}} dt \, \Big(- \partial_u H(q(t),p(t),u(t)) \cdot \delta u \Big).$$

A vector field $X \in \mathbb{W}$ is now a triple of functions

$$X = (X^q, X^p, X^u) \in C^\infty(\mathbb{M}, \mathbb{CF}) \times C^\infty(\mathbb{M}, \mathbb{CF}^*) \times C^\infty(\mathbb{M}, \mathbb{CU});$$

its value at the state (q,p,u) is $X(q,p,u) = (X^q(q,p,u), X^p(q,p,u), X^u(q,p,u))$. Associated with each vector field X is the derivation Xd defined by

$$Xdf := X^q \cdot \partial_q f + X^p \cdot \partial_p f + X^u \cdot \partial_u f.$$

It is again easy to check that this defines a commutative differential geometry. In particular, a general linear form ζ is described by a triple of functions $(\zeta_q, \zeta_p, \zeta_u) \in C^\infty(\mathbb{M}, \mathbb{CF}^*) \times C^\infty(\mathbb{M}, \mathbb{CF}^*) \times C^\infty(\mathbb{M}, \mathbb{CU})$ such that

$$X\zeta = X^q \cdot \zeta_q + X^p \cdot \zeta_p + X^u \cdot \zeta_u. \tag{18.24}$$

In analogy to the unconstrained case, we define the linear form θ by

$$(X\theta)(q,p,u) := X^q(q,p,u) \cdot p \ .$$

Thus $\theta = (p,0,0)$ and a similar calculation as before gives the exact 2-form

$$\omega := -d\theta = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

and

$$(YX\omega)(q,p,u) := X^q(q,p,u) \cdot Y^p(q,p,u) - Y^q(q,p,u) \cdot X^p(q,p,u).$$

Since no differentiation by the parameters u is involved, the 2-form ω is now degenerate and hence no longer symplectic. As a result, $\mathbb{E}(\omega)$ is strictly smaller than $\mathbb{E}$; a scalar field f is found to be compatible with ω and hence in $\mathbb{E}(\omega)$ only if $\partial_u f = 0$, i.e., f is independent of u. Thus $\mathbb{E}(\omega) = C^\infty(\mathbb{M})$ is again the Poisson algebra of scalar fields on phase space, with Lie product (18.17).

The Hamilton equations (18.19) remain valid, too; note that by the general theory, $H \angle f \in \mathbb{E}(\omega)$, although H depends on u.

If the Hamiltonian $H(q,p,u) = H(q,p)$ is independent of u, everything reduces to what we said about unconstrained Hamiltonian mechanics. Constrained Hamiltonian mechanics with unconstrained Hamiltonian $H_0(q,p)$ and u-independent holonomic constraints $C(q,p) = 0$ are obtained by introducing a vector u of Lagrange multipliers for the constraints and defining $H(q,p,u) = H_0(q,p) + C(q,p) \cdot u$. Note that $\partial_u H(q,p,u) = C(q,p)$ simply recovers the holonomic constraints. Thus, we see that the components of u which occur only linearly in H behave as multipliers of u-independent holonomic constraints.

Note that there is another class of models for conservative Hamiltonian dynamics, defined by so-called **nonholonomic constraints**. There the constrained dynamics is not given by (18.20) but instead by

$$\dot{q} = \frac{dq}{dt} = \partial_p H(q,p), \quad \dot{p} = \frac{dp}{dt} = -\partial_q H(q,p) + A(q)u, \quad 0 = \partial_p H(q,p) \cdot A(q),$$

where $A(q)$ maps a multiplier vector $u \in \mathbb{U}$ to an element from $\mathbb{F}$, and the Hamiltonian H again defines the energy. The energy is conserved since $\frac{d}{dt}H(q,p) = \partial_q H(q,p) \cdot \dot{q} + \partial_p H(q,p) \cdot \dot{p} = \partial_p H(q,p) \cdot A(q)u = 0$. However, now the dynamics can usually no longer be written in terms of a variational principle. Only the special **integrable** case where $A(q) = \partial_q C(q)$ corresponds to holonomic constraints of the form $C(q) = 0$ and a modified Hamiltonian $\widetilde{H}(q,p,u) := H(q,p) - C(q) \cdot u$, which agrees on the space of trajectories with H. The most general conservative Hamiltonian system may have both holonomic and nonholonomic constraints; the reader may wish to write down the defining equations and generalize the above discussion accordingly.

18.4 Lagrangian mechanics

Frequently, and especially in relativistic field theory, a classical system is defined in terms of the Lagrangian approach to mechanics. We consider here the **autonomous** case only, where the Lagrangian is time-independent.

The basic object is now a **Lagrangian** $L \in \mathbf{C}^\infty(T\mathbb{M}_c)$, a function of points in the tangent space $T\mathbb{M}_c$ of a configuration manifold $\mathbb{M}_c$. As in the Hamiltonian case, we restrict our attention to the case where $\mathbb{M}_c$ is a nonempty, open subset of a convenient vector space $\mathbb{F}$ over $\mathbb{R}$. Then the tangent space is $T\mathbb{M}_c = \mathbb{M}_c \times \mathbb{F}$, points in $T\mathbb{M}_c$ are pairs (q,v) consisting of a configuration point $q \in \mathbb{M}_c$ and a tangent vector $v \in \mathbb{F}$ at q, referred to as **velocity**, and the Lagrangian is a function with function values $L(q,v)$.

The Lagrangian approach to mechanics can be represented in the framework of constrained Hamiltonian dynamics by taking $\mathbb{U} = \mathbb{F}$, and $u = v$. Then the choice

$$H(q,p,v) := up - L(q,v) \tag{18.25}$$

for the Hamiltonian gives unconstrained Lagrangian mechanics. Constrained Lagrangian mechanics with holonomic constraints $C(q,v) = 0$ is similarly obtained by taking $\mathbb{U} = \mathbb{F} \times \mathbb{U}_0$

and $u = (v, u_0)$ and $H(q, p, v, u_0) = pv - L(q, v) + u_0^T C(q, v)$, where u_0 is a Lagrange multiplier. However, in the following, we only discuss the unconstrained Lagrangian case.

Applying the general machinery of Section 18.3 to (18.25), we find as dynamical equations the **Euler-Lagrange equations**

$$\dot{q} = v, \quad \dot{p} = \partial_q L(q, v), \quad p = \partial_v L(q, v); \tag{18.26}$$

and the action (18.12) reduces on the submanifold defined by $\dot{q} = v$ to

$$I(q) := \int_{\underline{t}}^{\overline{t}} dt\ L(q(t), \dot{q}(t)). \tag{18.27}$$

The Hamiltonian (18.25) is time invariant since

$$(p \cdot \dot{q})^\bullet = \dot{p} \cdot \dot{q} + p \cdot \ddot{q} = L_q \cdot \dot{q} + L\dot{q} \cdot \ddot{q} = L(q, \dot{q})^\bullet = \dot{L}.$$

It is easily verified directly that the condition for $I(q)$ to be stationary at the path q gives again the Euler-Lagrange equations (18.26); this is usually taken as the starting point of the Lagrangian approach.

18.4.1 Example. The Lagrangian $L(q, v) = \frac{1}{2}mv^2 - \frac{1}{2}kq^2$ defines the harmonic oscillator, as can be seen by writing down the Euler-Lagrange equations. Note that the action need not be bounded below, as can be seen from the path $q(t) = s(1-t^2)$ in $[\underline{t}, \overline{t}] = [-1, 1]$, where $I(q) = (4m - \frac{8}{15}k)s^2$ diverges to $-\infty$ when $k > 7.5m$ and $s \to \infty$. Thus, it is inappropriate to refer to the stationary action principle as principle of least action, as often done for historical reasons.

If we change a Lagrangian $L(q, v)$ to

$$\widetilde{L}(q, v) := L(q, v) + v\dot{\partial}_q \phi(q)$$

for some smooth function ϕ, the action $I(q)$ remains unchanged apart from a boundary term arising through integration by parts. As a result, the new equations of motions and the old ones are equivalent. On the other hand, the momentum changes from p to $\widetilde{p} = p + \partial_q \phi(q)$. This does not affect the equation of motion in the form (18.19) since the transformation from p to $\tilde{p}$ is a canonical transformation leaving the Lie product invariant. Indeed, it is not difficult to see that the more general substitution of $p' = p + \chi(q)$ for p preserves the Lie product iff the Jacobian $\partial_q \chi(q)$ is a symmetric matrix. Necessity follows since for constants $a, b \in \mathbb{F}$,

$$a \cdot p' \angle b \cdot p' = a \cdot \chi(q) b - b \cdot \chi(q) a$$

must vanish, and sufficiency can be established by a more involved computation.

We may work directly in the tangent manifold and define the linear form

$$\theta_L = p = \partial_{\dot{q}} L,$$

$$\theta_L(X) := Xp, \tag{18.28}$$

and the canonical 2-form

$$\omega_L = -d\theta_L.$$

Then $d\omega_L = -ddp = 0$ implies that ω_L is closed, and hence Theorem 18.1.3 applies. If ω_L is non-degenerate, we can solve for $\dot{q}$ in terms of p, q and get the Hamiltonian picture in the traditional way. The Poisson algebra becomes the standard Poisson algebra on the cotangent bundle. If ω_L is degenerate, we cannot solve for $\dot{q}$ and compatibility restricts the space $\mathbb{E}(\omega_L)$ of quantities.

$$p = L_{\dot{q}} \in \mathbb{E} \otimes \mathbb{CF}$$

is the **canonical momentum**.

On $\mathbb{E} = C^\infty(T\mathbb{M})$, any Lagrangian $L = L(q, \dot{q})$ defines a Lie product on $\mathbb{E}(\omega_L)$ which induces the Euler-Lagrange dynamics defined by the action $I = \int dtL$.

We rearrange the canonical 2-form as

$$\omega_L = dq \wedge dp = dq \wedge (p_q dq + p_{\dot{q}} d\dot{q}).$$

The condition for $f \in \mathbb{E}(\omega_L)$ to be compatible with ω requires the existence of a Hamiltonian vector field X_f with

$$\frac{\partial f}{\partial \dot{q}} = G dq(X_f), \quad \frac{\partial f}{\partial q} = -G d\dot{q}(X_f), \tag{18.29}$$

with the symmetric **Hessian matrix**

$$G := \partial_q^2 L = \partial_q \partial_v L = \frac{\partial p}{\partial \dot{q}} \tag{18.30}$$

Case 1. In the *regular* case, i.e., if the Hessian matrix is invertible, we can solve the constraint equation $p = \partial_v L$ at least locally for v, getting an equation $\dot{q} = v(q, p)$. In this case, we find from (18.29) that

$$f \angle g = \frac{\partial f}{\partial q} \cdot G^{-1} \frac{\partial g}{\partial \dot{q}} - \frac{\partial g}{\partial q} \cdot G^{-1} \frac{\partial f}{\partial \dot{q}}, \tag{18.31}$$

where f, g are functions of q and $\dot{q}$. Note that

$$L_v(q, v(q, p)) = p,$$

and

$$H(q, p) = pv(q, p) - L(q, v(q, p))$$

has derivatives

$$H_p = v(q, p) + pv_p(q, p) - L_v(q, v(q, p))v_p(q, p) = v(q, p) = \dot{q},$$

$$H_q = pv_q(q, p) - L_q(q, v(q, p)) - L_v(q, v(q, p))v_q(q, p) = -L_q(q, \dot{q}) = -\dot{p},$$

so that

$$\frac{d}{dt} f(q, p) = f_p \dot{p} + f_q \dot{q} = -f_p H_q + f_q H_p = H \angle f,$$

with the canonical Lie product on phase space.

Since $H = (p|\dot{q}) - L$, we have for solutions q

$$\frac{\partial H}{\partial \dot{q}} = \Big(\frac{\partial p}{\partial \dot{q}}\Big|\dot{q}\Big) + p - L_{\dot{q}} = \frac{\partial p}{\partial \dot{q}}\dot{q},$$

$$\begin{aligned}\frac{\partial H}{\partial q} &= \Big(\frac{\partial p}{\partial q}\Big|\dot{q}\Big) - \frac{\partial L}{\partial q} = \Big(\frac{\partial p}{\partial q}\Big|\dot{q}\Big) - \dot{p} \\ &= \Big(\frac{\partial p}{\partial q}\Big|\dot{q}\Big) - \Big(\Big(\frac{\partial p}{\partial q}\Big|\dot{q}\Big) + \Big(\frac{\partial p}{\partial \dot{q}}\Big|\ddot{q}\Big)\Big) = -\Big(\frac{\partial p}{\partial \dot{q}}\Big|\ddot{q}\Big).\end{aligned}$$

Hence

$$X_H = \Big(\frac{d}{dt}q\Big|\partial_q\Big) + \Big(\frac{d}{dt}\dot{q}\Big|\partial_{\dot{q}}\Big)$$

and

$$H\angle g = dg(X_H) = \Big(\frac{\partial g}{\partial q}\Big|\dot{q}\Big) + \Big(\frac{\partial g}{\partial \dot{q}}\Big|\ddot{q}\Big) = (g(q,\dot{q}))^{\bullet} = \dot{g},$$

so that H generates the dynamics.

Case 2. In the *singular* case, i.e., when the Hessian matrix (18.30) is not invertible, condition (18.1) is nontrivial, not all $f(q,\dot{q})$ are compatible with ω and hence in the Poisson algebra. Then (18.31) only holds for the generalized inverse and (18.29) requires that the partial derivatives are in the range of G. The Poisson manifold (or orbifold?) is the set of orbits of the gauge group; cf. M/R p. 325. Restrict $\mathbb{E}$ accordingly, as in the symplectic case:]

The resulting Lie product (cf. (18.4)) is

$$f\angle g = dg(X_f) = \frac{\partial g}{\partial q}dq(X_f) + \frac{\partial g}{\partial \dot{q}}d\dot{q}(X_f). \tag{18.32}$$

Note that the standard treatment in terms of symplectic manifolds requires regularity. In the singular case, complicated additional assumptions and arguments are needed to bring theories with gauge symmetries (which are always singular) into the framework of symplectic geometry.

Chapter 19

Hamiltonian quantum mechanics

In this chapter, Hamiltonian quantum mechanics is described in differential geometric, classical terms. In particular, this enables one to formulate dynamics for mixed quantum-classical systems in which – as in the Born-Oppenheimer approximation in quantum chemistry – slow degrees of freedom are modelled classically, while the fast motion (typically of electrons) is modelled by quantum mechanics.

Also discussed is the relation between classical mechanics and quantum mechanics in terms of quantization procedures.

19.1 Quantum dynamics as symplectic motion

As a particular case of dynamics in the Poisson algebra of a symplectic form we discuss here the dynamics of wave functions and expectations in quantum mechanics.

We consider the special case of the unconstrained setting of Section 18.2 where $\mathbb{M}_c = \mathbb{F}$. Then $\mathbb{H} = \mathbb{C}\mathbb{F} \cong \mathbb{M}$ is a complex Euclidean space in which we may do quantum mechanics. The isomorphism between $\mathbb{H}$ and $\mathbb{M}$ as real vector spaces is made explicit by writing

$$\psi = q + \iota p \in \mathbb{C}\mathbb{F}, \tag{19.1}$$

where

$$\iota := \frac{i}{\hbar}. \tag{19.2}$$

Then

$$\overline{\psi} = q - \iota p, \tag{19.3}$$

and the Hermitian inner product in $\mathbb{H}$ is

$$\phi^* \psi = \overline{\phi} \cdot \psi. \tag{19.4}$$

We may regard arbitrary smooth functions of ψ and $\overline{\psi}$ as functions of q and p by writing (with slight abuse of notation)

$$f(\psi, \overline{\psi}) = f(q + \iota p, q - \iota p). \tag{19.5}$$

The chain rule then implies the relations

$$\partial_\psi + \partial_{\overline{\psi}} = \partial_q, \tag{19.6}$$

$$\iota(\partial_\psi - \partial_{\overline{\psi}}) = \partial_p \tag{19.7}$$

for the partial derivatives. Using these, it is an easy matter to rewrite the Lie product (18.17) in the form

$$f \angle g = \iota(f_\psi \cdot g_{\overline{\psi}} - g_\psi \cdot f_{\overline{\psi}}). \tag{19.8}$$

Now we consider the classical Hamiltonian

$$H_c(\psi, \overline{\psi}) := \psi^* H \psi,$$

where $H \in \operatorname{Lin} \mathbb{H}$ is a quantum Hamiltonian. Then we find

$$\dot{\psi} = H_c \angle \psi = -\iota H \psi, \tag{19.9}$$

giving the **Schrödinger equation**

$$i\hbar \dot{\psi} = H\psi \tag{19.10}$$

as classical Hamiltonian equation of motion for the state vector $\psi \in \mathbb{H}$. Thus, quantum mechanics may be discussed in a classical framework. The variational principle for classical Hamiltonian systems discussed in the context of (18.12), rewritten for the present situation, is called the **Dirac-Frenkel variational principle**. It was first used by Dirac [73] and Frenkel [92], and found numerous applications; a geometric treatment is given in Kramer & Saraceno [157]. The action takes the form

$$I(\psi, \overline{\psi}) := \int_{\underline{t}}^{\overline{t}} dt \; \psi^*(t) \Big(i\hbar \frac{d}{dt} - H) \Big) \psi(t); \tag{19.11}$$

setting its variation to zero indeed recovers (19.10). The Dirac-Frenkel variational principle plays an important role in approximation schemes for the dynamics of quantum systems. In many cases, a viable approximation is obtained by restricting the state vectors $\psi(t)$ to a linear or nonlinear manifold of easily manageable states $|z\rangle$ (for example **coherent states**) parameterized by classical parameters z which can often be given a physical meaning. Inserting the ansatz $\psi(t) = |z(t)\rangle$ into the action (19.11) gives an action for the path $z(t)$, and the variational principle for this action defines an approximate classical Lagrangian (and hence conservative) dynamics for the parameter vector $z(t)$. Thus, the Dirac-Frenkel variational principle fits in naturally with the interpretation in Section 10.4 of the parameter vectors characterizing a state as the natural observables. An important application of this situation are the **time-dependent Hartree-Fock equations** which are at the heart of dynamical simulations in quantum chemistry.

We note that $\psi^*\psi$ is a constant of the motion, hence we may restrict the dynamics (19.10) to **normalized state vectors** ψ satisfying $\psi^*\psi = 1$. In this case, we may interpret the function $A_c \in \mathbb{E}$ defined for $A \in \operatorname{Lin} \mathbb{H}$ by

$$A_c(\psi, \overline{\psi}) := \psi^* A \psi = \langle A \rangle$$

as the classical **value** of the quantity A in the pure state defined by the normalized state vector ψ, or, equivalently, by the rank one density matrix

$$\rho = \psi\psi^*. \tag{19.12}$$

The Lie product of two values is again a value, since one easily calculates

$$\langle A\rangle\angle\langle B\rangle = \langle \iota[A,B]\rangle = \langle A\angle B\rangle, \tag{19.13}$$

where the Lie product on the right hand side is the quantum bracket. In particular, the dynamics of the values is given by the **Ehrenfest equation**

$$\frac{d}{dt}\langle A\rangle = \langle H\rangle\angle\langle A\rangle = \langle H\angle A\rangle = \frac{i}{\hbar}\langle [H,A]\rangle. \tag{19.14}$$

In the special case, where $H = T(p) + V(q)$ is expressible as a sum of a kinetic energy operator $T(p)$ depending on a momentum vector p and of a potential energy operator $V(q)$ depending on a position vector q, whose components are operators satisfying the traditional **canonical commutation rules**

$$q_j\angle q_k = p_j\angle p_k = 0, \quad p_j\angle q_k = \delta_{jk},$$

the special cases of the Ehrenfest equation,

$$\frac{d}{dt}\langle q\rangle = \langle \partial_p H(q,p)\rangle = \langle \partial_p T(p)\rangle, \quad \frac{d}{dt}\langle p\rangle = -\langle \partial_q H(q,p)\rangle = -\langle \partial_q V(q)\rangle,$$

often called the **Ehrenfest theorem**, are due to Ehrenfest [78]. The Ehrenfest equation, here derived in the Schrödinger picture, is valid also in the Heisenberg picture (or even more general interaction pictures); the dynamical objects of physical interest are neither the states nor the quantities, but the values. We may also compute the dynamics of the density matrix (19.12), and find the **Liouville equation**

$$i\hbar\dot\rho = [H(p,q),\rho]. \tag{19.15}$$

More generally, it is not difficult to check that taking (19.13) as a definition of the Lie product of values in arbitrary states (not necessarily pure states as in the above derivation) indeed turns the family of $\langle A\rangle$ with $\langle\cdot\rangle$ ranging over states defined by

$$\langle A\rangle = \operatorname{tr}\rho A \tag{19.16}$$

for some strongly integrable density matrix ρ and A ranging over the elements of $\operatorname{Lin}\mathbb{H}$ into a Lie algebra. Therefore, the Ehrenfest equation is valid for arbitrary states, not only for pure states. By inserting (19.16) into the Ehrenfest equation and comparing coefficients, one also sees that the Liouville equation (19.15) remains valid.

19.2 Quantum-classical dynamics

There are many systems of practical interest which are treated in a hybrid quantum-classical fashion. The most important example is the Born-Oppenheimer approximation, where

nuclei are treated classically, while electrons remain quantized. Another truly quantum-classical system is a quantum Boltzmann equation with spin; here the spin is still an operator, represented by 4×4 matrices parameterized by classical phase space variables. On the other hand, the quantum-Boltzmann equation for spin zero is already a purely classical equation, since its dynamical variables are all commuting.

In the Liouville picture, where the density matrices are the dynamical variables, the basic equations for a large class of quantum-classical models are the **generalized Liouville equation**

$$i\hbar\dot{\rho} = [H(p,q), \rho],$$

and the **generalized Hamilton equations**

$$\dot{q} = \operatorname{tr} \rho \partial_p H(p,q),$$

$$\dot{p} = -\operatorname{tr} \rho \partial_q H(p,q).$$

Here $H \in C^\infty(\mathbb{M}, \operatorname{Lin} \mathbb{H})$ is an operator valued function on a classical phase space $\mathbb{M}$. Thus $H(p,q)$ is, for any fixed vectors p, q, a linear operator on some Euclidean space $\mathbb{H}$, the **density matrix** $\rho = \rho(t)$ is a time-dependent trace-class operator on $\mathbb{H}$, and $q = q(t), p = p(t)$ are classical, time-dependent vectors, not quantum objects. The classical quantities are the functions of the values

$$\langle f(p,q) \rangle = \operatorname{tr} \rho f(p,q)$$

where f is a (p,q)-dependent operator on $\mathbb{H}$. Expressed in terms of values, we have

$$\dot{q} = \Big\langle \partial_p H(p,q) \Big\rangle, \quad \dot{p} = -\Big\langle \partial_q H(p,q) \Big\rangle,$$

which looks like the Ehrenfest theorem, except that on the left hand side we have classical variables and no expectations. The equations are conservative equations for the evolution of values (the value $\langle H \rangle$ of the energy is conserved); dissipative systems and stochastic systems can be also modelled, but this is beyond the scope of the present exposition.

The quantum-classical dynamics preserves the rank of the density ρ. In particular, if ρ has the rank 1 form

$$\rho = \psi\psi^* \tag{19.17}$$

at some time, it has at any time the form (19.17) with time-dependent ψ. The fact that ρ has trace 1 translates into the statement that the state vector ψ is normalized to $\psi^*\psi = 1$. One easily checks that the Liouville equation holds iff the state vector psi, determined by (19.17) up to a phase, satisfies the Schrödinger equation

$$i\hbar\dot{\psi} = H(p,q)\psi.$$

In terms of the state vector, values take the familiar form

$$\langle f(p,q) \rangle = \psi^* f(p,q) \psi.$$

The reader is invited to formulate a Hamiltonian description of quantum-classical systems, by starting with a symplectic dynamics in which only a part of the position and momentum variables are complexified into a quantum state vector, and to derive the corresponding

Poisson algebra. Now the Lie product is the tensor product of that of the classical subsystem and that of the quantum subsystem treated as a classical Hamiltonian system. The **Ehrenfest equation** still has the form

$$\frac{d}{dt}\langle A\rangle = \langle H\rangle\angle\langle A\rangle,$$

but the right hand side no longer simplifies to the value of a commutator; instead, one gets a nonlinear dependence on values. Such nonlinearities are common for reduced descriptions coming from a pure quantum theory by coarse graining. Usually, quantum-classical systems are regarded as reduced descriptions, and the same phenomenon occurs. There are plenty of other examples of practical importance, the primary one being the **Schrödinger-Poisson equations** in semiconductor modeling.

19.2.1 Examples. We mention two important examples, molecular quantum chemistry and a spinning electron.

(i) The **Born-Oppenheimer approximation** of the dynamics of molecules, widely used in quantum chemistry, is a typical quantum-classical system of the above kind. The nuclei are described by classical phase space variables, while the electrons are described quantum mechanically by means of a state vector ψ in a Hilbert space of antisymmetrized electron wave functions.

(ii) A **spinning electron**, while having no purely classical description, can be modelled quantum-classically by classical phase space variables p, q and a quantum 4-component spin. Then, with α, β as in the Dirac equation,

$$H(p,q) = \alpha\cdot p + \beta m + eV(q) \tag{19.18}$$

is a 4×4 matrix parameterized by classical 3-vectors $p = p(t)$ and $q = q(t)$, $\rho = \rho(t)$ is a positive semidefinite 4×4 matrix of trace 1, and the trace in the above equation is just the trace of a 4×4 matrix.

One gets the equations from Dirac's equation and Ehrenfest's theorem by an approximation involving coherent states for position and momentum. Note that this is just a toy example. More useful field theoretic quantum-classical versions lead to **Vlasov equations** for (p,q)-dependent 4×4 densities, describing a fluid of independent classical electrons of the form (19.18). With even more realism, one needs to add also a collision term accounting for interactions, resulting in a **quantum Boltzmann equation**; and for even more accurate modeling, (19.18) is no longer adequate but needs additional dissipative terms.

The quantum-classical dynamics, given in the Schrödinger picture, can also be written in the Heisenberg picture. The equivalent Heisenberg dynamics is

$$\frac{d}{dt}f = \partial_q f\langle\partial_p H\rangle - \partial_p f\langle\partial_q H\rangle + \frac{i}{\hbar}[H,f]$$

where now $\langle\bullet\rangle$ is the fixed Heisenberg state. From this, one can immediately see that everything depends only on values by applying $\langle\bullet\rangle$ to this equation:

$$\frac{d}{dt}\langle f\rangle = \langle\partial_q f\rangle\langle\partial_p H\rangle - \langle\partial_p f\rangle\langle\partial_q H\rangle + \langle\frac{i}{\hbar}[H,f]\rangle.$$

This is now a fully classical equation for classical values of the quantum-classical hybrid model considered.

In the interpretation given in Chapter 10, densities are irreducible objects describing a single quantum system, not stochastic entities that make sense only under repetition. (This is analogous to the way phase space densities appear in the Boltzmann equation, though the analogy is not very deep.)

In general, values in the quantum-classical dynamics are to be interpreted as objects characterizing a single quantum system, in the sense of the consistent experiment interpretation, and not as the result of averaging over many realizations.

By design, in the Heisenberg picture, the state does not take part in the dynamics. What is new, however, compared to pure quantum dynamics is that the Heisenberg state occurs explicitly in the differential equation. In practical applications, the Heisenberg state is fixed by the experimental setting; hence this state dependence of the dynamics is harmless. However, because the dynamics depends on the Heisenberg state, calculating results by splitting a density at time $t = 0$ into a mixture of pure states no longer makes sense. One gets different evolutions of the operators in different pure states, and there is no reason why their combination should at the end give the correct dynamics of the original density. (And indeed, this will usually fail.) This splitting is already artificial in pure quantum mechanics since there is no natural way to tell of which pure states a mixed state is composed of. But there the splitting happens to be valid and useful as a calculational tool since the dynamics in the Heisenberg picture is state independent.

In contrast to the pure quantum case, there is now a difference between averaging results of two experiments ρ_1, ρ_2 and the results of a single experiment ρ given by $(\rho_1 + \rho_2)/2$. That, in ordinary quantum theory, the two are indistinguishable in their statistical properties is a coincidental consequence of the linearity of the Schrödinger equation, and the resulting state independence of the Heisenberg equation; it does no longer hold in effective quantum theories where nonlinearities appear due to a reduced description.

19.3 Deformation quantization

There are many ways to **quantize** a classical system, i.e., to relate to a dynamical description of a classical system a corresponding quantum version. This process is far from unique, but there are a number of well-explored (and only sometimes equivalent) routes for doing this. Whether a particular quantization is useful depends on how well the resulting quantum system describes the intended application – something outside the scope of our discussion.

An important algebraic approach to quantization is **Berezin quantization**, also called the **method of orbits**. Here classical Poisson representations of Lie algebras are lifted to unitary representations. We only hint at the constructions, and refer for details to Berezin

[31], Bar-Moshe & Marinov [22], Landsman [169], and Kirillov [152]. The construction of the Lie–Poisson algebra in Section 12.5 from a Lie $*$-algebra $\mathbb{L}$ implies that the dual of $\mathbb{L}$ becomes in a natural way a Poisson manifold; the corresponding symplectic leaves are the so-called **co-adjoint orbits**, the orbits of the universal covering group corresponding to $\mathbb{L}$ in its co-adjoint action on $\mathbb{L}^*$. The canonical Poisson algebras on the co-adjoint orbits carry an **irreducible Poisson representation** of $\mathbb{L}$, and any irreducible Poisson representation of $\mathbb{L}$ arises in this way (up to equivalence). Thus, classifying the co-adjoint orbits is the classical analogue of classifying irreducible unitary representations. The quantization constructions mentioned above rely on close relations between co-adjoint orbits, coherent states over Lie groups, and irreducible unitary representations. These relations can even be generalized further, replacing the Lie algebra structure by a purely geometric setting, which then leads to the framework of **geometric quantization**, cf. Woodhouse [294].

Another possibility is **deformation quantization** which deforms a commutative product into a so-called **Moyal product**; for definitions and details, see, e.g., Rieffel [235]. Alternatively, deformation quantization may be viewed as a deformation of the quantities in a Poisson algebra $\mathbb{E}$. This is the procedure we shall discuss in more detail.

The deformation can be obtained by embedding $\mathbb{E}$ into the algebra $\operatorname{Lin}\mathbb{E}$, identifying $f \in \mathbb{E}$ with the multiplication mapping M_f which maps g to

$$M_f\{g\} := fg,$$

writing for emphasis the arguments (in $\mathbb{E}$) of operators from $\operatorname{Lin}\mathbb{E}$ (often referred to as **superoperators**, to distinguish them from operators acting on $\mathbb{E}$ itself) in curly braces.

Recall the linear operator $\mathrm{ad}_f \in \operatorname{Lin}\mathbb{E}$ defined by

$$\mathrm{ad}_f\{g\} := f\angle g, \tag{19.19}$$

For $f \in \mathbb{E}$, we define the **quantization** $\widehat{f}$ of f by

$$\widehat{f} := f - \frac{i\hbar}{2}\mathrm{ad}_f \in \operatorname{Lin}\mathbb{E}. \tag{19.20}$$

Note that the quantization preserves nonlinear operations (product and Lie product) only up to terms of formal order $O(\hbar)$. This reflects the ordering ambiguity in traditional quantization procedures.

For an arbitrary Gibbs state on $\operatorname{Lin}\mathbb{E}$, the expectation

$$\langle\widehat{f}\rangle = \langle f\rangle - \frac{i\hbar}{2}\langle\mathrm{ad}_f\rangle$$

differs from those of f by a term of numerical order $O(\hbar)$, justifying an interpretation in terms of deformation.

19.3.1 Proposition. *For f, g in a not necessarily commutative Poisson algebra $\mathbb{E}$,*

$$[\mathrm{ad}_f, g] = [f, \mathrm{ad}_g] = f\angle g, \tag{19.21}$$

$$[\mathrm{ad}_f, \mathrm{ad}_g] = \mathrm{ad}_{f\angle g}. \tag{19.22}$$

$$[\widehat{f}, g] = [f, \widehat{g}] = [f, g] - \frac{i\hbar}{2} f\angle g. \tag{19.23}$$

$$[\widehat{f}, \widehat{g}] = [f, g] - i\hbar f\angle g - \frac{\hbar^2}{4}\mathrm{ad}_{f\angle g}, \tag{19.24}$$

Proof. We have, for all $h \in \mathbb{E}$,

$$\begin{aligned} [\mathrm{ad}_f, g]\{h\} &= \mathrm{ad}_f\{gh\} - g\mathrm{ad}_f\{h\} \\ &= f\angle gh - g(f\angle h) = (f\angle g)h, \end{aligned}$$

hence $[\mathrm{ad}_f, g] = f\angle g$. Therefore, also $[f, \mathrm{ad}_g] = -[\mathrm{ad}_g, f] = -g\angle f = f\angle g$, so that (19.21) holds. Similarly,

$$\begin{aligned} [\mathrm{ad}_f, \mathrm{ad}_g]\{h\} &= \mathrm{ad}_f\{\mathrm{ad}_g\{h\}\} - \mathrm{ad}_g\{\mathrm{ad}_f\{h\}\} \\ &= f\angle(g\angle h) - g\angle(f\angle h) \\ &= (f\angle g)\angle h = \mathrm{ad}_{f\angle g}\{h\} \end{aligned}$$

by (S5), hence (19.22) holds. (19.23) follows from

$$[\widehat{f}, g] = \left[f - \frac{i\hbar}{2}\mathrm{ad}_f, g\right] = [f, g] - \frac{i\hbar}{2}[\mathrm{ad}_f, g] = [f, g] - \frac{i\hbar}{2} f\angle g,$$

and

$$[f, \widehat{g}] = -[\widehat{g}, f] = -[g, f] + \frac{i\hbar}{2} g\angle f = [f, g] - \frac{i\hbar}{2} g\angle f.$$

Finally, since

$$\begin{aligned} [\widehat{f}, \widehat{g}] &= \left[f - \frac{i\hbar}{2}\mathrm{ad}_f, g - \frac{i\hbar}{2}\mathrm{ad}_g\right] \\ &= [f, g] - \frac{i\hbar}{2}[\mathrm{ad}_f, g] - \frac{i\hbar}{2}[f, \mathrm{ad}_g] + \left(\frac{i\hbar}{2}\right)^2 [\mathrm{ad}_f, \mathrm{ad}_g], \end{aligned}$$

(19.24) follows from (19.21) and (19.22). □

To actually quantize a classical theory, one may choose a Lie algebra of relevant quantities generating the Poisson algebra, quantize its elements by the above rule, express the classical action as a suitably ordered polynomial expression in the generators, and use as quantum action this expression with all generators replaced by their quantizations.

In general, the above recipe for phase space quantization gives an approximate Poisson isomorphism, up to $O(\hbar)$ terms.

We now show that, however, Lie subalgebras are mapped into (perhaps slightly bigger) Lie algebras defining an abelian extension , and that one gets a true isomorphism for all embedded Heisenberg Lie algebras and all embedded abelian Lie algebras.

19.3.2 Theorem. ***(Quantization Theorem)***
If $\mathbb{E}$ is commutative then, with

$$M_f\{g\} := fg, \quad Q_f\{g\} := \widehat{f}\{g\} = fg - \frac{i\hbar}{2} f\angle g,$$

the quantum Lie product

$$A\angle B = \iota[A, B] \quad \text{for } A, B \in \operatorname{Lin}\mathbb{E}$$

satisfies, for $f, g \in \mathbb{E}$,

$$Q_f\angle Q_g = M_{f\angle g} - \frac{i\hbar}{4}\mathrm{ad}_{f\angle g} = \frac{1}{2}(M_{f\angle g} + Q_{f\angle g}), \tag{19.25}$$

$$Q_f\angle M_g = M_f\angle Q_g = \frac{1}{2}M_{f\angle g}. \tag{19.26}$$

Any Lie subalgebra $\mathbb{L}$ of $\mathbb{E}$ defines a Lie algebra

$$\widehat{\mathbb{L}} = \{M_{f\angle g} + Q_h \mid f, g, h \in \mathbb{L}\} \tag{19.27}$$

under the quantum Lie product. If $\mathbb{L}$ is an abelian Lie algebra or a Heisenberg Lie algebra then Q is a Lie isomorphism between $\mathbb{L}$ and $\widehat{\mathbb{L}}$.

Proof. Since $\mathbb{E}$ is commutative, the first term in (19.24) and (19.23) vanishes, and multiplication by $\iota = i/\hbar$ gives (19.25) and (19.26). The final statement is immediate from (19.25) and (19.26). □

Note that by the so-called **Groenewold-van Hove Theorem** (Groenewold [113], van Hove [277], Gotay et al. [108]), no quantization procedure can exist which possesses all features desirable from a naive point of view. The present quantization procedure sacrifices the exact preservation of commutation rules.

19.4 The Wigner transform

We now specialize the preceding to the standard symplectic Poisson algebra $\mathbb{E} = C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$. Thus, $\mathbb{E}$ is a commutative Poisson algebra of phase space functions as discussed in Section 18.2. in this very important case, which covers N-particle quantum mechanics, the embedding discussed in Section 19.3 turns out to be equivalent to standard quantization.

The equivalence is given in terms of the so-called Wigner transform. The Wigner transform relates kernels of linear integral operators over $\mathbb{R}^n$ to corresponding phase space functions. It therefore mediates between a quantum (operator) ansd a classical (phase space) description of the same situation, and is heavily used in semiclassical approximations of quantum mechanics. For example (though this is outside the scope of the present book), they turn

the Heisenberg equation of motion for quantum field expectations (combined with certain approximations) into quantum kinetic equations on phase space.

The basic idea is to rewrite a kernel $K(x,y)$ as a function of the mean coordinate $q = (x+y)/2$ and the difference $q' = x - y$, and then Fourier transform with respect to q' to get a function of q and a momentum vector p.

In the present special case, phase space quantization amounts to using the reducible representation

$$\widehat{p} = p - \frac{i\hbar}{2}\partial_q, \quad \widehat{q} = q + \frac{i\hbar}{2}\partial_p$$

of the canonical commutation rules on the Hilbert space of square integrable functions on phase space instead of the traditional irreducible **position representation** by

$$\widetilde{p} = -i\hbar\partial_x, \quad \widetilde{q} = x$$

on the Hilbert space of square integrable functions of configuration space, or of the irreducible **momentum representation** by

$$p' = p, \quad q' = i\hbar\partial_p$$

on the Hilbert space of square integrable functions of momentum space. Since the momentum representation is obtained from the position representation by the simple canonical transformation which interchanges x and p and then writing $q' = -\widetilde{p}$, $p' = \widetilde{q}$, it is enough to discuss in the following the transformation to the position representation.

By quantizing in phase space, one gives up irreducibility (and hence the description of a state by a *unique* density) but gains in simplicity. This may be compared to the situation in gauge theory, where the description by gauge potentials introduces some arbitrariness with which one pays for the more elegant formulation of the field equations but which does not affect the observable consequences.

We now show that these representations are related by a **Wigner transform** (cf. Wigner [292]).

We consider the quantization of the commutative Poisson algebra $\mathbb{E} = C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ with standard Poisson bracket (18.17). Since for $f = f(p,q)$ we have

$$p\angle f = \partial_q f, \quad q\angle f = -\partial_p f, \tag{19.28}$$

the quantization rule amounts to

$$\widehat{p} = p - \frac{i\hbar}{2}\partial_q, \quad \widehat{q} = q + \frac{i\hbar}{2}\partial_p. \tag{19.29}$$

By (19.25),

$$\widehat{p}_\mu \angle \widehat{q}_\nu = p_\mu \angle q_\nu = \delta_{\mu\nu}. \tag{19.30}$$

Thus we have a unitary representation of the Heisenberg algebra $H(n)$ by linear operators on the phase space $\Omega = \mathbb{R}^n \times \mathbb{R}^n$, equipped with the standard inner product. To relate this representation to the traditional position representation given by

$$\widetilde{p} = -i\hbar\partial_x, \quad \widetilde{q} = x, \tag{19.31}$$

we introduce the **Wigner transform**

$$\widetilde{f}(x,y) := \int dp e^{\iota p^T(x-y)} f\Big(p, \frac{x+y}{2}\Big) \tag{19.32}$$

of a function $f \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$.

19.4.1 Theorem. *The Wigner transform has the inverse transform*

$$f(p,q) = h^{-n} \int d\xi e^{-2\iota p^T \xi} \widetilde{f}(q+\xi, q-\xi), \tag{19.33}$$

where

$$h = 2\pi\hbar, \quad n = \dim p = \dim q, \tag{19.34}$$

and satisfies the rules

$$\widetilde{\widehat{p}f} = \widetilde{p}\widetilde{f}, \quad \widetilde{\widehat{q}f} = \widetilde{q}\widetilde{f}. \tag{19.35}$$

Proof. We have

$$\begin{aligned}
\int d\xi e^{-2\iota p^T \xi} \widetilde{f}(q+\xi, q-\xi) &= \int d\xi e^{-2\iota p^T \xi} \int dk e^{2\iota k^T \xi} f(k,q) \\
&= \int dp \Big(\int d\xi e^{2\iota (k-p)^T \xi} \Big) f(k,q) \\
&= \int dp\ h^n \delta(k-p) f(k,q) = h^n f(p,q),
\end{aligned}$$

proving (19.33). (19.35) follows from

$$\begin{aligned}
\widetilde{p}\widetilde{f}(x,y) &= -i\hbar\partial_x \int dp e^{\iota p^T(x-y)} f\Big(p, \frac{x+y}{2}\Big) \\
&= -i\hbar \int dp e^{\iota p^T(x-y)} \Big(\iota p + \frac{1}{2}\partial_q\Big) f\Big(p, \frac{x+y}{2}\Big) \\
&= \int dp e^{\iota p^T(x-y)} (p - \frac{i\hbar}{2}\partial_q) f\Big(p, \frac{x+y}{2}\Big) \\
&= \int dp e^{\iota p^T(x-y)} \widehat{p} f\Big(p, \frac{x+y}{2}\Big) = \widetilde{\widehat{p}f}(x,y)
\end{aligned}$$

and

$$\begin{aligned}
\widetilde{\widehat{q}f}(x,y) &= \int dp e^{\iota p^T(x-y)} \Big(\frac{x+y}{2} + \frac{i\hbar}{2}\partial p\Big) f\Big(p, \frac{x+y}{2}\Big) \\
&= \int dp e^{\iota p^T(x-y)} \Big(\frac{z+y}{2} - \frac{i\hbar}{2}\iota(x-y)\Big) f\Big(p, \frac{x+y}{2}\Big) \\
&= \int dp e^{\iota p^T(x-y)} x f\Big(p, \frac{x+y}{2}\Big) \\
&= x \int dp e^{\iota p^T(x-y)} f\Big(p, \frac{x+y}{2}\Big) = x\widetilde{f}(x,y) = \widetilde{q}\widetilde{f}(x,y).
\end{aligned}$$

□

Thus the Wigner transform provides an isomorphism between the two representations. Note that the phase space representation is highly redundant since the position representation does not act at all on the y-coordinate. The redundancy is apparent from the fact that the algebra generated by $\widehat{p}$ and $\widehat{q}$ is much smaller than $\operatorname{Lin}\mathbb{E}$, and in fact isomorphic (modulo convergence issues) to $\operatorname{Lin} C^\infty(\mathbb{R}^n)$ via the Wigner transform. However, this redundancy is very helpful since it makes the classical limit and the approximation by semiclassical techniques much simpler.

The Wigner transform can be applied to all nonlinear PDEs of Schrödinger or Dirac type. These have the form

$$I(\psi\psi^*)\psi = 0, \quad \psi \in C^\infty(\mathbb{R}^n), \tag{19.36}$$

where I is an operator-valued function of the density matrix

$$\widetilde{\rho} := \psi\psi^* \tag{19.37}$$

and can be rewritten in terms of it as the equation

$$I(\widetilde{\rho})\widetilde{\rho} = 0$$

which after an inverse Wigner transform becomes an equation

$$\bar{I}(\rho)\rho = 0 \tag{19.38}$$

in phase space. However, (19.37) loses the rank 1 condition implicit in (19.36), hence corresponds to a "mixing" of pure states.

19.4.2 Proposition. *The bilinear inner product*

$$(f|g) = \int dpdq\ f(p,q)g(p,q) \tag{19.39}$$

satisfies

$$(f|g) = \left(\frac{2}{h}\right)^n \int dxdy\ \widetilde{f}(x,y)\widetilde{g}(y,x). \tag{19.40}$$

Proof. This follows from

$$\begin{aligned}
\int dxdy\widetilde{f}(x,y)\widetilde{g}(y,x) &= \int dxdy \int dpe^{\iota p^T(x-y)} f\Big(p, \frac{x+y}{2}\Big) \int dke^{\iota k^T(y-x)} g\Big(k, \frac{y+x}{2}\Big) \\
&= \int dpdkdxdye^{\iota(p-k)^T(x-y)} f\Big(p, \frac{x+y}{2}\Big) g\Big(k, \frac{x+y}{2}\Big) \\
&= \int dpdkdqdwe^{\iota(p-k)^T w} f(p,q)g(k,q) \\
&= \int dpdkdq\Big(\frac{h}{2}\Big)^n \delta(p-k) f(p,q)g(k,q) \\
&= \Big(\frac{h}{2}\Big)^n \int dpdq\ f(p,q)g(p,q) = \Big(\frac{h}{2}\Big)^n (f|g).
\end{aligned}$$

□

Under conjugation, we have directly from (19.32),

$$\widetilde{f}^*(x,y) = \overline{\widetilde{f}(y,x)} \quad \Leftrightarrow \quad f^*(p,q) = \overline{f(-p,q)}, \tag{19.41}$$

indicating that the complex combination

$$z = q + ip$$

behaves naturally.

19.4.3 Proposition. *The* ***conditional expectation*** *of an operator $A \in S(\Omega, \mathbb{L})$ at fixed x or k, respectively, defined by*

$$\langle A \rangle_x := \int dk \rho(k,x) A, \quad \langle A \rangle_k := \int dx \rho(k,x) A, \tag{19.42}$$

satisfies

$$\langle A(\mathbf{p}) \rangle_k = A(k) \langle 1 \rangle_k, \qquad \langle A(\mathbf{q}) \rangle_x = A(x) \langle 1 \rangle_x \tag{19.43}$$

and

$$\langle A \rangle := \int dk dx A \rho(k,x) = \int dk \langle A \rangle_x = \int dx \langle A \rangle_k. \tag{19.44}$$

Thus $\mathbf{p}$ *is the momentum operator and* $\mathbf{q}$ *the position operator.*

Proof. The proof is straightforward. □

19.4.4 Theorem. *With the pointwise convolution*

$$(f * g)(p,q) = \int dk f(k,q) g(p-k,q), \tag{19.45}$$

we have for the pointwise product

$$\widetilde{f}\widetilde{g} = \widetilde{f * g}. \tag{19.46}$$

Proof. By (19.33), we have $\widetilde{f}\widetilde{g} = \widetilde{e}$, where

$$\begin{aligned}
h^n e(p,q) &= \int d\xi e^{-2\iota p^T \xi} \widetilde{f}(q+\xi, q-\xi) \widetilde{g}(q+\xi, q-\xi) \\
&= \int d\xi e^{-2\iota p^T \xi} \int dk e^{2\iota k^T \xi} f(k,q) \int dl e^{2\iota l^T \xi} g(l,q) \\
&= \int dk dl \Big(\int d\xi e^{2\iota (k+l-p)^T \xi} \Big) f(k,q) g(l,q) \\
&= \int dk dl \; h^n \delta(k+l-p) f(k,q) g(l,q) \\
&= h^n \int dk \; f(k,q) g(p-k,q) = h^n (f * g)(p,q).
\end{aligned}$$

□

A comparison with (19.35) shows that, formally,

$$p * f = \widehat{p} f, \quad q * f = \widehat{q} f.$$

For a fully localized phase space function, (19.32) implies directly

$$f(p,q) = f(q) \quad \Leftrightarrow \quad \widetilde{f}(x,y) = h^n f(x)\delta(x-y). \tag{19.47}$$

The symbol formulation. To extend the quantization rule to arbitrary smooth functions we need the symbol formulation of $\widehat{p}$ and $\widehat{q}$.

Let $\Omega = \mathbb{R}^m \times \mathbb{R}^m$ the classical phase space, and let

$$j = i\hbar/2. \tag{19.48}$$

19.4.5 Proposition. *For every distribution ρ on Ω,*

$$\rho(k,x) = \int \widehat{\rho}(k+p, x+q) e^{-p\cdot q/j} dp dq, \tag{19.49}$$

where

$$\widehat{\rho}(p,q) = (\pi\hbar)^{-2m} \int \rho(k+p, x+q) e^{k\cdot x/j} dk dx. \tag{19.50}$$

Proof. We use the formula

$$\int f(q) e^{-p\cdot q/j} dp dq = (\pi\hbar)^m f(0), \tag{19.51}$$

and find for $\widehat{\rho}$ defined by (19.50):

$$\begin{aligned}
& \int \widehat{\rho}(k+p, x+q) e^{-p\cdot q/j} dp dq \\
= \; & (\pi\hbar)^{-2m} \int \rho(k'+k+p, x'+x+q) e^{k'\cdot x' - p\cdot q)/j} dk' dx' dp dq \\
= \; & (\pi\hbar)^{-2m} \int \rho(k+p', x+q') e^{p'\cdot q'/j} e^{-p\cdot q'/j} e^{-p'\cdot q/j} dp dq' dq dp' \\
= \; & (\pi\hbar)^{-m} \int \rho(k, x+q') e^{-p\cdot q'/j} dp dq' \\
= \; & \rho(k,x).
\end{aligned}$$

We used the substitution $k' = p' - p,\ x' = q' - q$. □

19.4.6 Proposition. *For every Schwartz function A on phase space Ω, the symbol $A(\mathbf{p},\mathbf{q})$ defined by*

$$A(\mathbf{p},\mathbf{q})\rho(k,x) := \int_\Omega A(k+p,x-q)\widehat{\rho}(k+p,x+q)e^{-p\cdot q/j}dpdq \tag{19.52}$$

is consistent with the interpretation

$$\mathbf{p} = k + j\partial_x, \qquad \mathbf{q} = x - j\partial_k \tag{19.53}$$

when A is a normally ordered polynomial acting on $\rho(k,x)$ where all $\mathbf{p}_\mu$ are to the right of all $\mathbf{q}_\nu$. Moreover, we have the canonical commutation rules (CCR)

$$\iota[\mathbf{p}_\mu,\mathbf{q}_\nu] = \delta_{\mu\nu}. \tag{19.54}$$

Proof. We can rewrite (19.49) as

$$\rho(k,x) = \int \widehat{\rho}(k',x')e^{-(k'-k)\cdot(x'-x)/j}dk'dx',$$

and find inductively for a monomial $\mathbf{q}^\alpha\mathbf{p}^\beta$ (with multiexponents)

$$\begin{aligned}\mathbf{q}^\alpha\mathbf{p}^\beta\rho(k,x) &= \int (k')^\alpha(2x-x')^\beta\widehat{\rho}(k',x')e^{-(k'-k)\cdot(x'-x)/j}dk'dx' \\ &= \int (k+p)^\alpha(x-q)^\beta\widehat{\rho}(k+p,x+q)e^{-p\cdot q/j}dpdq.\end{aligned}$$

Now take linear combinations and limits to find (19.52).

The CCR follow since (with $f_u = \partial f/\partial u$)

$$\begin{aligned}p_\mu q_\nu f &= p_\mu(x_\nu f - jf_{k_\nu}) = k_\mu(x_\nu f - jf_{k_\nu}) + j(x_\nu f - jf_{k_\nu})_{x_\nu} \\ &= k_\mu x_\nu f + j(\delta_{\mu\nu}f + x_\nu f_{x_\mu} - k_\mu f_{k_\nu}) - j^2 f_{k_\nu}x_\mu,\end{aligned}$$

$$\begin{aligned}q_\nu p_\mu f &= q_\nu(k_\mu f + jf_{x_\mu}) = x_\nu(k_\mu f + jf_{x_\mu}) - j(k_\mu f + jf_{x_\mu})k_\nu \\ &= k_\mu x_\nu f + j(-\delta_{\mu\nu}f + x_\nu f_{x_\mu} - k_\mu f_{k_\nu}) - j^2 f_{k_\nu}x_\mu,\end{aligned}$$

hence

$$[p_\mu,q_\nu]f = p_\mu q_\nu f - q_\nu p_\mu f = 2j\delta_{\mu\nu}f = i\hbar\delta_{\mu\nu}f.$$

This also implies (19.53). □

Write $\mathrm{Jm}(f) := \iota(f - f^*)$, so that

$$\mathrm{Jm}(a+jb) := b \quad \text{if } a,b \in \mathbb{E}_0 \text{ are Hermitian.}$$

19.4.7 Proposition. *If*

$$\rho(-k,x) = \overline{\rho(k,x)} \quad \text{for all } (k,x) \in \Omega \tag{19.55}$$

then the dynamics

$$\dot{\rho} = \{H, \rho\}, \tag{19.56}$$

where

$$\{H, \rho\} = \frac{1}{2j}\left(H\rho - (H\rho)^*\right) = \mathrm{Jm}(H\rho) \tag{19.57}$$

leaves the total density $\langle 1 \rangle$ *invariant. Moreover, if for all* A *we have* $\langle A^* A \rangle \geq 0$ *at time* $t = 0$ *then* $\langle A^* A \rangle \geq 0$ *at all times* $t \geq 0$.

19.4.8 Proposition. ***(Classical limit)***

In the limit $j \to 0$,

$$A(\mathbf{p}, \mathbf{q}) = A(k, x) + O(\hbar),$$

and

$$\{H(\mathbf{p}, \mathbf{q}), \rho\}(p, q) = \partial_p H \partial_q \rho - \partial_q H \partial_p \rho + O(\hbar)$$

reduces to the classical Poisson bracket.

Note that

$$\{p, \rho\} = \rho_q, \ \{q, \rho\} = -\rho_p$$

so this is consistent with

$$\dot{\rho} = (\dot{q}\partial_q + \dot{p}\partial_p)\rho = H_p \rho_q - H_q \rho_p$$

from Hamiltonian dynamics.

To get the density in a position representation, write

$$\underline{\rho}(x, x') = \int \widehat{\underline{\rho}}(p, x') e^{p \cdot x / i\hbar} dp$$

where

$$\widehat{\underline{\rho}}(p, x') = (2\pi\hbar)^{-m} \int \underline{\rho}(x, y) e^{-p \cdot x / i\hbar} dx$$

For normal ordered H, we have

$$H(\underline{\mathbf{p}}, \underline{\mathbf{q}}) \underline{\rho}(x, y) = (2\pi\hbar)^{-m} \int H(p, x) \widehat{\underline{\rho}}(p, y) e^{p \cdot x / i\hbar} dp.$$

.

Similarly,

$$\underline{\rho}(k + p, k - p) := \int \rho(k, x) e^{p \cdot x / j} dx,$$
$$\rho(k, x) = (\pi\hbar)^{-m} \int \underline{\rho}(k + p, k - p) e^{-p \cdot x / j} dx$$

defines a CCR isomorphism with the momentum representation.

Note that in the position and momentum representation,

$$\underline{\rho}^*(x, x') = \overline{\underline{\rho}(x', x)}, \quad \underline{\rho}^*(k, k') = \overline{\underline{\rho}(k', k)}$$

while in the phase repesentation,

$$\rho^*(k,x) = \overline{\rho(-k,x)}.$$

This becomes natural in an analytic representation $z = x + ik$.

For numerical calculation, approximate $H \in S(\Omega, \mathbb{E}_0)$ by trigonometric functions (complex exponentials). This gives finite difference formulas. The initial density ρ can be just given, or it can be regularized (using a Husimi function? GM-MP 1.24)

Part VI

Representations and spectroscopy

Chapter 20

Harmonic oscillators and coherent states

Part VI applies the concepts introduced so far to the study of the dominant kinds of elementary motion in a bound system, vibrations of oscillators (described by Poisson representations of the Heisenberg group), rotations of rigid bodies (described by Poisson representations of the rotation group), and their interaction. On the quantum level, quantum oscillators are always bosonic systems, while spinning systems may be bosonic or fermionic depending on whether or not the spin is integral. The analysis of experimental spectra, concentrating on the mathematical contents of the subject, concludes our discussion.

This chapter is a detailed study of harmonic oscillators (bosons, elementary vibrations), both from the classical and the quantum point of view. We introduce raising and lowering operators in the symplectic Poisson algebra, and show that the classical case is the limit $\hbar \to 0$ of the quantum harmonic oscillator.

The representation theory of the single-mode Heisenberg algebra is particularly simple since by the Stone–von Neumann theorem, all unitary representations are equivalent. We find that the quantum spectrum of a harmonic oscillator is discrete and consists of the classical frequency (multiplied by $\hbar$) and its nonnegative integral multiples (overtones, excited states).

We shall work in the representation where the harmonic oscillator Hamiltonian is diagonal, which gives rise to the ladder operators mediating between neighboring eigenstates. We introduce Dirac's bra-ket notation, and deduce the basic properties of the bosonic Fock spaces, first for a single harmonic oscillator and then for a system of finitely many harmonic modes.

We then introduce coherent states, an overcomplete basis representation in which not only the Heisenberg algebra, but the action of the Heisenberg group is explicitly visible. Coherent states are quantum states that behave as classically as possible, thereby making a bridge between the quantum system and classical systems. The coherent state representation is

particularly relevant for the study of quantum optics, but we only indicate its connection to the modes of the electromagnetic field.

20.1 The classical harmonic oscillator

The classical one-dimensional harmonic oscillator without damping, introduced in Section 5.2, is defined by the Hamiltonian

$$H = \frac{p^2}{2m} + V(q)\,, \tag{20.1}$$

where $V(q)$ is quadratic and bounded from below, so that there are constants q_0, V_0 and $k > 0$ with

$$V(q) = V_0 + \frac{k}{2}(q - q_0)^2\,.$$

The number k is called the **stiffness**; the greater the constant k, the more difficult is it to move away from equilibrium. The Hamilton equations are:

$$\dot{q} = \frac{p}{m}\,, \quad \dot{p} = -V'(q) = -k(q - q_0)\,.$$

A complex exponential ansatz shows that the solution of the Hamilton equations is:

$$q(t) = q_0 + 2\,\mathrm{Re}(e^{i\omega t}x)\,, \quad p(t) = \mathrm{Re}(i\omega m e^{i\omega t}x)\,,$$

where x is a complex number depending on the initial conditions, and

$$\omega = \sqrt{\frac{k}{m}},$$

is the **frequency** of the harmonic oscillator. It is convenient to express the variables in terms of a so-called complex **normal mode**, the function $a(t)$ defined by

$$a(t) := \sqrt{\frac{k}{2\omega}}(q(t) - q_0) + i\frac{p(t)}{\sqrt{2m\omega}}\,.$$

One can recover q and p through

$$q(t) = q_0 + \frac{1}{2}\sqrt{\frac{2\omega}{k}}(a(t) + a^*(t))\,, \quad p(t) = \frac{1}{2i}\sqrt{2m\omega}(a(t) - a^*(t))\,, \tag{20.2}$$

hence the description by a normal mode is equivalent to the original description. Differentiating $a(t)$ and using $\dot{q} = p/m$, we obtain

$$\dot{a}(t) = \sqrt{\frac{k}{2\omega}}\frac{p(t)}{m} - \frac{i}{\sqrt{2m\omega}}k(q(t) - q_0) = -i\omega a(t)\,.$$

We conclude that $a(t)$ has to obey

$$a(t) = a(0)e^{i\omega t}\,.$$

We calculate the Lie product of a and a^* and find

$$\begin{aligned} a\angle a^* &= \frac{\partial a}{\partial p}\frac{\partial a^*}{\partial q} - \frac{\partial a^*}{\partial p}\frac{\partial a}{\partial q} \\ &= 2i\sqrt{\frac{k}{2\omega}}\frac{1}{\sqrt{2m\omega}} \\ &= i\,, \end{aligned}$$

that is, we obtain the relation

$$a\angle a^* = i\,. \tag{20.3}$$

The relation (20.3) is called the **canonical commutation relation** (CCR) for the harmonic oscillator. More generally, one finds for the Lie product of general functions f, g of a and a^* the formula

$$f\angle g = i\frac{\partial f}{\partial a}\frac{\partial g}{\partial a^*} - i\frac{\partial f}{\partial a^*}\frac{\partial g}{\partial a}. \tag{20.4}$$

This will be seen later as a special case of a general principle for constructing so-called Lie–Poisson algebras from a Lie algebra.

20.2 Quantizing the harmonic oscillator

For a classical harmonic oscillator, the Lie product in the CCR (20.3) is defined via the Poisson bracket. To quantize the harmonic oscillator, all we do is replace the Lie product in the CCR by its quantum analogue. Thus we postulate the existence of an operator a and its conjugate a^* with the relation

$$\frac{i}{\hbar}[a, a^*] = i\,,$$

equivalently

$$[a, a^*] = \hbar\,. \tag{20.5}$$

Note that equation (20.5) has the right behavior under $\hbar \to 0$, since in the limit that $\hbar$ goes to zero, we have to end up in the classical regime, where the operators a and a^* become functions on phase space and hence commute.

Equation (20.5) defines a $*$-algebra, i.e., an associative algebra with unity and an involution $*$, generated by a with the relation $aa^* - a^*a = \hbar$. Later we look for representations in a Hilbert space, where the involution then corresponds to Hermitian conjugation. But already at this level, we call expressions in a and a^* operators.

The quantum mechanical Hamiltonian for the harmonic oscillator is the operator given by direct substitution of the p and q from (20.2):

$$\begin{aligned} H &= \omega\Big(\frac{a-a^*}{2i}\Big)^2 + \omega\Big(\frac{a+a^*}{2}\Big)^2 + V_0 \\ &= \tfrac{1}{2}\omega(aa^* + a^*a) + V_0 \\ &= \omega a^*a + \tfrac{1}{2}\omega\hbar + V_0\,. \end{aligned} \tag{20.6}$$

Since only differences in energy are important, one often chooses $V_0 = -\frac{1}{2}\hbar\omega$ to get the simple formula $H = \omega a^* a$.

In the classical theory we have commuting variables a and a^* with a Lie product $a \angle a^* = i$. That is, we have a commutative $*$-Poisson algebra. In the quantum theory we have an associative algebra generated by a and a^* with the relation $aa^* - a^*a = \hbar$. Since in the quantum theory two seemingly different polynomial expressions (such as aa^* and $a^*a + \hbar$) can be the same, there is a need for a preferred ordering of a and a^* in monomials. The **normal ordering** is that ordering of a and a^* in monomials where all a^*'s are moved to the left of the a's. It is easy to see that every noncommutative polynomial in a and a^* can be normally ordered by repeated use of the relation $aa^* = a^*a + \hbar$; in the process of normal ordering, lower degree monomials are generated with higher powers of $\hbar$. We give the following proposition that guarantees that taking $\hbar \to 0$ we recover the classical theory:

20.2.1 Proposition. *Let f and g be noncommutative polynomials in a, a^* and $\hbar$. Viewing f and g as polynomials in commuting variables a and a^*, one can calculate $f \angle g$ using* (20.4). *As noncommutative polynomials one can calculate the commutator $[f, g] = fg - gf$. The two results are related by:*

$$\frac{i}{\hbar}[f, g] = f \angle g + O(\hbar)\,. \tag{20.7}$$

One expresses this relation by saying that the quantum Lie product is a ***deformation*** *of the classical Lie product.*

Proof. The order of the a and a^* does not matter since changing the order we generate powers of $\hbar$. We use induction on the degree of the polynomials. For degree zero and one, (20.7) holds. Suppose it holds for degree of f smaller than n and degree of g one. If we write $f = a^*S + Ta$ for some normally ordered polynomials S and T with degrees smaller than n, we see that for $g = a^*$:

$$\begin{aligned} i[a^*S + Ta, a^*] &= ia^*[S, a^*] + i\hbar T + i[T, a^*]a \\ &= \hbar a^* S \angle a^* + i\hbar T + \hbar T \angle a^* a + O(\hbar^2) \\ &= \hbar(a^*S)\angle a^* + \hbar(Ta)\angle a^* + O(\hbar^2)\,, \end{aligned}$$

and the result holds for f arbitrary and $g = a^*$. For $g = a$ it goes similar. Suppose the claim holds for all g with degree k, with $0 \le k \le n$. Then for degree $n+1$ let us write $g = aP + a^*Q + R$, where P, Q and R are polynomials of degree strictly less than $n+1$. Then we have:

$$\begin{aligned} \frac{i}{\hbar}[f, g] &= \frac{i}{\hbar}[f, aP + a^*Q + R] \\ &= \frac{i}{\hbar}[f, a]P + \frac{i}{\hbar}a[f, P] + \frac{i}{\hbar}[f, a^*]Q + \frac{i}{\hbar}a^*[f, Q] + \frac{i}{\hbar}[f, R] \\ &= f \angle aP + af \angle P + f \angle a^*Q + a^* f \angle Q + f \angle R + O(\hbar) \\ &= f \angle (aP) + f \angle (a^*Q) + f \angle R + O(\hbar) \\ &= f \angle (aP + a^*Q + R) + O(\hbar)\,. \end{aligned} \tag{20.8}$$

And the proof is complete. □

Extension to the anharmonic case. The anharmonic oscillator can in principle be treated in a similar fashion. Since the classical Lie product (the Poisson bracket) is the same, we may proceed exactly as before, except that the formulas involving the Hamiltonian are no longer valid. In particular, since the frequency ω was determined by the Hamiltonian, it is now an arbitrary constant. Thus there are multiple, inequivalent ways of defining the quantities $a(t)$. Indeed, there is even more freedom since the only important property to be preserved is the canonical commutation relation.

Generalizing the affine form of $a(t)$ in the harmonic case, we choose it as an arbitrary affine combination of $q(t)$ and $p(t)$,

$$a = \lambda + \mu q + i\nu p \tag{20.9}$$

for suitable complex numbers μ, ν and λ. As can be easily verified, the canonical commutation relations (20.3) are reproduced, so that the classical Lie product takes again the form (20.4), exactly when the restriction

$$2\,\mathrm{Re}\,\mu\overline{\nu} = 1$$

holds. Having made a choice, we obtain a classical Hamiltonian $H = H(a, a^*)$ in terms of a and a^*. Using the Heisenberg dynamics and (20.4), we obtain

$$\dot{a}(t) = H\angle a(t) = -i\frac{\partial H}{\partial a^*}\,. \tag{20.10}$$

We remark that if (20.3) holds for $t = 0$ then it holds for all t. Indeed, the derivative of the left-hand side of (20.3) vanishes identically.

Using a different choice of the parameters defining a we get a different variable a', which is affinely related to the original a,

$$a' = \alpha + \beta a + \gamma a^*\,. \tag{20.11}$$

The requirement that a' satisfies the same commutation relations as a leads to the restriction

$$|\beta|^2 - |\gamma|^2 = 1. \tag{20.12}$$

A transformation of the form (20.11) satisfying (20.12) is called a **Bogoliubov transformation**. Bogoliubov transformations have important applications; for example, they were at the heart of Hawkings' proof that black holes radiate. The generalization of Bogoliubov transformations to systems of oscillating electron pairs in metals is an important ingredient for the theory of Cooper pairs, which explains superconductivity effects in metals at low temperature.

Different choices of the coefficients in the definition of a lead of course to different forms of $H(a, a^*)$; this means that different Hamiltonians $H(a, a^*)$ can describe the same oscillator. The particular choice above for the harmonic oscillator is the one leading to $H(a, a^*) = E_0 + \omega a^* a$, for which the dynamics (20.10) takes the simple form $\dot{a} = -i\omega a$. In theoretical physics there are different operators a_k and a_k^* labeled by some parameter k. One tries to find by means of Bogoliubov transformations the simplest form of the Hamiltonian. The

preferred form is the form where H is diagonalized: $H = \sum_k a_k^* a_k + \ldots$, where the dots contain terms of higher order in the operators a_k and a_k^*.

The quantization of an anharmonic oscillator is done as in the harmonic case. For each classical Hamiltonian polynomial in a and a^*, there is a unique normally ordered quantum version. However, when modeling the same system both in a classical and in a quantum setting, the coefficients of the quantum system in a normal ordering of the operators must be taken to depend on $\hbar$, and the form of this dependence is not determined by the quantum-classical correspondence. Therefore, the best fit of coefficients of H to experimental data will generally produce different optimal values in the classical and the quantum case. In a quantum field theory, the coefficients will also be dependent on the scale at which frequencies remain unresolved, giving so-called **running coupling constants** which play an important role in renormalization techniques.

20.3 Representations of the Heisenberg algebra

We saw at the end of Section 20.1 that the Heisenberg algebra $t(3, \mathbb{C})$ can be considered as being generated by $1, a$, and a^* where a and a^* satisfy the CCR $a \angle a^* = i$.

In the classical case, we know a realization of these commutation relations in terms of a Poisson bracket. In the quantum case, we must find a representation in terms of operators in a Hilbert space. The representations of physical interest are the unitary representations, which represent the one as identity and behave properly under the $*$-operation. In this section we construct a unitary representation of the Heisenberg algebra.

In the quantized version of a classical theory the functions on phase space become elements of some associative algebra $\mathbb{E}$. For a representation we want to realize the algebra $\mathbb{E}$ as a subalgebra of an algebra of linear operators.

The approach of Schrödinger (1926) to this problem was to take as Hilbert space the space of square integrable complex-valued functions ψ on $\mathbb{R}^3$; then the Schrödinger equation for the dynamics of a pure state takes the form of a wave equation, which was familiar to physicists at that time and hence came to dominate quantum mechanics. The approach taken by Schrödinger proved to be very successful and is also presented in many quantum physics textbooks, since (for a single particle) the real-valued function $|\psi(x)|^2$ has an intuitive semiclassical probability interpretation (discussed in Section s.motQM). For multiparticle systems, the intuitive advantages of Schrödinger's representation is no longer given, as the wave functions are no longer in physical space $\mathbb{R}^3$ but, for n particles, in an abstract $3n$-dimensional configuration space. For systems involving an unconserved number of particles, in particular for interactions with light, and for systems in the thermodynamic limit, things are even more complicated since the configuration space becomes infinite-dimensional, and the wave function representation becomes unwieldy – instead one usually resorts to the techniques of quantum field theory. Nevertheless, there are interesting papers using the resulting functional Schrödinger equation to illuminate the relations between classical solitons and quantum bound states (see, e.g., Jackiw [135]).

One year earlier than Schrödinger, Heisenberg invented his infinite-dimensional matrix algebra. We present Heisenberg's approach since it generalizes easily to the most complex quantum systems, including the universe as a whole.

We now look at an arbitrary unitary representation $J : \mathbb{L} \to \operatorname{Lin} \mathbb{H}$ in a Euclidean space $\mathbb{H}$ satisfying

$$J(a^*) = J(a)^*, \quad J(1) = 1.$$

We shall write the operators corresponding to a and a^* in the representation again by a and a^* (rather than using $J(a)$, etc.), in order to avoid clumsy notation. This will not cause problems since the representation turns out to be faithful. Then the operator

$$n := \frac{1}{\hbar} a^* a,$$

for reasons that will soon be apparent, is called the **number operator**, satisfies the commutation relations

$$[a, n] = a\,, \quad [a^*, n] = -a^*\,,$$

as is easily checked. This implies that the vector space generated by 1, a, a^* and n is closed under the commutator, and hence forms a Lie $*$-algebra $\mathbb{L}$ with the quantum Lie product, called the **oscillator algebra** $os(1)$. In this section (as always when classifying unitary representations), it will be more convenient to work directly with commutators.

We now illustrate an important technique in representation theory, which in many cases of interest provides all irreducible representations of a certain kind. See Section 22.4 for some other applications.

We define the **Verma module** corresponding to a complex number λ by

$$V_\lambda = \{\psi \in \overline{\mathbb{H}} \mid n\psi = \lambda\psi\}\,,$$

where the Hilbert space $\overline{\mathbb{H}}$ is the closure of $\mathbb{H}$. If V_λ is nontrivial, it contains a nonzero vector, λ is an eigenvalue of n, and any nonzero $\psi \in V_\lambda$ is a corresponding eigenvector. Thus the nonzero Verma modules are just the eigenspaces of the eigenvalues of n. Since we consider here only unitary representations where * is the adjoint, this implies that

$$\lambda = \frac{\psi^* n \psi}{\psi^* \psi} = \frac{\|a\psi\|^2}{\hbar \|\psi\|^2} \geq 0$$

is real and nonnegative. Noting that in general n is Hermitian, we now make the slightly stronger assumption that n is self-adjoint as a densely defined operator of the Hilbert space $\overline{\mathbb{H}}$. Then the spectral theorem implies that the infimum

$$\widehat{\lambda} = \inf_{\psi \neq 0} \frac{\psi^* n \psi}{\psi^* \psi}$$

is a real and nonnegative number, attained for some $\widehat{\psi} \neq 0$, and $\widehat{\psi}$ is an eigenvector of n corresponding to the eigenvalue $\widehat{\lambda}$. Thus $V_{\widehat{\lambda}} \neq 0$. Now consider an arbitrary λ with $V_\lambda \neq 0$ and a nonzero $\psi \in V_\lambda$. Then $na\psi = (\lambda - 1)a\psi$, hence $a\psi \in V_{\lambda-1}$. If $a\psi = 0$ then

$$\lambda \psi^* \psi = \psi^* n \psi = \frac{1}{\hbar} \psi^* a^* a \psi = 0,$$

hence $\lambda = 0$; and if $a\psi \neq 0$ then $V_{\lambda-1} \neq 0$, and $\lambda - 1$ is an eigenvalue of n. In the latter case, we can repeat the step once, or more often. But since all eigenvalues are nonnegative, this can happen only a finite number of times, and ultimately we must end up with the other alternative. Hence zero is an eigenvalue (in particular $\widehat{\lambda} = 0$) and $\lambda - n = 0$ for some nonnegative integer n. Thus the only possible eigenvalues are nonnegative integers. That all these actually are eigenvalues follows by a similar argument. Indeed, with ψ as before, we have

$$na^*\psi = ([n, a^*] + a^*n)\psi = (n+1)a^*\psi = (\lambda+1)a^*\psi,$$

hence $a^*\psi \in V_{\lambda+1}$. Since

$$\|a^*\psi\|^2 = \psi^* a a^* \psi = \psi^*(\hbar + a^*a)\psi = \hbar\|\psi\|^2 + \|a\psi\|^2 \geq \hbar\|\psi\|^2 > 0,$$

$V_{\lambda+1} \neq 0$ and $a^*\psi$ is an eigenvector for the eigenvalue $\lambda + 1$. By induction, we reach all positive integers from $V_{\widehat{\lambda}} = V_0$. Thus we have proved the following theorem:

20.3.1 Theorem. *In a representation in which n is self-adjoint, a Verma module V_λ of the oscillator algebra $\mathbb{L}$ is nonzero if and only if λ is a nonnegative integer.*

In particular, the spectrum of the Hamiltonian $H = \omega a^* a$ of a quantum harmonic oscillator consists of the nonnegative integral multiples of $\omega\hbar$.

The results obtained justify the following terminology. The operator a is called a **lowering operator**, since its application to an eigenstate of the number operator n lowers the associated eigenvalue by one. The operator a^* is called a **raising operator**, since its application to an eigenstate of the number operator n raises the associated eigenvalue by one. Together, the operators a and a^* are called **ladder operators**. A unit vector in the Verma module V_0 is called a **ground state** (in the second quantized language of quantum field theory a **vacuum vector**). For a **ground state**, i.e., a nonzero vector $\psi \in V_0$, we have $n\psi = 0$, hence $\|a\psi\|^2 = \psi^* a^* a\psi = \hbar\psi^* n\psi = 0$ and therefore $a\psi = 0$. Thus the ground state is annihilated by the lowering operator. Therefore a is also called an **annihilation operator**; if this term is used then a^* is called a **creation operator**.

20.4 Bras and Kets

In his groundbreaking work on quantum mechanics, Dirac introduced a notation for vectors and operators that is widely used by physicists but is quite different from what mathematicians are used to. Dirac's bra-ket calculus is not very well defined in the way actually used by physicists, since the basis vectors considered in the calculus do not necessarily lie in the Hilbert space in which everything should happen from a strictly axiomatic point of view.

We define here a precise version of Dirac's bra-ket calculus, which can also satisfy mathematicians. Instead of working in a Hilbert space we consider a fixed dense subspace which we denote by $\mathbb{H}$. Thus $\mathbb{H}$ is a vector space with a Hermitian inner product $\langle\cdot|\cdot\rangle$, antilinear in the first argument and linear in the second, such that $\langle\psi|\psi\rangle$ is always real and nonnegative, and the relation

$$\langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle \tag{20.13}$$

holds, where α^* denotes the complex conjugate of a number $\alpha \in \mathbb{C}$. The inner product defines a Euclidean norm $\|\psi\| := \sqrt{\langle\psi|\psi\rangle}$, and the Hilbert space is the closure $\overline{\mathbb{H}}$ of $\mathbb{H}$ in the topology induced by this norm. We refer to the elements of $\mathbb{H}$ as **smooth vectors** since they correspond in the important special case $\mathbb{H} = C^\infty(\mathbb{R})$ to arbitrarily often differentiable functions.

Every smooth vector ψ defines a continuous linear functional, denoted by ψ^*, which maps $\phi \in \mathbb{H}$ to the complex number

$$\psi^*(\phi) := \langle\psi|\phi\rangle. \tag{20.14}$$

Dirac's idea was to turn this formula into a more suggestive form by splitting the bracket $\langle\psi, \phi\rangle$ into a **bra** $\langle\psi|$, standing for ψ^*, and a **ket** $|\phi\rangle$, standing for ϕ, and deleting the now superfluous parentheses. Then the formula becomes

$$\langle\psi|\,|\phi\rangle := \langle\psi|\phi\rangle, \tag{20.15}$$

which just asks us to replace two adjacent vertical bars by a single one.

If $\mathbb{H}$ is itself a Hilbert space (and in particular, if the dimension of $\mathbb{H}$ is finite) then it is not difficult to see that all continuous linear functionals arise in this way. However, in many interesting infinite-dimensional vector spaces $\mathbb{H}$, the situation is different. For example, if $\mathbb{H} = C^\infty(\mathbb{R})$ and $z \in \mathbb{R}$ then the mapping δ_z which maps $\psi \in \mathbb{H}$ to

$$\delta_z(\psi) := \psi(z)$$

is a continuous linear functional which cannot be obtained as ψ^* for some smooth vector ψ.

We can accommodate this in the bra-ket calculus by allowing as bras *all* continuous linear functionals rather than only those which have the form ψ^* with $\psi \in \mathbb{H}$. We simply need to label the continuous linear functional as bras $\langle\psi|$ with symbols ψ from a set $\mathbb{H}^*$ such that the functionals of the form ψ^* with $\psi \in \mathbb{H}$ get the label ψ. The set $\mathbb{H}^*$ can be made canonically into a vector space containing $\mathbb{H}$ as a subspace by requiring the mapping $* : \psi \to \psi^* := \langle\psi|$ to be antilinear. Then $\mathbb{H}^* = \mathbb{H}$ in case $\mathbb{H}$ is a Hilbert space, but in general $\mathbb{H}$ may be a proper subspace of $\mathbb{H}^*$. Since the inner product extends continuously from $\mathbb{H}$ to the Hilbert space completion $\overline{\mathbb{H}}$, every element of $\overline{\mathbb{H}}$ defines a continuous linear function. Thus, in general, the Hilbert space $\overline{\mathbb{H}}$ sits somewhere in between $\mathbb{H}$ and $\mathbb{H}^*$,

$$\mathbb{H} \subseteq \overline{\mathbb{H}} \subseteq \mathbb{H}^*. \tag{20.16}$$

Frequently, some extra "nuclear" structure on $\mathbb{H}$ is assumed which turns (20.16) into a so-called **Gelfand triple** or **rigged Hilbert space** (see, e.g., Maurin [190], Bohm & Gadella [38], and for applications to resonances Kukulin et al. [165]); however, on the level of our discussion, we don't need this extra structure.

If $\mathbb{H} = C^\infty(\mathbb{R})$, physicists call the vectors $\psi \in \mathbb{H}^*$ **wave functions** – well being aware that they are not always functions in the standard sense –, and write them with a dummy argument x as $\psi(x)$. For example, they consider δ_z to be a **shifted delta function**, and write it as $\delta(x - z)$.

A wave function which is in the Hilbert space $\overline{\mathbb{H}} \subseteq \mathbb{H}^*$ is called **normalizable**, the remaining wave functions are called **non-normalizable**. In mathematical terms, the normalizable

wave functions are equivalence classes of square integrable functions, with two functions being regarded as equivalent when they differ only on a set of measure zero. The shifted delta functions are examples of non-normalizable wave functions.

For a general Euclidean space $\mathbb{H}$, we refer to the elements of $\mathbb{H}^*$ as **rough vectors** since they correspond in the special case $\mathbb{H} = C^\infty(\mathbb{R})$ to functions that are less smooth, possibly not even continuous, and possibly (as in case of the δ_z) not functions at all.

Having extended the bra-ket notation to allow rough vectors as labels in bras, the symmetry property (20.13) is lost. To restore that, we simply extend the inner product to enforce the validity of (20.13) by defining $\langle\psi|\phi\rangle := \langle\phi|\psi\rangle^*$ if $\phi \in \mathbb{H}^*$ and $\psi \in \mathbb{H}$. This can be done consistently, and implies that now kets can be labeled by rough vectors, too. But now the formula (20.15) makes trouble. What is $\langle\psi|\phi\rangle$ when both ϕ and ψ are rough vectors? In general, there is no solution; this product cannot be always defined. However, one can consistently define it in certain cases, namely when ϕ is in some subspace $\tilde{\mathbb{H}}$ of $\mathbb{H}^*$ and the linear functional ψ^* defined at first only on $\mathbb{H}$ can be extended to $\tilde{\mathbb{H}}$ by some limiting procedure. We won't list here the various possibilities; our usage of bras and kets will be restricted to cases where at least one of the two labels in an inner product is smooth.

The main use of Dirac's notation is for the specification of vectors and matrices in a particular representation of the algebra of quantities. We first review the notation in the case where a countable orthonormal basis of smooth states is available. In this case there is a countable set K of **labels** such that the basis consists of the kets $|k\rangle$ with $k \in K$, and orthogonality implies that

$$\langle j|k\rangle = \delta_{jk}\,,$$

and the **resolution of unity**

$$\sum_k |k\rangle\langle k| = 1\,.$$

In the finite-dimensional case, there is a close correspondence to the notation of linear algebra if we take $\langle k|$ to be the kth unit row vector with a 1 in position k and zeros elsewhere, and $|k\rangle$ to be its transpose, the kth unit column vector.

$$x = \sum_k x_k|k\rangle \quad \text{represents the vector } x = (x_k),$$

and

$$\langle k|x = x_k$$

gives the components of x.

$$A = \sum_{jk} |j\rangle A_{jk}\langle k| \quad \text{represents the matrix } A = (A_{jk}),$$

$$\langle j|A = \sum_k A_{jk}\langle k| \quad \text{represents } A_{j:}, \text{ the } j\text{th row of } A,$$

$$A|k\rangle = \sum_j |j\rangle A_{jk} \quad \text{represents } A_{:k}, \text{ the } k\text{th column of } A,$$

and

$$\langle j|A|k\rangle = A_{jk}$$

gives the matrix entries of A. Compared to the standard linear algebra notation there is no gain.

The situation is different when K is a structured set, for example a set of pairs (k, s) where k is a momentum label and s a spin label, or other such sets arising naturally in the dynamical symmetry approach of Section 23.6. Then the index notation becomes somewhat cumbersome to comprehend, and the more lengthy bra-ket notation is superior.

20.5 Boson Fock space

As we have seen in Section 20.3, every nice unitary representation of the oscillator algebra contains a ground state $\widehat{\psi}$ of norm 1, and hence the representation contains the vectors $(a^*)^k\widehat{\psi}$ $(k = 0, 1, 2, \ldots)$. Their span defines a Euclidean vector space $\mathbb{F}_+$ whose closure $\overline{\mathbb{F}}_+$ is a Hilbert space, called the **single mode bosonic Fock space**, or simply Fock space. Clearly, $\mathbb{F}_+$ is closed under the action of $\mathbb{L}$, hence we have a unitary representation of $\mathbb{L}$ on $\mathbb{F}_+$. It is not difficult to see that different choices of the ground state either define the same Fock space (if the ground states differ only by a phase) or orthogonal Fock spaces. Indeed, if $\mathbb{F} \subset \mathbb{F}_+$ is an invariant submodule, it needs to have a vector $\tilde{\psi}_0$, which necessarily coincides with the ground state of $\mathbb{F}_+$ up to a complex number. Thus an arbitrary unitary representation is a direct sum of Fock spaces. Thus the representations on a Fock space are *irreducible* representations. We shall show in a moment that the unitary representation on a Fock space is essentially unique. This is the content of the celebrated **Stone–Von Neumann theorem**, which actually is about the representation of the Heisenberg group.

Bosonic Fock spaces with more degrees of freedom are obtained by taking tensor products of the Fock space with one degree of freedom, and describe systems of quantum oscillators. As we shall see in Chapter 21, there is also a fermionic counterpart of Fock spaces, which are related to so-called Clifford algebras. The single mode case describes a so-called **qubit** and is simply the vector space $\mathbb{C}^2$; the general case is a tensor product of these, and describes systems of qubits.

We now study the structure of $\mathbb{F}_+$ for a given ground state $\widehat{\psi}$ of norm 1 in more detail. The properties found will lead to a construction of a Hilbert space which actually contains a representation of the Heisenberg algebra (which, so far, we simply had assumed).

20.5.1 Proposition. *The vectors*

$$|k\rangle := \frac{1}{k!}(a^*)^k\widehat{\psi} \quad (k = 0, 1, 2, \ldots) \tag{20.17}$$

satisfy the relations

$$a^*|k-1\rangle = k|k\rangle, \quad a|k\rangle = \hbar|k-1\rangle, \quad n|k\rangle = k|k\rangle,$$

$$\langle k|k'\rangle = \frac{\hbar^k}{k!}\delta_{kk'}.$$

Proof. The first relation is just definition. For the second observe that $a\widehat{\psi} = 0$ and $[a, (a^*)^k] = k(a^*)^{k-1}$. For the third, just combine $n = \frac{1}{\hbar}a^*a$ and the first and second relation. For the fourth relation we have $\langle k| = \frac{1}{k!}(\widehat{\psi})^* a^k$ and $\langle k|k'\rangle = 0$ if $k \neq k'$ since eigenvectors of a Hermitian operator corresponding to different eigenvalues are orthogonal. So only the normalization needs to be checked:

$$\langle k|k\rangle = \frac{1}{k^2}\langle k-1|aa^*|k-1\rangle = \frac{1}{k^2}\langle k-1|\hbar + \hbar n|k-1\rangle = \frac{\hbar}{k}\langle k-1|k-1\rangle\,.$$

Using induction the fourth equality follows. □

In the Fock space $\mathbb{F}_+$, the vectors are by definition the linear combinations

$$\psi = \sum_{k=0}^{\infty} \psi_k|k\rangle\,, \quad \psi_k \in \mathbb{C}\,.$$

Proposition 20.5.1 gives us the relations

$$(a\psi)_k = \hbar\psi_{k+1}\,, \quad (a^*\psi)_k = k\psi_{k-1}\,, \quad (n\psi)_k = k\psi_k\,, \tag{20.18}$$

and $\varphi^*\psi = (\sum \varphi_k|k\rangle)^* \sum \psi_l|l\rangle = \sum \frac{\hbar^k}{k!}\bar{\varphi}_k\psi_k$, hence

$$\varphi^*\psi = \sum \frac{\hbar^k}{k!}\bar{\varphi}_k\psi_k\,. \tag{20.19}$$

Equations (20.18) and (20.19) are an equivalent description of the equations of Proposition 20.5.1.

We now define $\mathbb{H}$ as the closure of $\mathbb{F}_+$. This makes $\mathbb{F}_+$ a dense subspace of $\mathbb{H}$, and we say that the operators a, a^* and n are **densely defined** in $\mathbb{H}$ (meaning that they are defined on a dense subspace). Previously we have seen that if the canonical commutation relations admit an irreducible representation, then it has to be of the form as described by Proposition 20.5.1. But now we can say more:

The set $\mathbb{H}$ of vectors $\psi \in \mathbb{C}^\infty$ with finite norm

$$\|\psi\| := \sqrt{\sum_{k=0}^{\infty} \frac{\hbar^k}{k!}|\psi_k|^2}$$

is a Hilbert space with inner product (20.19), on which the definitions 20.18 give densely defined operators a, a^*, n. The components of $a^*\psi$ grow significantly faster than those of ψ, so that $a^*\psi \in \mathbb{H}$ only for ψ in a proper subspace of $\mathbb{H}$. This subspace is dense, since it contains the dense subset of ψ with only finitely many nonzero entries. Note that the operators 1, a, a^* and n, and hence all elements of $\mathbb{L}$ are represented by infinite tridiagonal matrices, where only matrix elements in which the indices differ by at most one are nonzero. This is the representation of the quantum harmonic oscillator discovered by Heisenberg in his groundbreaking paper [123].

It is now easy to check that the operators 1, a, a^* and n satisfy the canonical commutation relations, that a^* is the Hermitian conjugate of a, and that $n = a^*a$. Thus we have a representation of $\mathbb{L}$. The representation is irreducible since acting repeatedly with $a^* \in \mathbb{L}$ on the vector $\widehat{\psi}$ with entries $\widehat{\psi}_k = \delta_{k0}$ (the ground state) gives a basis of $\mathbb{H}$. Combining this with the uniqueness statement obtained before, we arrive at the following theorem of Stone and Von Neumann (but essentially already obtained in [123]):

20.5.2 Theorem. *The canonical commutation relations admit an (up to equivalence) unique irreducible unitary representation on a Hilbert space such that the action of a, a^* and $n = a^*a$ is defined on a dense subspace and n is self-adjoint.*

The theorem holds with a similar proof for arbitrary finite-dimensional Heisenberg algebras coming from a nondegenerate alternating form. It fails spectacularly in infinite dimensions. In this case there are uncountably many inequivalent representations; see, e.g., Barton [27] for an (in spite of the title of the book) elementary discussion of these. Their existence is one of the main stumbling blocks for extending quantum mechanics to quantum field theory.

20.6 Bargmann–Fock representation

We present an important but easy representation of the Heisenberg algebra $h(n)$, which will be useful to us when we study coherent states in Section 20.7. Consider the vector space of complex polynomials in n variables $\mathbb{C}[z_1, \ldots, z_n]$. We then identify a_k and a_k^* with the operators defined by[1]

$$(a_k p)(z_1, \ldots, z_n) := z_k p(z_1, \ldots, z_n)\,,$$

and

$$(a_k^* p)(z_1, \ldots, z_n) := \frac{\partial}{\partial z_k} p(z_1, \ldots, z_n)\,.$$

It is easy to check that this indeed defines a representation. We can even make a unitary representation out of this. For that purpose we consider the vector space $\mathbb{H}$ of all entire functions on $\mathbb{C}^n$ with finite norm with respect to the inner product

$$\langle f|g\rangle = \int_{\mathbb{C}^n} \overline{f(z)} g(z) e^{-\bar{z}\cdot z}\,.$$

The space $\mathbb{H}$ with the above inner product is a Euclidean space; its closure is a Hilbert space, the multi-dimensional version of the Bargmann–Fock space described in Section 20.5.

The operators a_k and a_k^* are adjoints of each other. An orthogonal basis is given by the monomials:

$$\langle z_1^{k_1} \ldots z_n^{k_n} | z_1^{l_1} \ldots z_n^{l_n} \rangle = \prod_{i=1}^{n} k_i! \delta_{k_i, l_i}\,.$$

[1] Remember the transformations $a_k = \frac{p_k - i q_k}{\sqrt{2}}$ and $a_k^* = \frac{p_k + i q_k}{\sqrt{2}}$.

From the discussion in Section 13.1 it follows that the quadratic expressions modulo the linear expressions in the elements z_i and $\frac{\partial}{\partial z_k}$ form the Lie algebra $sp(2n, \mathbb{C})$. Taking all quadratic expressions (so not modding out by the linear polynomials) in the elements z_i and $\frac{\partial}{\partial z_k}$ one obtains a central extension of $isp(2n)$.

The above representation is irreducible (one sees rather quickly that starting with 1, acting with p_k gives all entire functions) and is called the Bargmann–Fock representation. By the Stone–Von Neumann theorem, which says that there is only one irreducible representation of the Heisenberg algebra, the Bargmann–Fock representation is up to isomorphism the only irreducible representation of the Heisenberg algebra.

We have seen in Section 13.1 that the quadratic expressions (modulo linear terms) in the q_i and the p_k rotate the generators q_i and p_k into each other under the action of the Lie product. In other words, the action of the quadratic expressions builds a representation of $sp(2n, \mathbb{C})$ inside the Bargmann–Fock representation. That this happens is not so strange. Let us consider the automorphism group of the Heisenberg algebra, consisting of all the invertible maps $h(n) \to h(n)$ preserving the Lie product. But from equation (13.1) we see that the automorphism group contains the group $Sp(2n, \mathbb{C})$. Now let us denote the above given Bargmann–Fock representation by $U : h(n) \to \mathrm{Lin}(H)$, then using $Sp(2n, \mathbb{C})$ we get a new representation of the Heisenberg algebra as follows. For each $g \in Sp(2n, \mathbb{C})$ we consider the representation

$$U_g : h(n) \to \mathrm{Lin}(H)\,, \quad U_g(x) = U(gx)\,.$$

Since $Sp(2n, \mathbb{C}) \subset \mathrm{Aut}(h(n))$ the U_g are indeed representations. But the unitary irreducible representation of $h(n)$ is unique, up to isomorphism, and hence there must be a unitary operator $R(g)$ such that

$$U_g = R(g)UR(g)^{-1}\,.$$

It is clear that the $R(g)$ are determined up to a sign. Thus $R(g)R(h) = \pm R(gh)$ and we say that the $R(g)$ form a **projective representation** of the group $Sp(2n, \mathbb{C})$. This representation is called the **metaplectic representation**. The operators $R(g)$ themselves form a group, closely related to the **metaplectic group** $Mp(2n, \mathbb{R})$, the universal covering group of the Lie algebra $sp(2n, \mathbb{R})$. The metaplectic group is a two-fold cover of $Sp(2n, \mathbb{R})$, hence has a center of order 2, while our group has the multiplicative group of the reals as center. Factoring out the positive reals leaves the metaplectic group.

20.7 Coherent states for the harmonic oscillator

Coherent states were introduced in 1963 by Glauber [105], who recognized their importance in quantum optics; he received in 2005 the Nobel prize for his work in this direction. But the notion of a coherent state (without the name) was already introduced by Erwin Schrödinger [248] in 1926 when he was looking for solutions to the Schrödinger equation that satisfy the **Heisenberg uncertainty relation**

$$\Delta p \Delta q \geq \frac{\hbar}{2}, \tag{20.20}$$

where Δx denotes the variance of a quantity x. Schrödinger was looking for states that were as classical as possible, having equality $\Delta p \Delta q = \frac{\hbar}{2}$. The coherent states, and only these satisfy equality; they therefore build a connection between classical physics and quantum physics that grew stronger as the notion of coherent states was extended to more general situations.

To introduce Glauber's coherent states, we remind the reader that for the harmonic oscillator we constructed the Fock space $\mathbb{H}$ of $\psi = (\psi_k)_{k\geq 0}$ satisfying

$$\sum_{k=0}^{\infty} \frac{\hbar^k}{k!} \overline{\psi}_k \psi_k < \infty \,. \tag{20.21}$$

One may regard ψ either as a vector with infinitely many components, or as an infinite sequence. Equivalently, in Dirac's bra-ket notation, the ψ_k's are the complex coefficients in the expansion of ψ with respect to an eigenbasis $|k\rangle$ of the number operator, $\psi = \sum \psi_k |k\rangle$. The inner product is given by

$$\varphi^* \psi = \sum_{k=0}^{\infty} \frac{\hbar^k}{k!} \overline{\varphi}_k \psi_k \,.$$

The operators a, a^* and n act as $(a\psi)_k = \hbar\psi_{k+1}$, $(a^*\psi)_k = k\psi_{k-1}$ and $(n\psi)_k = k\psi_k$. We now define a **coherent state** for the harmonic oscillator to be a vector of the form

$$|\lambda, z\rangle := (\overline{\lambda}, \overline{\lambda}\overline{z}, \overline{\lambda}\overline{z}^2, \ldots) \,; \quad (\lambda, z \in \mathbb{C})$$

in other words, a state ψ with coefficients $\psi_k = \overline{\lambda}\overline{z}^k$. By (20.17), we can write

$$|\lambda, z\rangle = \sum_{k=0}^{\infty} \overline{\lambda} \frac{\overline{z}^k}{k!} (a^*)^k \hat{\psi} \,,$$

where $\hat{\psi}$ is the ground state. Even more, we have

$$|\lambda, z\rangle = \sum_{k\geq 0} \bar{\lambda} \bar{z}^k |k\rangle \,, \tag{20.22}$$

and we see that $\psi \in \mathbb{H}$ since

$$\sum_{k\geq 0} \hbar^k |\lambda|^2 \frac{|z|^{2k}}{k!} = |\lambda|^2 e^{\hbar |z|^2} < \infty \,.$$

The inner product between two coherent states is given by

$$\langle \lambda', z' | \lambda, z\rangle = \sum_{k=0}^{\infty} \frac{\hbar^k z'^k \overline{z}^k}{k!} \lambda' \overline{\lambda} = \lambda' \overline{\lambda} e^{\hbar z' \overline{z}} \,.$$

It is easy to see that

$$\langle \lambda, z | n\rangle = \frac{\lambda \hbar^n z^n}{n!} \,.$$

Suppose ψ is an element of $\mathbb{H}$, then

$$\langle \lambda, z|\psi\rangle = \lambda \sum_{k=0}^{\infty} \frac{(\hbar z)^k}{k!}\psi_k \equiv \lambda\psi(z)\,, \tag{20.23}$$

which defines the function $\psi(z)$ corresponding to ψ. Conversely, given an analytic function g

$$g(z) = \sum_{k\geq 0} \frac{(\hbar z)^k}{k!} g_k\,,$$

with $\sum_{k\geq 0} \frac{\hbar^2|g_k|^2}{k!} < \infty$ we assign to g the element $\psi_g = (g_k)_{k\geq 0}$ in $\mathbb{H}$. We claim that $\psi \mapsto \psi(z)$ is a map from $\mathbb{H}$ to the set of analytic functions. In order to prove the claim we have to prove that the power series (20.23) converges everywhere. We calculate the radius of convergence R

$$R = \limsup_{k\to\infty} \frac{1}{\sqrt[k]{\frac{\hbar^k\psi_k}{k!}}} = \limsup_{k\to\infty} \sqrt[k]{\frac{k!}{\hbar^k\psi_k}} \to \infty$$

since ψ_k satisfies (20.21). Hence the function $\psi(z)$ is analytic everywhere. The state ψ is uniquely described by the function $\psi(z)$ in the sense that $\psi(z) = 0 \Leftrightarrow \psi = 0$, since

$$\frac{1}{\lambda\hbar^k}\frac{d^k}{dz^k}\psi(z)\Big|_{z=0} = \psi_k\,.$$

The inner product between φ and ψ now becomes

$$\varphi^*\psi = \sum_{k=0}^{\infty} \frac{1}{k!|\lambda|^2\hbar^k}\Big[\frac{d^k}{dz^k}\overline{\varphi}(z)\frac{d^k}{dz^k}\psi(z)\Big]_{z=0}\,.$$

So we can use the powerful theorems of complex analysis to deal with the states in the Hilbert space $\mathbb{H}$. For the relations between complex analysis and coherent states, including important generalizations to coherent states associated with other Lie groups, see Perelomov [216], Upmeier [274], Faraut & Koranyi [84].

Every element in $\mathbb{H}$ is a linear combination of coherent states, but the combination is in general not unique. For the harmonic oscillator a set of finitely many coherent states $|\lambda, z\rangle$ with different z is linearly independent, since suppose

$$|v\rangle := \sum_{i=1}^{n} |\lambda_i, z_i\rangle = 0\,, \quad \lambda_i \neq 0\,,$$

then it follows that

$$\langle \mu, w|v\rangle = \sum_{i=1}^{\infty} \mu\lambda_i e^{\hbar w z_i} = 0\,,$$

for all w. But a finite set of exponential functions is linearly independent. Hence it follows that a finite set of coherent states $|\lambda, z\rangle$ with different z is linearly independent. The set of linear combinations of finitely many coherent states is dense in $\mathbb{H}$. The coherent states

form a kind of a "basis", but an overcomplete set. Such a set is called a **frame**. Frames are widely used in wavelet analysis.

We now show that coherent states of unit norm have a basis-like property, expressed through a so-called resolution of the identity. To simplify the notation we put $\hbar = 1$. Next we define

$$|z\rangle = |e^{-\frac{1}{2}|z|^2}, z\rangle \,.$$

The vectors $|z\rangle$ have a unit norm; $\langle z|z\rangle = 1$. We calculate for an element $|f\rangle = \sum_k f_k|k\rangle$ the following

$$|z\rangle\langle z|f\rangle = \sum_{k,n} e^{-|z|^2}\bar{z}^n z^k \frac{f_k}{k!}|n\rangle \,.$$

The coefficient of each component $|n\rangle$ equals

$$\varphi_n = e^{-|z|^2} f(z)\bar{z}^n \,,$$

where $f(z)$ is defined as

$$f(z) = \sum_n \frac{z^n}{n!} f_n.$$

From the above discussion we know that $f(z)$ is analytic everywhere. Thus the vector $\sum_n \varphi|n\rangle$ is of finite norm;

$$\sum_n \frac{|\varphi_n|^2}{n!} = \sum_n e^{-2|z|^2}|f(z)|^2 \frac{|z|^{2n}}{n!} = e^{-|z|^2}|f(z)|^2 < \infty \,.$$

Hence $|z\rangle\langle z|f\rangle$ represents an element in $\mathbb{H}$ and we can integrate each component to get

$$\frac{1}{\pi}\int_{\mathbb{C}} |z\rangle\langle z|f\rangle d^2z = \frac{1}{\pi}\int_{\mathbb{C}} |z\rangle f(z) e^{-\frac{1}{2}|z|^2} dz = |f\rangle \,, \tag{20.24}$$

where the integration measure is $dz = d(\mathrm{Re}z)d(\mathrm{Im}z)$ and where we used

$$\int_{\mathbb{C}} \bar{z}^n z^m e^{-|z|^2} dz = \pi n! \delta_{n,m} \,. \tag{20.25}$$

In physics literature one writes the result (20.24) as

$$\frac{1}{\pi}\int |z\rangle\langle z| dz = 1 \,.$$

In mathematics, such an expression is called a **resolution of the identity**. The fact that the coherent states admit a resolution of the identity makes them useful. We now wish to show that the expansion of $|f\rangle$ in coherent states is unique, thereby proving that the coherent states make up a tight frame. We use (20.24) to compute the inner product of $|f\rangle$ with a coherent state $\langle w|$

$$\langle w|f\rangle = \frac{1}{\pi} e^{-\frac{1}{2}|w|^2} \int_{\mathbb{C}} e^{w\bar{z}-|z|^2} f(z) dz \,.$$

But f is an analytic function, so we first try $f = z^n$. Using (20.25) we obtain the identity

$$\frac{1}{\pi}\int_{\mathbb{C}} e^{-|z|^2} e^{w\bar{z}} z^m dz = w^m \,.$$

Hence we derive the more general identity for analytic functions

$$\frac{1}{\pi}\int_{\mathbb{C}} e^{-|z|^2} e^{w\bar{z}} f(z) dz = f(w) \,,$$

from which we obtain

$$f(w) = e^{\frac{1}{2}|w|^2} \langle w|f\rangle \,.$$

Hence the expansion of f in coherent states is unique, since if $f = 0$, then all the $\langle z|f\rangle = 0$ and the expansion vanishes identically. Note that the above discussion only works for analytic functions f. If we admit a non-analytic f we get for example

$$\int_{\mathbb{C}} |z\rangle \bar{z}^n e^{-\frac{1}{2}|z|^2} dz = 0 \,,$$

for all $n > 0$. There is a relation between coherent states and the Hilbert space $\mathbb{H}_{\mathbb{C}}$ of analytic functions $f : \mathbb{C} \to \mathbb{C}$ such that

$$\int_{\mathbb{C}} |f(z)|^2 e^{-|z|^2} dz < \infty \,,$$

for which the $(z^n)_{n\geq 0}$ form a basis. We refer the interested reader to Glauber [105], Segal [251], Bargmann [23, 24]. We just remark that if $f \in \mathbb{H}_{\mathbb{C}}$ and expand f as

$$f(z) = \sum_{n\geq 0} \frac{f_n z^n}{n!}$$

then

$$\begin{aligned} \int_{\mathbb{C}} |f(z)|^2 e^{-|z|^2} dz &= \int_{\mathbb{C}} \sum_{n,m\geq 0} \frac{\bar{z}^n z^m \bar{f}_n f_m}{n!m!} e^{-|z|^2} dz \\ &= \pi \sum_{n\geq 0} \frac{|f_n|^2}{n!} \,. \end{aligned}$$

Hence f defines an element in the Fock space $\mathbb{H}$. (We have assumed one can change the order of integration and summation, but that can be made rigorous, see Bargmann [23] for a readable explanation.) The above discussion on the uniqueness of the expansion of an analytic function in terms of coherent states was taken from Glauber [105], which is a very readable account on coherent states and the physics and mathematics behind them.

We now reinsert the constant $\hbar$ to see some of the behavior of the coherent states. Remember the formula for q

$$q = 2\omega m^{-\frac{1}{2}}(a + a^*) \,.$$

We see easily that

$$a|\lambda, z\rangle = \hbar\bar{z}|\lambda, z\rangle. \tag{20.26}$$

With a bit more work we see that

$$\langle\lambda, z|a^*|\lambda, z\rangle = \sum_{k,l} |\lambda|^2 \frac{z^i \overline{z}^j}{k!l!} \hat{\psi}^* a^k (a^*)^{l+1} \hat{\psi} = z|\lambda|^2 \sum_{k=0}^{\infty} \frac{|z|^{2k}}{k!} ,$$

from which it follows that

$$\langle\lambda, z|a^*|\lambda, z\rangle = z\langle\lambda, z|\lambda, z\rangle .$$

We thus see that we can associate the real part of z with the position;

$$\langle\lambda, z|q|\lambda, z\rangle = 2\omega m^{-\frac{1}{2}}(z + z^*)\langle\lambda, z|\lambda, z\rangle .$$

In a similar fashion the imaginary part of z is related to the momentum p. Let us pause for a while to see what the above means. The harmonic oscillator has a very symmetric shape. One can show that the wave functions which are eigenvectors of the number operator n respect the symmetry $q \to -q$ in the sense that if $q \to -q$ then they change with a factor $(-1)^n$ (see any introductory book on quantum mechanics, e.g., Griffiths [111]). This means that for all wave functions that are eigenfunctions of the number operator the average position is precisely in the middle, at q_0. Therefore the momentum has zero expectation value. The coherent states represent shifted states; their position is not in the middle. Note that we have used the Heisenberg picture where the states are time-independent. To see the time-dependent behavior of the coherent states, we consider the product

$$e^{-iHt}|\lambda, z\rangle .$$

If we now shift the lowest energy to zero (that is, we choose $V_0 = \frac{1}{2}\hbar\omega$), and use (20.22) and

$$e^{-i\frac{H}{\hbar}t}|n\rangle = e^{-i\omega nt}|n\rangle ,$$

we see

$$e^{-i\frac{H}{\hbar}t}|\lambda, z\rangle = |\lambda, ze^{-i\omega t}\rangle .$$

The coherent states thus swing from left to right in the potential with a frequency ω and with amplitude $|z|/2m\omega$. In order to see the action of the Heisenberg group on the coherent state, we calculate

$$(e^{\alpha n}\psi)_k = e^{\alpha k}\psi_k \quad \Rightarrow e^{\alpha n}|\lambda, z\rangle = |\lambda, e^{\alpha} z\rangle .$$

From $a|\lambda, z\rangle = \hbar\overline{z}|\lambda, z\rangle$ it follows that

$$e^{\alpha a}|\lambda, z\rangle = e^{\hbar\alpha\overline{z}}|\lambda, z\rangle = |e^{\hbar\alpha\overline{z}}\lambda, z\rangle .$$

Further, we have

$$e^{\overline{\alpha}a^*}|\lambda, z\rangle = \sum_{k,l} \frac{\overline{\alpha}^k (a^*)^k}{k!} \overline{\lambda} \frac{\overline{z}^l (a^*)^l}{l!} \hat{\psi} = \sum_k \overline{\lambda} \frac{\overline{\alpha + z}^k}{k!} (a^*)^k \hat{\psi} = |\lambda, z + \alpha\rangle ,$$

and also we have

$$e^{\alpha}|\lambda, z\rangle = |e^{\alpha}\lambda, z\rangle .$$

We summarize this and write

$$e^{\alpha n}|\lambda, z\rangle = |\lambda, e^{\alpha} z\rangle\,, \quad e^{\alpha a}|\lambda, z\rangle = |e^{\alpha\hbar z}\lambda, z\rangle \tag{20.27}$$

$$e^{\overline{\alpha} a^*}|\lambda, z\rangle = |\lambda, z+\alpha\rangle\,, \quad e^{\alpha}|\lambda, z\rangle = |e^{\alpha}\lambda, z\rangle\,. \tag{20.28}$$

We can apply arbitrary group elements by taking products.

The **Glauber coherent states** introduced in the present section for the Heisenberg group, can be generalized. Indeed, the concept of coherent states extends to a large class of Lie groups acting on so-called co-adjoint orbits of the group. In each case, the co-adjoint orbit provides a manifold of labels for the coherent states on which the group acts, and the coherent states span in an overcomplete fashion a Hilbert space on which the group acts as an irreducible highest weight representation. We shall discuss highest weight representations in Chapter 22, but cannot give details for the general case mentioned here. Instead, we refer the reader to the book by Perelomov [216] and to the extensive survey by Zhang et al. [300].

20.8 Monochromatic beams and coherent states

As indicated in Section 5.6 for the case of a beam of monochromatic light, the modes of the electromagnetic field play the role of the annihilation and creation operator of the quantum field. Classically the observables are functions on phase space, hence specified to a certain observable we have an operator on the configuration space. Namely a physical configuration is specified by giving the values of the observables, and to any observable we assign the operator that reads off the value of that observable. Thus if a configuration of a laser beam, which we suggestively denote $|\mathbf{E}\rangle$, is specified by an electric field $\mathbf{E}(x, y, z, t)$, then the operator $\mathcal{E}(x, y, z, t)$ reads off the values of the components of the electric field at the space-time point (x, y, z, t):

$$\mathcal{E}(x, y, z, t)|\mathbf{E}\rangle = \mathbf{E}(x, y, z, t)|E\rangle\,.$$

In the transition from classical mechanics to quantum mechanics the role of the operator $\mathcal{E}(x, y, z, t)$ is played by the operator's positive frequency part of the electromagnetic field. The above equation then tells us that $|\mathbf{E}\rangle$ is an eigenvalue of the annihilation operator.

In a classical system there are many photons and the number of photons need not be constant, due to absorption and due to the constant photon production of the laser. Hence, from a micromechanical point of view, the quantum number n is no longer a good quantum number to assign to a system resembling a laser. However we know that the electric field is nearly perfectly constant, and if the beam goes in one direction we can take the expression

$$\mathbf{E}(x, y, z, t) = a^* \mathbf{e}^{i\omega_k t}\mathbf{u}(\mathbf{x})\,,$$

for the electric field, where a^* is an annihilator operator. Since the classical state of the laser has a well-defined value of the electric field, the quantum state $|\mathbf{E}\rangle$ that mimics the

classical state the most is the one where

$$a^* \mathbf{e}^{i\omega_k t} \mathbf{u}(\mathbf{x}) |\mathbf{E}\rangle = \mathbf{E}(x, y, z, t) |\mathbf{E}\rangle \, .$$

But then $|\mathbf{E}\rangle$ is an eigenvector of a^*. This similarity between coherent states and classical states is what motivated Roy Glauber to investigate coherent states and apply his analysis to the (quantum and semiclassical) theory of light.

All this extends with suitable modifications to the other wave equations described in Sections 5.5 and 5.4. In each case, there are families of coherent states describing nearly classical ray-like behavior, and there are more exotic quantum states which behave quite unlike any classical system.

Chapter 21

Spin and fermions

This chapter discusses the quantum mechnaics of spinning systems, where the only relevant degrees of freedom correspond to rotation.

The quantum version of the classical rotator discussed in Section 12.4 can be obtained by looking for canonical anticommutation relations, which naturally produce the Lie algebra of a spinning top. As for oscillators, the canonical anticommutation relations have a unique irreducible unitary representation, which corresponds to a spin 1/2 representation of the rotation group. The multimode version gives rise to fermionic Fock spaces; in contrast to the bosonic case, these are finite-dimensional when the number of modes is finite. In particular, the single mode fermionic Fock space is 2-dimensional.

Many constructions for bosons and fermions only differ in the signs of certain terms, such as commutators versus anticommutators. For example, quadratic expressions in bosonic or fermionic Fock spaces form Lie algebras, which give natural representations of the universal covering groups of the Lie algebras $so(n)$ in the fermionic case and $sp(2n, \mathbb{R})$ in the bosonic case, the so-called spin groups and metaplectic groups, respectively. In fact, the analogies apart from sign lead to a common generalization of bosonic and fermionic objects in form of super Lie algebras, which, however are outside the scope of the book.

Apart from the Fock representation, the rotation group has a unique irreducible unitary representation of each finite dimension. We derive these spinor representations by restriction of corresponding nonunitary representations of the general linear group $GL(2, \mathbb{C})$ on homogeneous polynomials in two variables, and find corresponding spin coherent states.

21.1 Fermion Fock space

As we have seen in Section 12.4 the affine functions in the Poisson algebra of the spinning top make up the Lie algebra $u(2)$. One can thus expect that the quantization of the spinning top boils down to representation theory of $su(2)$ and $u(2)$ and indeed it does. In the following sections the representations of $su(2)$ and $u(2)$ play an important role. See for

example HUMPHREYS [131] or JACOBSEN [136] for a comparison of the methods used.

In this section, however, we look at a particular representation, the Fock representation of $u(2)$. It behaves in many respects like the Fock representation of the Heisenberg algebra, and gives the right generalization to the case of many fermionic modes, and in particular to quantum field theory.

In fact, there are many analogies between bosonic and fermionic systems – many formulas look alike, apart for the occurrence of additional minus signs in certain places.[1] Although very similar in many respects, there is a fundamental difference with basic representation theory of bosons and fermions. While bosons are characterized by canonical commutation relations, fermions are quantized using canonical anticommutation relations. We shall see in a moment that this naturally reproduces the Lie algebra $u(2)$ of a spinning top, and – just like for canonical commutation relations – uniquely fixes the representation.

We define a **signed commutator**

$$[f,g]_\pm := fg \mp gf\,;$$

the upper sign applies to 'bosonic' quantities f,g, and reproduces the ordinary commutator, $[f,g]_+ = [f,g]$, while the lower sign applies to 'fermionic' quantities f,g, and reproduces the **anticommutator**

$$[f,g]_- = fg + gf\,.$$

Often, the anticommutator is written instead as $\{f,g\}$, which looks like a Poisson bracket, so that we don't recommend this notation. In the theory of Lie superalgebras, the sign at the commutator is not written at all, since the context already determines the nature of the arguments, and hence implies the commutator sign.

To understand how anticommutators give rise to the $u(2)$ Lie algebra governing a spinning top, we impose the **canonical anticommutation relations** on operators a and $a^* = (a)^*$ in some Hilbert space

$$[a,a^*]_- = \hbar\,, \quad [a,a]_- = 0\,, \quad [a^*,a^*]_- = 0\,.$$

In particular we have $a^2 = (a^*)^2 = 0$. The algebra $\mathbb{E}$ spanned by $1, a$ and a^* is four-dimensional since these generators together with $aa^* - a^*a$ already span $\mathbb{E}$. Hence $\mathbb{E}$ is isomorphic to the algebra of complex 2×2-matrices; an explicit isomorphism is obtained by identifying a and a^* with the matrices

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

respectively and $aa^* - a^*a$ with σ_3. The Lie $*$-algebra $\mathbb{L}$ described by 1, a, a^* and $[a,a^*]$ is thus $u(2)$. Thus the anticommutation relation automatically produce the right Lie algebra for a spinning rigid body, and $u(2)$ is the fermionic analogue of the oscillator algebra $os(1)$.

[1] To see how this leads to the vast mathematical area of superalgebras and supergeometry we refer the interested reader to for example VARADARAJAN [280], SCHEUNERT [246], TUYNMAN [272], DELIGNE et al. [82] and references.

We can get the same result more formally on the quantum level in a way which is completely analogous to the bosonic case, by considering an arbitrary unitary representations of the canonical anticommutation relations, i.e., for linear operators a and a^* satisfying these relations. We introduce the operator

$$n := \hbar^{-1} a^* a \,,$$

and we let $\psi \in V_\lambda$ for some Verma module V_λ; as in Section 20.3, this means $n\psi = \lambda\psi$. We obtain

$$na\psi = \hbar^{-1} a^* a a \psi = 0 \,,$$

and hence $a\psi \in V_0$. Further,

$$na^*\psi = \hbar^{-1} a^* a a^* \psi = a^*\psi \,,$$

and therefore $a^*\psi \in V_1$. To compute λ we proceed

$$\hbar^2 n^2 \psi = a^* a a^* a \psi = \hbar a^* a \psi = \hbar^2 n \psi$$

and hence $\lambda^2 - \lambda = 0$, from which we deduce $\lambda = 0, 1$. Thus we have arrived at the remarkable conclusion that the canonical anticommutation relations lead to two-dimensional Hilbert spaces.

We take a basis vector $|0\rangle$ in V_0 and we define $|1\rangle = a^*|0\rangle$. The Lie $*$-algebra $\mathbb{L}$ acts on the space spanned by $|0\rangle$ and $|1\rangle$, which is isomorphic to $\mathbb{C}^2$. This representation is called the **Pauli representation**. In the above we have thus shown that the Pauli representation is the unique irreducible unitary representation of the canonical anticommutation relations. This is the fermionic analogue of the Stone–von Neumann theorem.

In analogy with the boson case, the representation space $\mathbb{C}^2$ is called the **single mode fermion Fock space**.

We shall see in Section 2.11 that the irreducible representations of $su(2)$ are in one-to-one correspondence with the (finite) dimension of the representation space. For historical reasons, this dimension is usually denoted by $2j + 1$, and j is called the **spin** of the representation. Clearly, the spin j is half a nonnegative integer. In particular, the single mode fermionic Fock space has dimension 2 and hence spin $j = 1/2$.

In general, cf. Section 3.14, elementary particles are associated with an irreducible representation of the Poincaré algebra (or in the nonrelativistic limit the Galileo algebra), which is characterized by mass and spin. The spin assigment in these representations is such that, in the massive case, the restriction to a center of mass frame at a fixed time gives an irreducible representation of the Lie algebra $so(3) = su(2)$ of the same spin. (The massless case is not related to $u(2)$.)

Elementary particles of integral spin (bosons) are represented by a bosonic Fock space, those of nonintegral spin (fermions) by a fermionic Fock space. This fact is a consequence of the so-called **spin-statistics theorem** which holds under certain causality assumptions related to Poincaré invariance of a field theory. Fermionic particles obey the Pauli exclusion principle (Pauli [212], Schwinger [250], Streater [264]).

21.2 Extension to many degrees of freedom

Suppose that the algebra of linear operators on some vector space $\mathbb{H}$ contains, for some linearly ordered set[2] M of labels, quantities a_j and a_j^* ($j \in M$) satisfying the relations

$$[a_j, a_k]_\pm = [a_j^*, a_k^*]_\pm = 0, \quad [a_j, a_k^*]_\pm = \delta_{jk}\,, \quad (j, k \in M). \tag{21.1}$$

For the upper sign (the bosonic case), these are just the canonical commutation relations defining a Heisenberg algebra corresponding to harmonic oscillators with finitely many degrees of freedom. For the lower sign (the fermionic case), the relations (21.1) generalize the canonical anticommutation relations which we have met for the spinning top; we thus expect to get an analogue of the spinning top with n degrees of freedom.

In this section, we consider the fermionic case. We first assume that we have a unitary faithful representation and deduce enough properties that determine the representation uniquely. Then we use the properties deduced to construct the representation.

The canonical anticommutation relations imply that

$$a_j a_k = -a_k a_j\,, \quad a_j^* a_k^* = -a_k^* a_j^*\,, \quad a_j a_k^* = \delta_{jk} - a_k^* a_j\,, \tag{21.2}$$

and again we have in particular $a_j^2 = (a_j^*)^2 = 0$. To find the unitary representations of physical interest, we assume – in analogy to the bosonic case of the canonical commutation relations – the existence of a nonzero vector ψ_0, the **ground state**, such that

$$a_j \psi_0 = 0 \quad \text{for all } j \in M\,. \tag{21.3}$$

We next define for any finite set $J = \{j_1, \ldots, j_l\}$ of distinct labels $j_1 < \ldots < j_l$ from M the vectors

$$|J\rangle := |j_1 \ldots j_l\rangle := a_{j_1}^* \cdots a_{j_l}^* \psi_0 \quad |\emptyset\rangle = \psi_0\,. \tag{21.4}$$

Since we want a faithful representation, we may assume that $|J\rangle \neq 0$. Indeed suppose $|J\rangle = 0$ for $J = \{j_1, \ldots, j_l\}$, then acting on $|J\rangle$ with $a_{j_{l-1}} \cdots a_{j_1}$ we see that $a_{j_l}^*$ acts as 0. Because of (21.2), we have

$$a_j|J\rangle = \begin{cases} \varepsilon_j(J)|J \setminus \{j\}\rangle & \text{if } j \in J, \\ 0 & \text{if } j \notin J, \end{cases} \qquad a_j^*|J\rangle = \begin{cases} 0 & \text{if } j \in J, \\ \varepsilon_j(J)|J \cup \{j\}\rangle & \text{if } j \notin J, \end{cases} \tag{21.5}$$

where the sign $\varepsilon_j(J)$ is defined to be $+1$ if there is an even number of indices in J that are smaller than j and -1 otherwise.

21.2.1 Proposition. *We have the following identities:*

$$\varepsilon_j(J \setminus \{j\}) = \varepsilon_j(J) \quad \textit{for } j \in J\,, \tag{21.6}$$

$$\varepsilon_j(J \cup \{j\}) = \varepsilon_j(J) \quad \textit{for } j \notin J\,, \tag{21.7}$$

$$\varepsilon_j(J)\varepsilon_k(J \cup \{j\}) = -\varepsilon_k(J)\varepsilon_j(J \cup \{k\}) \quad \textit{for } j, k \notin J\,,\ j \neq k\,, \tag{21.8}$$

$$\varepsilon_j(J)\varepsilon_k(J \setminus \{j\}) = -\varepsilon_k(J)\varepsilon_j(J \setminus \{k\}) \quad \textit{for } j, k \in J\,,\ j \neq k\,, \tag{21.9}$$

$$\varepsilon_j(J)\varepsilon_k(J \cup \{j\}) = -\varepsilon_k(J)\varepsilon_j(J \setminus \{k\}) \quad \textit{for } j \notin J\,, k \in J\,. \tag{21.10}$$

[2] A set M is a linearly ordered if there is a binary relation $\leq$ such that for all $m, n, p \in M$: (1) $m \leq m$, (2) $m \leq n$ and $n \leq m$ then $m = n$, (3) $m \leq n$ and $n \leq p$ then $m \leq p$, (4) either $m \leq n$ or $n \leq m$.

Proof. This is a straightforward consequence of the definition, taking into account when $\varepsilon_j(J)$ and $\varepsilon_k(J)$ change sign if an index is removed or added to J. □

We define $\mathbb{F}_-(M)$ to be the vector space spanned by the $|J\rangle$. By definition, $\mathbb{F}_-(M)$ consists of the finite linear sums of the elements $|J\rangle$.

21.2.2 Proposition.
(i) The vectors $|J\rangle$ are linearly independent.

(ii) The vector space $\mathbb{F}_-(M)$ is an irreducible representation space for the canonical anticommutation relations.

Proof. (i) Suppose that we have $\sum_J c_J|J\rangle = 0$ with finitely many nonzero coefficients. and let $J = \{j_1, \ldots, j_l\}$ $(j_1 < \ldots < j_l)$ be a set of maximal size among the sets with $c_J \neq 0$. In view of (21.5), multiplication by $a_{j_l} \cdots a_{j_1}$ leaves as only nonzero term $\pm c_J|\emptyset\rangle = 0$. Since the ground state ψ_0 is nonzero, we conclude that $c_J = 0$, contradiction. Therefore, the vectors (21.4) are linearly independent and form a basis of $\mathbb{F}_-(M)$.

(ii) Equations (21.5) imply that a_j and a_j^* map $\mathbb{F}_-(M)$ into itself. Irreducibility of the representations follows since the same argument used in (i) implies that any invariant subspace of $\mathbb{F}_-(M)$ containing a nonzero element contains the ground state, hence all $|J\rangle$, and hence all elements of $\mathbb{F}_-(M)$. □

Since the $|J\rangle$ form a basis of $\mathbb{F}_-(M)$, we may identify a vector $\psi \in \mathbb{F}_-(M)$ with the **fermion wave function** ψ defined on the finite subsets of M whose value at $J \subseteq M$ is the coefficient $\psi(J)$ in the basis expansion

$$\psi = \sum_{J \subseteq M} \psi(J)|J\rangle\,,$$

where the summation is over all finite subsets J of M. Note that only finitely many coefficients $\psi(J)$ are nonzero.

21.2.3 Proposition. *Under the assumption* (21.3), *the anticommutation relations* (21.2) *imply that the linear operators*

$$a(u) := \sum_{j \in M} u_j a_j, \quad a^*(u) := \sum_{j \in M} u_j a_j^*,$$

defined for all vectors u indexed by M which have only finitely many nonzero entries, act on fermion wave functions according to

$$(a(u)\psi)(J) = \sum_{j \notin J} \varepsilon_j(J) u_j \psi(J \cup \{j\})\,, \quad (a^*(u)\psi)(J) = \sum_{j \in J} \varepsilon_j(J) u_j \psi(J \setminus \{j\})\,. \tag{21.11}$$

Proof. We have

$$a_j\psi = \sum_J \psi(J) a_j|J\rangle = \sum_{J \ni j} \psi(J)\varepsilon_j(J)|J \setminus \{j\}\rangle = \sum_{J \not\ni j} \psi(J \cup \{j\})\varepsilon_j(J \cup \{j\})|J\rangle,$$

and using (21.7), we find

$$(a_j\psi)(J) = \begin{cases} 0 & \text{if } j \in J, \\ \varepsilon_j(J)\psi(J \cup \{j\}) & \text{if } j \notin J. \end{cases}$$

Taking linear combinations proves the first assertion. Similarly,

$$a_j^*\psi = \sum \psi(J)a_j^*|J\rangle = \sum_{J \not\ni j} \psi(J)\varepsilon_j(J)|J \cup \{j\}\rangle = \sum_{J \ni j} \psi(J \setminus \{j\})\varepsilon_j(J \setminus \{j\})|J\rangle\,.$$

Using (21.6), we find

$$(a_j^*\psi)(J) = \begin{cases} \varepsilon_j(J)\psi(J \setminus \{j\}) & \text{if } j \in J, \\ 0 & \text{if } j \notin J\,. \end{cases}$$

Taking linear combinations proves the second assertion. □

For a unitary representation, we need that a_j is the Hermitian conjugate of a_j^*, which is the case if and only if the $|J\rangle$ are orthonormal. Indeed, suppose $J \neq J'$, then we may assume there is $j \in J$ that is not in J' (else turn the role of J and J' around). But then $\langle J|J'\rangle = \langle J \setminus \{j\}|a_j|J'\rangle = 0$. Hence we may assume that $\mathbb{F}_-(M)$ has the inner product

$$\phi^*\psi = \sum_J \overline{\phi(J)}\psi(J)\,. \tag{21.12}$$

To show that unitary representations with the desired conjugation and anticommutation relations actually exist, we start with the space $\mathbb{F}_-(M)$ of complex valued functions ψ defined on finite subsets of an arbitrary set M such that only finitely many values $\psi(J)$ are nonzero. Then (21.12) defines an inner product on $\mathbb{F}_-(M)$, and the completion $\overline{\mathbb{F}_-(M)}$ of $\mathbb{F}_-(M)$ in the associated norm is a Hilbert space, called the **fermion Fock space** over M.

For a concise formulation of the result, we use a slightly more abstract notation. We introduce the Euclidean space $\mathbb{H}$ of vectors indexed by M with finite support, equipped with the bilinear form

$$u^T v := \sum_{k \in M} u_k v_k\,,$$

and write $\mathbb{F}_-\mathbb{H} := \mathbb{F}_-(M)$. In applications to quantum field theory, $\mathbb{H}$ becomes the infinite-dimensional single-particle Hilbert space, and the sums become integrals over momentum vectors, but the formulas below remain valid with an appropriate interpretation.

21.2.4 Theorem. *The relations* (21.11) *define two linear mappings* a, a^* *from* $\mathbb{H}$ *to the algebra* $\mathrm{Lin}(\mathbb{F}_-, \mathbb{H})$*, and we have*

$$(a(u))^* = a^*(\overline{u})\,, \tag{21.13}$$

$$a(u)a(v) + a(v)a(u) = 0\,, \qquad a^*(u)a^*(v) + a^*(v)a^*(u) = 0\,, \tag{21.14}$$

$$a(u)a^*(v) + a^*(v)a(u) = u^T v. \tag{21.15}$$

In particular, taking for u, v *vectors with a single nonzero entry, we find the canonical anticommutation relations* (21.2)*.*

Proof. From the definitions (21.11) and (21.12), we find

$$\phi^* a^*(\overline{u})\psi = \sum_J \overline{\phi(J)} \sum_{j\in J} \varepsilon_j(J)\overline{u}_j \psi(J\setminus\{j\})\,.$$

Renaming the $J\setminus\{j\}$ to J, we get in view of (21.6) and (21.7)

$$\begin{aligned}\phi^* a^*(\overline{u})\psi &= \sum_J \sum_{j\notin J} \varepsilon_j(J\cup\{j\})\overline{u}_j \overline{\phi(J\cup\{j\})}\psi(J)\\ &= \sum_J \sum_{j\notin J} \varepsilon_j(J)\overline{u}_j \overline{\phi(J\cup\{j\})}\psi(J) = (a(u)\phi)^*\psi\,.\end{aligned}$$

This implies (21.13). To prove (21.14), we note that in view of (21.8),

$$\begin{aligned}(a(u)a(v)\psi)(J) &= \sum_{j\notin J}\sum_{k\notin J\cup\{j\}} \varepsilon_j(J)\varepsilon_k(J\cup\{j\})u_j v_k \psi(J\cup\{j,k\})\\ &= -\sum_{k\notin J}\sum_{j\notin J\cup\{k\}} \varepsilon_k(J)\varepsilon_j(J\cup\{k\})u_j v_k \psi(J\cup\{j,k\})\\ &= -(a(v)a(u)\psi)(J)\,.\end{aligned}$$

This proves the first formula in (21.14), and the second formula follows with (21.13). Finally, to prove (21.15), we note that

$$(a(u)a^*(v)\psi)(J) = \sum_{j\notin J}\sum_{k\in J\cup\{j\}} \varepsilon_j(J)\varepsilon_k(J\cup\{j\})u_j v_k \psi(J\cup\{j\}\setminus\{k\})\,, \tag{21.16}$$

and

$$(a^*(v)a(u)\psi)(J) = \sum_{k\in J}\sum_{j\notin J\setminus\{k\}} \varepsilon_k(J)\varepsilon_j(J\setminus\{k\})u_j v_k \psi(J\setminus\{k\}\cup\{j\})\,. \tag{21.17}$$

The sets of pairs (j,k) over which the summation in the two equations is taken, contain the pairs with $j\notin J, k\in J$, for which the signs are opposite by (21.10). Thus the corresponding terms in the sums cancel when the two equations are added. The remaining terms consist in (21.16) of the terms with $k=j\notin J$ and in (21.17) of the terms with $j=k\in J$; for the corresponding terms in the sums, all signs are $+1$. Therefore, adding the two equations results in

$$(a(u)a^*(v)\psi)(J) + (a^*(v)a(u)\psi)(J) = \sum_{j\notin J} u_j v_j \psi(J) + \sum_{k\in J} u_k v_k \psi(J) = u^T v\psi(J)\,.$$

□

21.3 Exterior algebra representation

We now show another important realization of the anticommutation relations, equivalent to that of the preceding section but phrased in a different language familiar from differential geometry.

For any vector space $\mathbb{H}$ we consider the tensor algebra $\bigoplus \mathbb{H} = \mathbb{C} \oplus \mathbb{H} \oplus (\mathbb{H} \otimes \mathbb{H}) \ldots$, which is an associative algebra with unity where multiplication is the tensor product. We define the ideal $\mathbb{J}_{\mp}$ to be the ideal generated by the elements $v \otimes w \mp w \otimes v$ for $v, w \in \mathbb{H}$. The quotients

$$\mathbb{H}/\mathbb{J}_- = \bigvee \mathbb{H}\,, \quad \mathbb{H}/\mathbb{J}_+ = \bigwedge \mathbb{H}\,,$$

that we obtain by dividing out by the ideals $\mathbb{J}_{\mp}$ are equipped with a natural algebra structure, since we divided out by ideals. We call $\bigvee \mathbb{H}$ the **symmetric algebra** and $\bigwedge \mathbb{H}$ the **exterior algebra**. The product in the exterior algebra is written as $v \wedge w$ in place of vw, and is then called the **exterior product** or **wedge product**. The product $\wedge$ satisfies the anticommutative law

$$v \wedge w = -w \wedge v$$

for any two vectors $v, w \in \mathbb{H}$, but not for general elements of $\bigwedge \mathbb{H}$; $u \wedge v \wedge w = w \wedge u \wedge v$.

The symmetric algebra leads to a representation of the canonical commutation relations (see Section 20.6); the exterior algebra to one of the canonical anticommutation relations.

We concentrate on the latter, and restrict to finite-dimensional vector spaces. If $\mathbb{H}$ is a vector space of finite dimension n we may choose a basis $e_1, \ldots, e_n$. Using the anticommutation relations one easily verifies that the exterior algebra $\bigwedge \mathbb{H}$ has a basis consisting of the elements

$$1\,; \quad e_i\,; \quad e_i \wedge e_j \;\; (i < j)\,; \quad e_i \wedge e_j \wedge e_k \;\; (i < j < k)\,; \quad \ldots; \quad e_1 \wedge e_2 \wedge \cdots \wedge e_n\,,$$

making a total of 2^n basis vectors. Thus the dimension of $\bigwedge \mathbb{H}$ is 2^n. We now introduce operators a_k given by

$$a_k(\omega) = e_k \wedge \omega \quad \text{for } \omega \in \bigwedge \mathbb{H}\,;$$

in particular, $a_k(1) = e_k$. Similarly we define operators a_k^* as follows: On elements of the form $\omega = e_k \wedge \omega'$ we put

$$a_k^*(\omega) := a_k^*(e_k \wedge \omega') = \omega',$$

but if we cannot write ω into the form $\omega = e_k \wedge \omega'$ we put

$$a_k^*(\omega) := 0\,.$$

We now show that we have

$$a_k a_l^* + a_l^* a_k = \delta_{kl}\,. \tag{21.18}$$

First we assume that we cannot write ω in the form $e_k \wedge \omega'$ and neither in the form $e_l \wedge \omega''$. In this case we have

$$a_k \circ a_l^*(\omega) + a_l^* \circ a_k(\omega) = a_l^*(e_k \wedge \omega) = \delta_{kl}\omega\,.$$

If we can write ω as $e_k \wedge \omega'$ but not as $e_l \wedge \omega''$ then we have $k \neq l$ and

$$a_k \circ a_l^*(\omega) + a_l^* \circ a_k(\omega) = a_l^* \circ a_k(e_k \wedge \omega') = 0\,.$$

If $k = l$ and $\omega = e_k \wedge \omega'$ we have

$$a_k \circ a_k^*(\omega) + a_k^* \circ a_k(e_k \wedge \omega') = a_k \circ a_k^*(e_k \wedge \omega') = \omega\,.$$

In the last case, when $k \neq l$ but we can write $\omega = e_k \wedge e_l \wedge \omega$ we have

$$a_k \circ a_l^*(\omega) = a_k \circ a_l^*(-e_l \wedge e_k \wedge \omega') = 0$$

and

$$a_l^* \circ a_k(\omega) = a_l^* \circ a_k(e_k \wedge e_l \wedge \omega) = 0\,.$$

Putting it all together we indeed have (21.18).

Generalized to infinite dimensions, (21.18) is the basis for the description of fermion fields in quantum field theory.

21.4 Spin and metaplectic representation

In analogy to the bosonic case treated in Section 13.1, we now show that quadratic expressions in anticommuting operators a and a^* make up well-known finite-dimensional Lie algebras, in this case the orthogonal algebras $so(2n)$ and $so(2n+1)$.

The method of derivation is different however. It works for bosons and fermions simultaneously, with differences only in certain signs, and gives in the bosonic case a construction of the metaplectic representation of $sp(2n, \mathbb{R})$ and the central extension of $isp(2n, \mathbb{R})$. In the sequel, the upper signs apply for the bosonic case, and the lower signs apply for the fermionic case. We use coordinate-independent notation, so that the method can be taken over almost literally to the infinite-dimensional case.

We assume that we have a linear mapping $a : \mathbb{H} \to \mathbb{E}$ that assigns to each α from some vector space $\mathbb{H}$ an element $a(\alpha)$ in an associative algebra $\mathbb{E}$ with identity 1 such that

$$[a(\alpha), a(\beta)]_\pm = a(\alpha)a(\beta) \mp a(\beta)a(\alpha) \in \mathbb{C}\,. \tag{21.19}$$

For example, with the standard generators a_k, a_k^* in a bosonic or fermionic Fock space, we can take

$$a(\alpha) = \sum_k (\alpha_k a_k + \alpha_{-k} a_k^*).$$

For the bosonic case, (21.19) means that the Lie algebra that is obtained by equipping $\mathbb{E}$ with the commutator as Lie product, contains a central extension of a commutative algebra.

The ground state on $\mathbb{E}$ is a positive linear functional $\langle\cdot\rangle$ that satisfies $\langle 1\rangle = 1$. Linearity implies that there is a linear operator G satisfying

$$\langle a(\alpha)a(\beta)\rangle = \alpha^T G \beta\,;$$

(21.19) then implies that

$$a(\alpha)a(\beta) \mp a(\beta)a(\alpha) = \alpha^T J \beta\,.$$

where

$$J := G \mp G^T, \quad J^T = \mp J\,.$$

In Section 13.1, the bilinear form ω was represented by an antisymmetric nondegenerate $2n\times 2n$-matrix. This is the most interesting case, although in the first part of the discussion below J can be degenerate.

Any quadratic expression in the a_k and a_k^* is a sum of terms of the form $a(\alpha)a(\beta)$; this is nothing else than the statement that any matrix is a sum of matrices of the form $M = mn^T$ for some vectors m and n. We define the quadratic expression[3]

$$N(\alpha\beta^T) := \frac{1}{2}\Big(a(\alpha)a(\beta) - \alpha^T G\beta\Big)\,.$$

and extend them by linearity (using a basis it is easy to see that the extension is unique and well-defined). We thus have $\langle N(f)\rangle = 0$ for all quadratic expressions f. We also have

$$a(\alpha)a(\beta) = 2N(\alpha\beta^T) + \mathrm{tr}(G^T\alpha\beta^T)\,.$$

Remember that in Section 13.1 we considered the symmetric combination $2E_{ij} = p_iq_j + q_jp_i$. Motivated by this we restrict our attention to $f = \sum_i \alpha_i\beta_i^T$ such that $f^T = \pm f$. For a single term $f = \alpha\beta^T = \pm f^T$, we find

$$\begin{aligned}
2[N(f), a(\gamma)] &= a(\alpha)a(\beta)a(\gamma) - a(\gamma)a(\alpha)a(\beta)\\
&= \pm a(\alpha)a(\gamma)a(\beta) + a(\alpha)\beta^T J\gamma \mp a(\alpha)a(\gamma)a(\beta) - a(\beta)\gamma^T J\alpha\\
&= a(\alpha\beta^T J\gamma) - a(\beta\alpha^T J^T\gamma)\\
&= a(fJ\gamma - f^T J^T\gamma)\,,
\end{aligned}$$

so that by linearity,

$$[N(f), a(\gamma)] = N(f)a(\gamma) - a(\gamma)N(f) = a(fJ\gamma)$$

for $f = \pm f^T$. Similarly for $g = \gamma\delta^T = \pm g^T$ we find

$$\begin{aligned}
2[N(f), N(g)] &= [N(f), a(\gamma)]a(\delta) + a(\gamma)[N(f), a(\delta)]\\
&= a(fJ\gamma)a(\delta) + a(\gamma)a(fJ\delta)\\
&= 2N(fJ\gamma\delta^T) + \mathrm{tr}(G^T fJ\gamma\delta^T) + 2N(\gamma(fJ\delta)^T) + \mathrm{tr}(G^T\gamma(fJ\delta)^T)\\
&= 2N(fJg - gJf) + \mathrm{tr}(G^T(fJg - gJf)),
\end{aligned}$$

so that again by linearity,

$$\begin{aligned}
[N(f), N(g)] &= N(fJg - gJf) + \frac{1}{2}\,\mathrm{tr}(G^T(fJg - gJf))\\
&= N(fJg - gJf) + \frac{1}{2}\,\mathrm{tr}((G \pm G^T)fJg)\,.
\end{aligned}$$

Writing

$$(s, \alpha, f) = N(f) + a(\alpha) + s1,$$

[3]In infinite dimensions, this amounts to a renormalization step that is conventionally described as "subtracting infinite constants" arising at a later stage of the development. Our formulas are renormalized from the outset, and no infinite constants arise.

we find for the bosonic case

$$[(s,\alpha,f),(s',\alpha',f')] = \big(\tfrac{1}{2}\operatorname{tr}((G+G^T)fJf') + \alpha^T J\alpha', fJ\alpha' - f'J\alpha, fJf' - f'Jf\big)$$

and for the fermionic case

$$[(s,\alpha,f),(s',\alpha',f')] = \big(S(f,f',\alpha,\alpha'), fJ\alpha' - f'J\alpha, fJf' - f'Jf + 2(\alpha\alpha'^T - \alpha'\alpha^T)\big)\ ,$$

where

$$S(f,f',\alpha,\alpha') = \tfrac{1}{2}\operatorname{tr}\Big((G-G^T)fJf'\Big) + \alpha^T J\alpha'.$$

Fermionic case. To exploit these formulas, we first focus on the fermionic case, and assume that J is nondegenerate; without loss of generality, we may choose J to be the $2n\times 2n$ identity matrix, $J=1$.

We consider the Lie algebra $\mathbb{L}$ defined by the quadratic elements modulo the constant term; that is, we factor out the center. We write (α,f) for the equivalence class of (s,α,f). The quadratic expressions f are antisymmetric, $f^T=-f$, and thus correspond to $so(2n,\mathbb{C})$. Let us consider the map $u:\mathbb{L}\to sl(2n+1,\mathbb{C})$ defined by

$$u:(\alpha,f)\mapsto \begin{pmatrix} f & 2^{-1/2}\alpha \\ 2^{-1/2}\alpha^T & 0 \end{pmatrix}.$$

The map u is injective and preserves the Lie product and thus is an isomorphism onto its image. The image under u of $\mathbb{L}$ is the Lie algebra $so(2n+1,\mathbb{C})$. It can easily be seen that matrices in the image satisfy

$$\begin{pmatrix} f & \alpha \\ \alpha^T & 0 \end{pmatrix}^T \hat{J} + \hat{J}\begin{pmatrix} f & \alpha \\ \alpha^T & 0 \end{pmatrix} = 0\,, \quad \hat{J} = \begin{pmatrix} J & 0 \\ 0 & -1 \end{pmatrix}\,,$$

since, for fermions, J is the $2n\times 2n$ identity matrix. Restricting this basis to the real numbers we obtain the real form $so(2n,1)$. Summarizing, we have thus established that the quadratic elements (with center) form a central extension of $so(2n+1,\mathbb{C})$. The purely quadratic expressions (no linear and constant terms) form the Lie algebra $so(2n,\mathbb{C})$. Note that the group $O(2n,\mathbb{C})$ is the automorphism group of the algebra defined by the relation

$$b_k b_l^* + b_l^* b_k = \delta_{kl}\,. \tag{21.20}$$

Going to the 'real' basis $c_k = b_k + b_k^*$, $c_{k+n} = i(b_k - b_k^*)$, we see that the real Lie group $O(2n)$ preserves the relations (21.20).

For a finite number of generators, the canonical anticommutation relations have a unique faithful unitary representation. Therefore as in Section 20.6 we can say something interesting about the automorphism group of the algebra defined by (21.20). Performing a rotation $b_k \mapsto b_k' := \sum g_{kl} b_l$ with $g=(g_{kl})$ an element of $SO(2n)$ on the generators b_k we get another representation of the canonical anticommutation relation, but since this representation is unique, there exists a unitary transformation $U(g)$ that relates the obtained representation with the original representation: $b_k' = U(g)b_kU(g)^{-1}$, where we simply wrote b_k for the representation of b_k. Again, $U(g)$ is not unique for a given g, since $-U(g)$ also does the job.

In this way we get a double cover of the group $SO(2n)$, called the **spin group** $Spin(2n)$, just as in Section 20.6 we obtained the metaplectic cover.

Bosonic case. For the bosonic case we may proceed in an analogous way. Again, we assume that J is nondegenerate; this time, the normal form can be taken without loss of generality as an antisymmetric $2n \times 2n$-matrix J that squares to -1.

We again form the Lie algebra $\mathbb{L}$ of inhomogeneous quadratic expressions and factor out the center. We then apply the map to the equivalence classes (α, f)

$$u : (\alpha, f) \mapsto \begin{pmatrix} Jf & \alpha \\ 0 & 0 \end{pmatrix} .$$

It is clear that

$$(Jf)^T J + J(Jf) = -f^T + f = 0 \,,$$

so that the map u is an isomorphism from $\mathbb{L}$ to $isp(2n)$. We thus see that the inhomogeneous quadratic quantities form a central extension of the Lie algebra $isp(2n)$.

Chapter 22

Highest weight representations

This chapter discusses highest weight representations, providing tools for classifying many irreducible representations of interest. We extend the ladder technique used in Section 20.3 for determining the unitary representations of the oscillator algebra to some other small Lie algebras of interest, and indicate how the ideas generalize further.

The basic ingredient is a triangular decomposition, which exists for all finite-dimensional semisimple Lie algebras, but also in other cases of interest such as the oscillator algebra, the Heisenberg algebra with the harmonic oscillator Hamiltonian adjoined.

We look in detail at 4-dimensional Lie algebras with a nontrivial triangular decomposition (among them the oscillator algebra and $so(3)$), which behave almost like the oscillator algebra. As a result, the analysis leading to Fock spaces generalizes without problems, and we are able to classify all irreducible unitary representations of the rotation group. Various related material concerning $SO(3)$ and its universal covering group $SU(2)$ is also included.

22.1 Triangular decompositions

Let $\mathbb{L}$ be a Lie $*$-algebra. A **triangular decomposition** of $\mathbb{L}$ consists of Lie subalgebras $\mathbb{L}_-$, $\mathbb{L}_0$ and $\mathbb{L}_+$ of $\mathbb{L}$ satisfying the properties[1]

(T1) $\mathbb{L} \;=\; \mathbb{L}_- \oplus \mathbb{L}_0 \oplus \mathbb{L}_+$,

(T2) $\mathbb{L}_0 \angle \mathbb{L}_\pm \;\subseteq\; \mathbb{L}_\pm$,

(T3) $\mathbb{L}_0^* = \mathbb{L}_0,\;\; \mathbb{L}_\pm^* = \mathbb{L}_\mp$,

(T4) $\mathbb{L}_0$ is abelian and contains the center $Z(\mathbb{L})$.

[1]Note that the present concept of a triangular decomposition is less demanding and hence more general than in the treatment by Moody & Pianzola [193]. Their additional restrictions allow them to extend much of the finite-dimensional semisimple theory outlined below to the infinite-dimensional case.

Triangular decompositions generalize the properties of annihilation and creation operators in the oscillator algebra $os(1)$ to more general Lie algebras. The terminology derives from the following motivating examples.

22.1.1 Examples. (i) In the Lie algebra $\mathbb{L} = gl(n, \mathbb{C}) = \mathbb{C}^{n\times n}$, we can define a triangular decomposition by defining $\mathbb{L}_0$ to be the Lie subalgebra of diagonal matrices, $\mathbb{L}_+$ to be the Lie subalgebra of strictly upper triangular matrices, and $\mathbb{L}_-$ to be the Lie subalgebra of strictly lower triangular matrices. Verification of the axioms is straightforward.

(ii) The oscillator algebra $os(1)$ has a triangular decomposition, given by

$$\mathbb{L}_- = \mathbb{C}\, a\,, \quad \mathbb{L}_0 = \mathbb{C}\, 1 + \mathbb{C}\, n\,, \quad \mathbb{L}_+ = \mathbb{C}\, a^*\,.$$

A **triangulated Lie algebra** is a Lie $*$-algebra with a distinguished triangular decomposition. We call the number $\operatorname{rk}\mathbb{L} := \dim \mathbb{L}_0/Z(\mathbb{L})$ the **rank**, and $\deg \mathbb{L} := \dim \mathbb{L}_\pm$ the **degree** of the triangulated Lie algebra $\mathbb{L}$. The elements of the dual space[2] $\mathbb{L}_0'$ are called **weights**. A **highest weight representation** is a representation J of $\mathbb{L}$ on a vector space $\mathbb{V}$ with a distinguished element 1, called the **ground state**[3], such that

(HW1) $J(\alpha)1 = 0$ for all $\alpha \in \mathbb{L}_-$, and

(HW2) $J(\alpha)1 \in \mathbb{C}$ for all $\alpha \in \mathbb{L}_0$.

The elements of $\mathbb{L}_-$ thus behave like annihilation operators. The defining properties imply that

$$w(\alpha) := J(\alpha)1\,, \quad \text{for } \alpha \in \mathbb{L}_0\,,$$

defines a weight $w \in \mathbb{L}_0'$, called the **highest weight** of the representation. A highest weight representation is irreducible if and only if the elements $a_1^* \dots a_k^* 1$ with $a_1, \dots, a_k \in \mathbb{L}_-$ span a dense subspace of $\mathbb{V}$. In an irreducible highest weight representation with highest weight w, all Casimir elements C of $\mathbb{L}$ have a fixed value $C(w) \in \mathbb{C}$.

The **spectrum** of $\mathbb{L}$ is the set $\Sigma(\mathbb{L})$ of weights w for which a unitary group representation exists, whose associated infinitesimal representation is a highest weight representation of $\mathbb{L}$ with highest weight w. The spectrum of $\mathbb{L}$ determines the possible spectra of each Casimir element C in arbitrary unitary representations of the universal covering group of $\mathbb{L}$, since the possible eigenvalues are precisely the possible $C(w)$ where w ranges over the spectrum of $\mathbb{L}$.

Note that a weight w belongs to the spectrum of $\mathbb{L}$ iff there is a unitary (cf. Definition 13.2.1) highest weight representation of $\mathbb{L}$ with highest weight w. In this case, there is a Euclidean inner product on $\mathbb{V}$, and without loss of generality, the ground state 1 may be assumed to be normalized.

[2]Since in the context of Lie $*$-algebras, the notation V^* for the dual of V is ambiguous, we use in this section a prime to indicate the dual.

[3]In a quantum field theory context, the ground state is referred to as the **vacuum**.

The semisimple case. There are many examples of triangulated Lie algebras, related to finite-dimensional semisimple Lie algebras (see the outline below) and to important classes of infinite-dimensional Lie algebras.

We mention without proof (which can be found in many places, e.g., FUCHS & SCHWEIGERT [95], FULTON & HARRIS [96], HUMPHREYS [131], JACOBSEN [136], KNAPP [154], KIRILLOV [151]) a number of facts about finite-dimensional semisimple Lie algebras.

All finite-dimensional semisimple real Lie algebras have a triangular decomposition, which is unique up to automorphisms. In this case, $\mathbb{L}_0$ is a Cartan subalgebra (a maximal abelian subalgebra generated by diagonal matrices in the adjoint representation, for some choice of basis), which is unique up to conjugation, and the Lie algebra $\mathbb{L}$ decomposes as

$$\mathbb{L} = \mathbb{L}_0 \oplus \bigoplus_{\alpha\in\Delta} \mathbb{L}_\alpha \,,$$

where $\Delta \subset \mathbb{L}_0'$ is the set of **roots**. The roots are nonzero elements of the dual of the Cartan subalgebra such that the Cartan subalgebra acts diagonally on $\mathbb{L}_\alpha$:

$$h\angle x = \alpha(h)x \,, \quad h \in \mathbb{L}_0, \quad x \in \mathbb{L}_\alpha \,.$$

$\mathbb{L}_\alpha$ is always 1-dimensional; any nonzero element in $\mathbb{L}_\alpha$ is called a **root generator**. For each root $\alpha \in \Delta$ the negative $-\alpha$ is also a root: for all $\alpha \in \mathbb{L}^*$, if $\mathbb{L}_\alpha \neq 0$, then $\mathbb{L}_{-\alpha} \neq 0$. Therefore there exists a choice of ordering such that Δ can be written as the union of the set of positive roots Δ^+ and the set of negative roots Δ^- and $\Delta^- = -\Delta^+$, in such a way that the cone of nonnegative linear combinations from Δ^+ and Δ^- intersect in 0 only. One defines

$$\mathbb{L}_\pm = \bigoplus_{\alpha\in\Delta^\pm} \mathbb{L}_\alpha \,,$$

and finds (using further properties of the roots) that the semisimple Lie algebra is a triangulated Lie algebra.

22.1.2 Example. Take $\mathbb{L} = sl(n, \mathbb{C})$, the Lie algebra of $n \times n$ matrices with trace zero. Let us we write E_{ij} for the matrix that is 1 on the (i, j)-entry and zero everywhere else. Then the diagonal matrices that have trace zero make up the Cartan subalgebra, which is thus spanned by the matrices $E_{ii} - E_{i+1,i+1}$ for $1 \leq i \leq n-1$ so that the rank is $n-1$. We have for $h = \mathrm{diag}(h_1, \ldots, h_n) \in \mathbb{L}_0$ in the Cartan subalgebra and for E_{ij} with $i \neq j$

$$h\angle E_{ij} = (h_i - h_j)E_{ij} \,.$$

Hence the roots are of the form $\lambda_i - \lambda_j$ where λ_i reads off the ith diagonal entry of an element of the Cartan subalgebra. We can choose a root $\lambda_i - \lambda_j$ to be positive if $i < j$. Then $\mathbb{L}_+$ are the upper triangular matrices, and $\mathbb{L}_-$ the lower triangular matrices. The positive root generators are E_{ij} with $i < j$.

Associated with each semisimple Lie algebra is a **weight lattice**, which is a discrete additive subgroup of $\mathbb{L}_0'$ and whose elements are called **integral weights**. Additionally, there is a

distinguished subset of the weight lattice, which is closed under addition and whose elements are called **dominant integral weights**. In terms of these:

(i) For each weight w, there is a Lie representation with w as highest weight.

(ii) A highest weight representation is finite-dimensional if and only if the highest weight is dominant and integral.

(iii) For compact finite-dimensional Lie algebras, that is finite-dimensional Lie algebras with a negative definite Cartan–Killing form (these are automatically semisimple, see Lemma 13.5.1), a highest weight representation is unitary if and only if it is finite-dimensional. The inner product is then uniquely determined by the requirement that the ground state 1 is normalized.

(iv) The Lie algebra induces a unitary representation of the universal covering group $\mathbb{G}$ if and only if w is a dominant integral weight. Thus the spectrum of $\mathbb{L}$ consists of all dominant integral weights of $\mathbb{L}$.

In the context of an integrable classical theory associated with $\mathbb{L}$, (iv) is equivalent to the **Bohr–Sommerfeld quantization condition**. (This folklore result is never stated in a precise form, but see, e.g., Voros [281], Kochetov [155], and Gadiyar [97].)

22.2 Triangulated Lie algebras of rank and degree one

We have seen that the oscillator algebra $os(1)$ has a triangular decomposition of rank and degree 1. A general triangulated Lie $*$-algebra of rank and degree 1 with center $\mathbb{C}$ must be the direct sum of the algebras

$$\mathbb{L}_- = \mathbb{C}a\,, \quad \mathbb{L}_+ = \mathbb{C}a^*\,, \quad \mathbb{L}_0 = \mathbb{C} + \mathbb{C}h\,,$$

where h is a fixed element in $\mathbb{L}_0 \setminus \mathbb{C}$. The center $\mathbb{C}$ commutes with everything, but h in general does not, which is the case we consider here. Then we may rescale h to obtain

$$a\angle h = ia\,.$$

The operation $*$ then gives

$$a^*\angle h = -ia^*\,.$$

For the Lie product of a and a^* we introduce complex numbers u and v and write

$$a\angle a^* = i(uh + v)\,,$$

but noting that $(a\angle a^*)^* = -a\angle a^*$ we see that $u, v \in \mathbb{R}$. It is easy to check that for all $u, v \in \mathbb{R}$ the Jacobi identities are fulfilled and hence for all real numbers u, v we have a Lie $*$-algebra.

For the two-parameter family of Lie $*$-algebras just defined there are essentially four different cases;

1. $u = v = 0$. This is the Lie $*$-algebra $iso(2) \oplus \mathbb{C}$.

2. $u = 0$, $v = \pm 1$. If $u = 0$ we can rescale the a and a^* as $a \mapsto \lambda a$ and $a^* \mapsto \lambda^* a^*$ to get $v = \pm 1$. By complex conjugation of the algebra we then can choose the sign of v and we find the Lie $*$-algebra $os(1)$. For the oscillator algebra we have $h \sim a^* a$.

3. $u = 1$ and $v = 0$. This Lie $*$-algebra is $so(2,1) \oplus \mathbb{C}$. If u and v are both nonzero, we can redefine h as $h \to \alpha h + \beta$ for some $\alpha, \beta \in \mathbb{C}$ to obtain this case or the next one.

4. $u = -1$ and $v = 0$. This is the Lie $*$-algebra $so(3) \oplus \mathbb{C}$.

Note that the elements a and a^* are abstract vectors from the point of view of Lie algebras. That means that we cannot say that a^* is the conjugate of a; it is only in Lie $*$-algebras, in the $*$-Poisson algebras and in their unitary representations that we can say that a^* is the Hermitian conjugate of a. It is for these reasons that we have treated case 3 and case 4 separately. In a unitary representation we have $J(f \angle g) = \frac{i}{\hbar}(J(f)J(g) - J(g)J(f))$, so that $J(f)^* = J(f^*)$ makes sense.

As alluded before $so(2,1)$ and $so(3)$ are isomorphic as complex Lie algebras. If we define in $so(2,1)$ the elements $r = ia$, $s = ia^*$ we obtain the relations

$$h \angle r = -ir\,, \quad h \angle s = is\,, \quad r \angle s = -a\,,$$

which defines case 4 of the list above: $so(3)$. However, the map from $so(2,1)$ to $so(3)$ does not preserve the $*$-operation, since $r^* = (ia)^* = -ia^* \neq s$. That means that $so(2,1)$ and $so(3)$ are not isomorphic as Lie $*$-algebras.

Among the triangulated Lie algebras of rank and degree 1 listed above, the most interesting cases for both classical and quantum mechanics are $os(1)$ and $so(3) \oplus \mathbb{C}$. As we have seen, the oscillator algebra $os(1)$ is related to the harmonic oscillator. The algebra $so(3) \oplus \mathbb{C}$ involves infinitesimal ordinary rotations and arises when dealing with the spinning top, as explained in Chapter 20. The algebra $so(2,1) \oplus \mathbb{C}$ is less prominent in classical mechanics although it arises in the analysis of the celestial 2-body problem. The algebra $so(2,1) \oplus \mathbb{C}$ has important applications to exactly solvable problems in quantum mechanics, and even appears in so-called gauged supergravity theories.

22.3 Unitary representations of $SU(2)$ and $SO(3)$

We now discuss the unitary representations of the Lie groups $SU(2)$ and $SO(3)$. The method presented below is often encountered in quantum physics textbooks. In Section 22.4 we discuss the highest weight representations of triangulated Lie algebras of rank and degree 1, which shows a great similarity with the discussion here.

Since the group $SU(2)$ is compact it has an invariant **Haar measure** $d\mu(g)$. Therefore we can integrate over the group in an invariant way; invariance of the Haar measure means

$\int f(hg)d\mu(g) = \int f(g)d\mu(g)$. If $SU(2)$ acts on a vector space V with an inner product $\langle , \rangle_0$ we can integrate over the group to get an invariant inner product;

$$\langle v, w\rangle = \int_{SU(2)} \langle g \cdot v, g \cdot w\rangle_0 d\mu(g)\,,$$

where we denoted the action of $g \in SU(2)$ on $v \in V$ by $g \cdot v$. It is a direct consequence of the invariance of the Haar measure that the inner product $\langle , \rangle$ is $SU(2)$-invariant. Hence we have realized $SU(2)$ by unitary matrices; every representation of $SU(2)$ is equivalent to a unitary representation.

Since the group $SU(2)$ is compact and simply connected there is a one-to-one correspondence between the representations of the group and the representations of the Lie algebra $su(2) \cong so(3)$. The Lie algebra consists of antihermitian matrices but multiplying them by i we obtain Hermitian matrices and we may use the Pauli matrices to describe $su(2)$. Finding all representations of the Lie algebra $su(2)$ therefore gives all representations of $SU(2)$.

We put $t_i = \frac{1}{2}\sigma_i$ for $i = 1, 2, 3$ and define $L_\pm = (t_1 \pm it_2)$ and obtain a triangulated algebra with trivial center;

$$t_3 \angle L_\pm = \pm L_\pm\,, \quad L_+ \angle L_- = 2t_3\,.$$

In a unitary representation we require that t_3 is Hermitian and $L_\pm^* = L_\mp$. If v is an eigenvector of t_3 with eigenvalue α, then $L_- v$ is an eigenvector of t_3 with eigenvalue $\alpha - 1$. For a finite-dimensional representation we cannot lower the eigenvalue forever and hence there exists a vector v with $L_- v = 0$. Assume that we have $t_3 v = \alpha v$ for some complex number α. Acting on v with L_+ we get vectors with eigenvalues $\alpha, \alpha + 1, \alpha + 2, \ldots$. Again this series has to terminate. Thus, there is an eigenvector w with eigenvalue $\alpha + N$ that is annihilated by L_+. Since t_3 is Hermitian, vectors with different eigenvalues are orthogonal and hence linearly independent. Thus the $N+1$ vectors with eigenvalues $\alpha, \ldots, \alpha+N$ form an irreducible representation. The trace of t_3 is zero, since $\operatorname{tr} t_3 = -i \operatorname{tr}(t_1 t_2 - t_2 t_1)$. But then the sum of the eigenvalues should vanish:

$$0 = \sum_{n=0}^{N} \alpha + n = (N+1)\alpha + \frac{1}{2}N(N+1) = \frac{1}{2}(N+1)(2\alpha + N)\,.$$

It follows that $\alpha = -N/2$. Therefore the eigenvalues are the integers $-\frac{N}{2}, -\frac{N}{2}+1, \ldots, \frac{N}{2} - 1, \frac{N}{2}$. Conversely, for all integers N we find a representation by giving vectors e_α with $-N/2 \le \alpha \le N/2$ and defining the action of t_3 and $L_\pm$ by the above rules. We then recover t_1 and t_2 by $t_1 = \frac{1}{2}(L_+ + L_-)$ and $t_2 = \frac{1}{2i}(L_+ - L_-)$. We can thus label the finite-dimensional representations of $su(2)$ by half-integers $j = 0, 1/2, 1, 3/2, 2, \ldots$. We denote them by D_j; note that we have $j = N/2$. The dimension of the representation D_j is $2j + 1$ and the eigenvalues of t_3 are $-j, -j+1, \ldots, j-1, j$. The Casimir J^2 defined by

$$J^2 = t_1 t_1 + t_2 t_2 + t_3 t_3 = L_+ L_- - t_3 + t_3 t_3$$

has the value $j(j+1)$ on the representation D_j since acting on the state v with eigenvalue $-j$

$$J^2 v = (L_+ L_- - t_3 + t_3 t_3)v = (0 + j + j^2)v = j(j+1)v\,.$$

The number j is called the spin of the representation. Clearly D_j is irreducible.

The representations that correspond to nonintegral j cannot be lifted to representations of $SO(3)$. Although the Lie algebras $su(2)$ and $so(3)$ are isomorphic, the groups $SO(3)$ and $SU(2)$ are not! As mentioned before, $SU(2)$ is the universal covering group of $SO(3)$. In fact, we have $SO(3) = SU(2)/\mathbb{Z}_2$. That means that there is an action of $\mathbb{Z}_2$ on $SU(2)$, such that $SO(3)$ is the manifold $SU(2)$ with the points that are related by the $\mathbb{Z}_2$-action identified. In Section 3.4 we gave details on how $SO(3)$ and $SU(2)$ are related by a 2-1 map $SU(2) \to SO(3)$. If a representation of $SU(2)$ is such that $\mathbb{Z}_2$-related points have the same image under the representation we have a well-defined representation for $SO(3)$; this thus precisely corresponds to the $\mathbb{Z}_2$-invariant representations. It turns out that only the representations with integer l correspond to $\mathbb{Z}_2$-invariant representations. In physics, particles are represented by fields that take values in an $su(2)$-representation. The representations D_j for $j = 1/2, 3/2, 5/2, \ldots$ correspond to fermions and for $j = 0, 1, 2, \ldots$ to bosons.

22.4 Some unitary highest weight representations

For the quantum theory one considers the unitary highest weight representations. We investigate the unitary highest weight representations for the triangulated Lie algebras of rank and degree 1 listed in Section 22.2. We thus look for a realization of operators a, a^*, h and 1 such that 1 acts as the identity, h acts diagonally and is Hermitian, a^* is the adjoint of a and the following relations hold (see (11.21) and Definition 13.2.1):

$$[a, n] = \hbar a\,, \quad [a^*, n] = -\hbar a^*\,, \quad [a, a^*] = \hbar(un + v)\,.$$

Furthermore, we assume there is a vector $|0\rangle$ with

$$a|0\rangle = 0\,, \quad n|0\rangle = \alpha|0\rangle\,.$$

By acting with a^* on $|0\rangle$ we obtain the other vectors in the representation. We define

$$|k\rangle = \frac{(\hbar a^*)^k}{k!}|0\rangle\,,$$

so that

$$a^*|k-1\rangle = \hbar k|k\rangle\,.$$

It follows that

$$n|k\rangle = \hbar(k+\alpha)|k\rangle\,.$$

We have $a|k\rangle = c_k|k-1\rangle$ and we want to determine c_k. Since $aa^* = [a, a^*] + a^*a$ we find

$$\hbar k c_k|k-1\rangle = aa^*|k-1\rangle = \hbar\Big((uh+v) + (k-1)c_{k-1}\Big)|k-1\rangle\,,$$

from which it follows

$$kc_k - (k-1)c_{k-1} = \hbar(uk + u\alpha + v)\,,$$

which is solved by

$$\begin{aligned} kc_k &= 0 + (1c_1 - 0c_0) + (2c_2 - 1c_1) + \ldots + (kc_k - (k-1)c_{k-1}) \\ &= \hbar k\Big(\hbar\alpha u + v + \tfrac{1}{2}\hbar u(k+1)\Big)\,, \end{aligned}$$

so that

$$a|k\rangle = \Big(\alpha\hbar u + v + \tfrac{1}{2}\hbar u(k+1)\Big)|k-1\rangle\,.$$

The vectors $|k\rangle$ are orthogonal, as in the case of the harmonic oscillator. So we suppose $\langle j|k\rangle = N_k\delta_{jk}$, and calculate $\langle j|a^*|k\rangle$ in two ways:

$$\langle j|a^*|k\rangle = (k+1)\langle j|k+1\rangle,$$

$$\langle j|a^*|k\rangle = (v + \bar{\alpha}\hbar u + \tfrac{1}{2}\hbar u(k+1))\langle j-1|k\rangle.$$

Choosing $k = j-1$ we find

$$j\hbar N_j = \big(v + u\hbar\bar{\alpha} + \tfrac{1}{2}(j+1)u\hbar\big)\,N_{j-1}\,.$$

For a representation we require that $N_j \geq 0$ for all j. We may normalize $N_0 = 1$ and it follows that we must have $\alpha \in \mathbb{R}$. To have a faithful representation we need $|1\rangle \neq 0$ and thus $N_1 > 0$. We distinguish further two cases:

Case 1: $u \geq 0$. By assumption ψ_0 is a nonzero vector and thus has a positive norm. But then all N_j are positive. Hence we find nonzero vectors for all $j \in \mathbb{N}_0$. An example of this case is given by $so(2,1)$, which is a noncompact Lie algebra. More generally, noncompact Lie algebras (defined by having a Cartan–Killing form that is not negative definite) do not admit a finite-dimensional unitary representation.

Case 2: $u < 0$. In this case N_j can become negative, unless it becomes zero for some integer j_m. Thus $(j_m + 1) + 2(\bar{\alpha} + \frac{v}{\hbar u})$. In this case we thus have a finite-dimensional unitary representation for every integer $j_m = 0, 1, 2, \ldots$. The dimension of the representation is $j_m + 1$. If $j_m = 0$ the vector $|1\rangle$ is already zero, and hence a^* operates as 0 in this representation. Therefore, if $j_m \geq 1$ the representations are faithful.

For the triangulated Lie algebras of rank and degree 1, there is a Casimir operator of the form $C = \hbar a^* a - q(n)$ for some quadratic $q(n)$. From Section 22.3 we know that $so(3)$ has the Casimir $J^2 = 2aa^* + n^2 + in$. And for the algebra $os(1)$ the element $C = \hbar a^* a - n$ is a Casimir. For the harmonic oscillator we then have $C = 0$, since n is precisely $\hbar a^* a$. For $so(2,1)$ this does not work; there is no analogue of the number operator with only integer eigenvalues. That is, the Lie algebra $so(2,1)$ does not admit a discrete Casimir.

Chapter 23

Spectroscopy and spectra

This final chapter applies the Lie theoretic structure to the analysis of quantum spectra. After a short history of some aspects of spectroscopy, we look at the spectrum of bound systems of particles. We show how to obtain from a measured spectrum the spectrum of the associated Hamiltonian, and discuss qualitative results on vibrations (giving discrete spectra) and chemical reactions (giving continuous spectra) that come from the consideration of simple systems and the consideration of approximate symmetries. The latter are shown to result in a clustering of spectral values.

The structure of the clusters is determined by how the irreducible representations of a dynamical Lie algebra split when the algebra is reduced to a subalgebra of generating symmetries. The clustering can also occur in a hierarchical fashion with fine splitting and hyperfine splitting, corresponding to a chain of subgroups. As an example, we discuss the spectrum of the hydrogen atom.

23.1 Introduction and historical background

In this chapter we show some features of spectra and spectroscopy. In the preceding chapters we discussed properties of systems. The Hamiltonian of a system has a spectrum consisting of the eigenvalues, but in practice we don't see this spectrum, but the energy differences. One perturbs the system by shining light on it for example and then observes some response. The responses give rise to the observed spectrum, the study of which is spectroscopy.

To study the structure of molecules and atoms, we often rely on destructive methods. The destructive nature of the experiments in chemistry was taken as a primitive distinction between chemistry and physics. Nowadays the situation is different. In high-energy physics, one also shoots particles at each other such that the original particles are destroyed and energy is converted into the creation of other particles. On the other side, in chemistry new laser-techniques are used where molecules are kept intact, and information about the structure of the molecular bonds is obtained.

With spectroscopy one can study properties of materials and mixtures without destructing the sample. There are crudely speaking two kinds of spectra, relying on different experimental methods. An emission spectrum is obtained by putting a system in a state of high energy. The system then falls back to a state with lower energy, and the energy difference is emitted in the form of light. Of course, in order to emit light, the system needs to interact with light. The kind of interaction then dictates which transitions are possible and hence which frequencies are emitted. For the absorption spectrum one more or less does the converse. One puts a system into a beam of (nearly) white light. The system then absorbs light and re-emits it again, but then in all directions.

In the 19th century Kirchhoff used an invention of the German chemist Robert Bunsen to heat up elements in a flame to study the emitted light. He passed light through a prism to study the intensity of light at different wavelengths. It turned out that the emitted spectrum of an element had quite clearly defined lines at certain wavelengths. In 1859 Kirchhoff pointed out that all the elements that he had been studying had a different emission spectrum. Hence disentangling the lines of an emission spectrum can help in finding the components an unknown mixture is made of. Figure 23.1 gives as example an emission and an absorption spectrum of Helium.

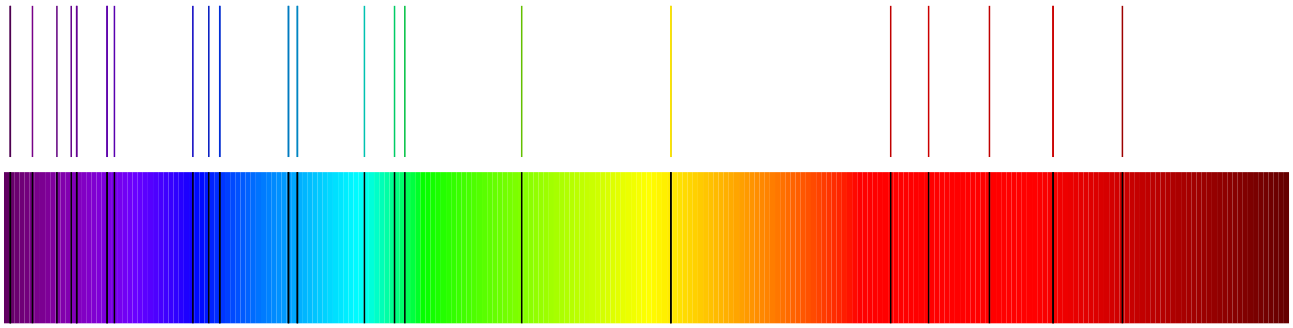

Figure 23.1: The emission (upper) and absorption (lower) spectrum of Helium.

Already much earlier, Isaac Newton had used in 1670-1672 a prism to study the decomposition of white light into a spectrum of different colors. In 1814 Joseph von Fraunhofer invented the spectroscope and identified 574 dark lines in the light of the sun. In fact, the Fraunhofer experiment can already be done with primitive equipment. On a sunny, cloudless day one sits in a dark room with one little hole through which the sun shines. In the beam of sunlight one places a prism and lets the light after the prism fall onto a white piece of paper. The observed spectrum can be seen to display dark lines; in Figure 23.1 the lines corresponding to helium are displayed. The Fraunhofer lines are a manifestation of the absorption spectrum. It was Kirchhoff who later explained the origin; light from the sun has to pass the atmosphere of the sun. In the atmosphere the elements that are present absorb certain parts of sunlight, at well-defined frequencies and re-emit it later, but then in all directions. Therefore the sunlight going in the forward direction – that is, away from the core of the sun – has lost intensity at certain well-defined frequencies. In this way, Kirchhoff showed that the atmosphere of the sun contained among others hydrogen

and sodium. The reason why the sunlight is almost white before entering the atmosphere of the sun we will not explain. When the light of the sun reaches the earth it is already so diluted that the elements in the earths' atmosphere give almost unobservable absorption lines. Therefore, the dark lines in the spectrum of the sun are due to the suns' atmosphere and not the earths' atmosphere.

In 1868, the French astronomer Pierre-Jules-Cesar Janssen observed a line in the spectrum of the sun that did not match any element known by then. The reason he observed it and not Fraunhofer was because Janssen used the better observing circumstances that a solar eclipse offers. Normally, the sun is too bright, but when the moon blocks the solar disc, one sees solely the atmosphere of the sun. The astronomer Joseph Norman Lockyear concluded that the new line must represent a new element. They tossed the name helium, from the Greek word "helios", which means sun. It was not until 1895 that the physicist John William Strutt, Lord Rayleigh – or in short John Rayleigh – proved that helium is also present on earth; he found it in samples of the mineral clevite. He exposed the mineral to some acids that reacted with the material thereby producing gasses. Then he studied the contents of the gas mixtures, and he found that helium was present. The reason why he found helium was explained later. Clevite is a mineral that contains uranium. The element uranium is radio-active; it can emit α-particles, which are the nuclei of helium atoms.

23.2 Spectra of systems of particles

We distinguish two kinds of spectra:
1. The spectrum in the sense of spectroscopy is the collection of frequencies emitted or absorbed by the system in its interaction with light or other electromagnetic (infrared, radio, X-ray) radiation.
2. The spectrum of a physical system is the collection of allowed energy values – the set of eigenvalues of the associated Hamiltonian.

The relation between the two is as follows. The observed spectrum (of spectroscopy) consists of the energy differences of the system: the observed spectra are of the form $\hbar\omega_{mn} = E_m - E_n$, where the energy levels of the system are E_n. In most systems the spectrum is discrete. Hence also the observed spectrum is discrete.

For systems that are made of constituents that can break apart, the spectrum contains continuous parts. Consider for example a molecule of two atoms like H_2. At a certain frequency the molecule can break apart. Then the energy of the photon can also be put into the kinetic energy of both H-atoms, which is a continuous parameter.

If the Hamiltonian has some imaginary eigenvalues λ, then $\mathrm{Im}\,\lambda < 0$ and the modes corresponding to λ are decaying modes. In a dissipative environment this results in energy loss, and the system can move from higher energy to lower energy.

On the other hand, a system can also be excited. It then absorbs energy from the environment. A typical example of excitation is an atom interacting with light. The energy levels of the atom are discrete, and hence only with a fine-tuned frequency the atom can absorb

a photon and attain a state with more energy. The energy difference between the ground state and the state with the second lowest energy is called the energy gap. If a photon has the frequency with the energy corresponding to the energy gap, it can be absorbed by the atom and the atom can be excited to the state above the ground state.

An excited atom cannot move down to a state with lower energy due to energy conservation, unless there is interaction with light. Incorporating interaction with light into the Hamiltonian makes the energies acquire a small imaginary part, representing the possibility to decay. If an atom jumps down in energy, it emits a photon with the same energy. This process is called spontaneous emission. The nice feature of spontaneous emission is that we can observe it.

The interaction with light is not just any arbitrary interaction. The interaction term V_{int} in the Hamiltonian

$$H_{\text{tot}} = H_{\text{atom}} + H_{\text{env}} + V_{\text{int}}$$

needs to respect some symmetries like Galilean invariance. The result is that not all transitions but only a selected set of transitions is allowed. The rules that dictate which transitions are allowed are therefore called **selection rules**.

The interaction is often treated as a perturbation. The justification is that the interaction term in the Hamiltonian is small compared to the other terms. One introduces a dimensionless variable λ and re-writes V_{int} as $V_{int}(\lambda) = \lambda V_{int}$. One recalculates the spectrum and expands it in λ to find

$$E_k(\lambda) = E_k(0) + \lambda \Delta E_k^1 + \lambda^2 \Delta E_k^2 + \dots .$$

Since the interaction is small, the first order correction often gives the interaction with light accurately enough. Using the techniques of perturbation theory one then finds the possible transitions, i.e. the selection rules, and the probabilities of the transitions. The probabilities gives the dominance in the observed spectrum; if a transition A is more probable than a transition B this will result in more spontaneous emission along transition A. Therefore the peak in the spectrum corresponding to A is bigger than the peak corresponding to B.

Observed spectra are often displayed by plotting, as in Figure 23.2, on the horizontal axis the frequency and on the vertical axis the observed intensity. Due to imperfections in measuring methods one never observes a real peak, but always a smeared out peak, that is, peaks have a width. However, there can be many reasons why a peak has a certain width. Imagine for example that one measures the spontaneous emission of a gas contained in cylinder. The gas atoms are moving around in the cylinder, with different velocities with respect to the measuring device. For each atom the spectrum is shifted due to the Doppler effect, known from a similar effect with sound, which can be observed when an ambulance passes by. Since one measures the emission of a whole population of atoms, the measured peak is a superposition of peaks that are distributed around a certain frequency. That is, the Doppler effect broadens a peak.

Technical imperfections of the measuring device also broaden peaks. Making the measuring equipment more and more accurate one can try to get a better and better resolved spectrum.

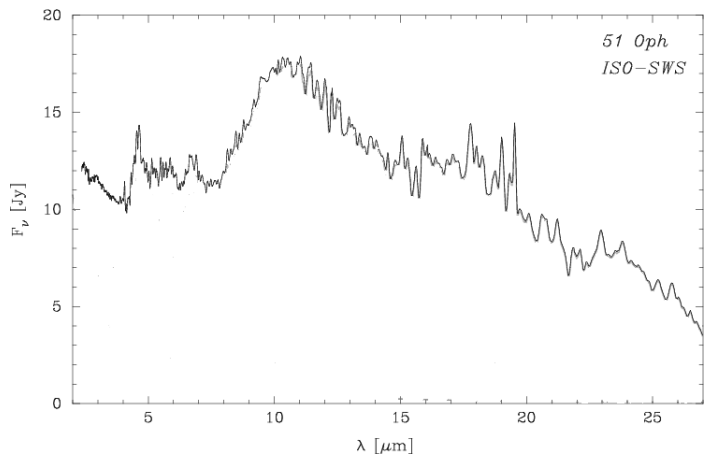

Figure 23.2: An example of a spectrum.

Doing this one might see that broad peaks resolve into a group of smaller peaks. One sees therefore more structure.

The result of a measurement is a list of data, the frequencies ω_l. Using the data one wants to obtain information of the system under study. If one knows the system already quite well, for example if one knows the parametric form of the Hamiltonian but not the precise values of the parameters, one may fit the measured energies to obtain a set of parameters that describes the measurements best. One therefore has to solve a data analysis problem. For each label l one has to find energies $E_{k(l)}$ and $E_{j(l)}$ with

$$\omega_l \approx E_{j(l)} - E_{k(l)},$$

within the experimental accuracy. Therefore, one solves the least-squares problem of minimizing the sum

$$S(E, j, k) := \sum_l q_l \Big(\frac{E_{j(l)} - E_{k(l)}}{\hbar \omega_l} - 1 \Big)^2 ,$$

for some weight factors q_l related to the inverse of the accuracy of the measurement of ω_l.

In general, both the list E of energy levels E_i and the functions j, k which determine the **assignment** of spectroscopic lines to transitions are unknown, and must be determined by minimizing $S(E, j, k)$. Usually, one starts with a preliminary list E of energy levels, and assigns each line l to a transition which minimizes the lth term, breaking ties arbitrarily. This defines preliminary assignment functions j, k. Fixing these turns the problem of minimizing $S(E, j, k)$ into a least squares problem for finding the energy levels, resulting in an improved E. Clearly, each cycle decreases the value of $S(E, j, k)$. The process is stopped when the assignments no longer change. Then $S(E, j, k)$ has reached a local minimum. Multiple lists of trial energy levels may be used to increase the likelihood that the assignment found corresponds to a global minimum. Frequently, one first assigns a subset of lines to a subset of levels to find good starting values.

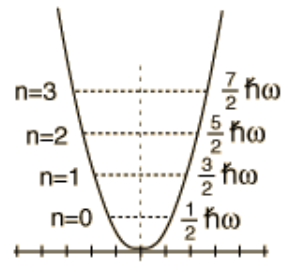

Figure 23.3: Harmonic oscillator potential, with the eigenvalues indicated.

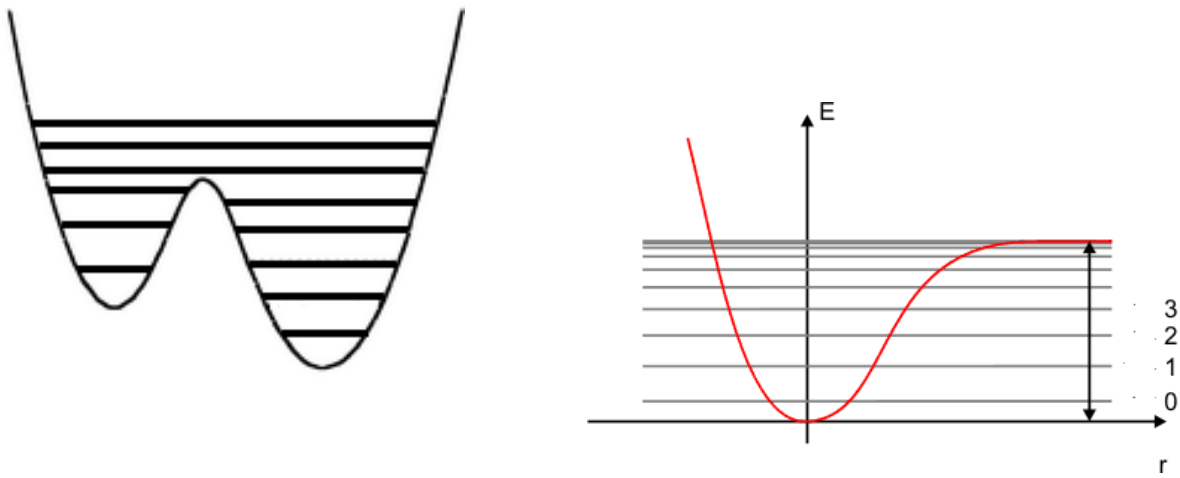

Figure 23.4: On the left a double well potential with the first energy levels indicated. On the right the Morse potential; the bound states have discrete energy but above the dissociation energy the spectrum is continuous.

23.3 Examples of spectra

The geometry of the molecule or atom under consideration strongly influences the spectrum, since the geometry determines the potential.

Consider a molecule of two atoms. We assume that the excitations inside each atom are of another magnitude than the excitations of the bond between the atoms. In that case we may consider the molecule as two balls connected by a spring. The spectrum is as in Figure 23.3, and the observed spectrum consists of one peak.

Consider now a system that has two local minima. An example of this would be a molecule C_2H_4 of which two versions exist, the cis and trans molecules. The molecular bond between the two C-atoms then behaves around each local minimum as a harmonic oscillator in some approximation. For higher energies however the two states start to interact and the molecule can change from cis to trans and vice versa. A typical spectrum then looks like Figure 23.4.

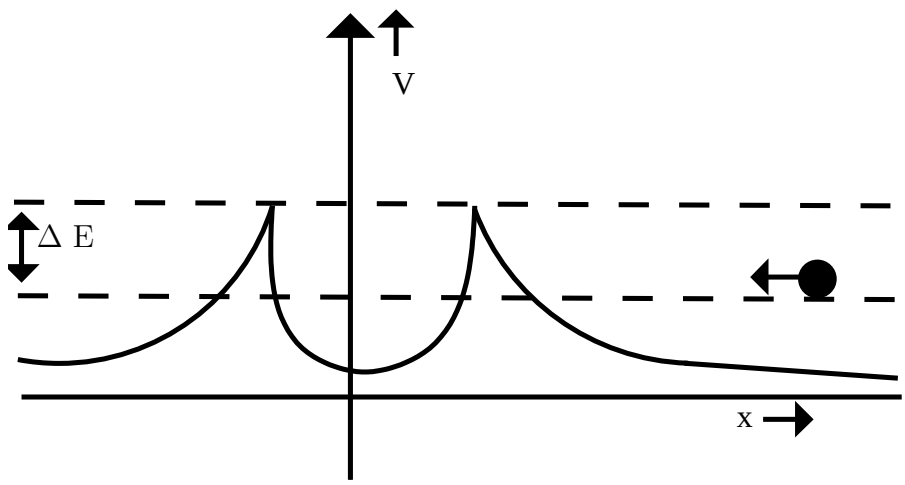

Figure 23.5: Sketch of the potential a proton experiences in the force field of a nucleus.

When there are asymptotically free states, one says that the system admits **dissociation**. Free states have continuous kinetic energy and hence the spectrum contains continuous parts. A potential showing dissociation is the Morse potential given by

$$V(r) = \alpha(e^{-\beta r} - \gamma)^2 - \alpha\gamma^2 \, , r \geq 0$$

where r is the atomic distance and α, β, and γ are positive parameters, see Figure 23.4. The potential of the H_2 molecule discussed above is another example. Above the dissociation energy the spectrum is continuous; the bound states have discrete energy.

Quantum physics has a remarkable feature compared to classical mechanics, called **tunneling**. If a particle is in a local minimum at energy E_1 and another minimum is available with energy level $E_0 < E_1$, then (in a semiclassical particle view) there is a nonzero probability that the particle "travels through the barrier" and ends up in the local minimum with lower energy. For example, the potential of the C_2H_4-molecule discussed above admits tunneling since the potential has two local minima. The probability of tunneling decreases with the height of the barrier between the two energy levels. Another example where tunneling occurs is in nuclear physics; the potential of Figure 23.5 represents the energy a proton feels in the potential field of a nucleus. The diameter of the nucleus is roughly the distance between the two peaks in Figure 23.5. The difference to the C_2H_4-molecule is here that the tunneling takes place between two states one of which is not integrable. Tunneling can go in two different directions; one direction is where the proton is shot at the nucleus with too little energy to classically penetrate the nucleus, the other direction is where the proton is inside the nucleus and classically cannot get out. In the latter case, there is a certain probability that the proton escapes the nucleus. This explains qualitatively the stochastic behavior of radio-active decay.

As another example, consider a chemical reaction of the form $AB + C \to A + BC$, that is, the molecule AB splits off a part B that then attaches to C to form BC. Here there are

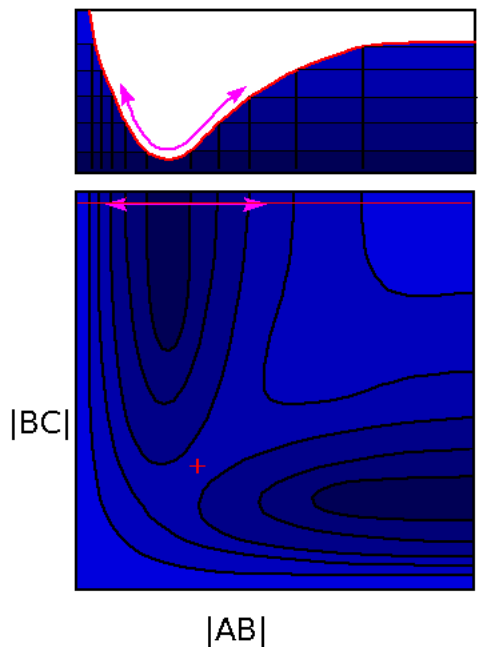

Figure 23.6: 2D-Plot of the potential experienced in a chemical reaction $AB+C \to A+BC$. The potential depends on the distances $|AB|$ and $|BC|$. The upper part shows a cross-section of the potential. The red marker is the saddle point.

two important parameters. The distance $|AB|$ between A and B and the distance $|BC|$ between B and C. A possible potential is plotted in Figure 23.6. The plot shows two valleys separated by a saddle point, marked by a red cross. The horizontal valley corresponds to $|BC|$ constant, hence to the state $A + BC$. The other valley corresponds to $AB + C$, and at the saddle point part B is exchanged.

23.4 Dynamical symmetries

As discussed before, when one looks at a poorly resolved spectrum, one sees some rough features of the system under study. Improving the resolution allows one to study more structure of the system.

A similar process happens when one studies a hydrogen atom in an external magnetic field. Upon increasing the magnetic field one sees that many lines of the original spectrum split into several close lines. Thus what first seems to be one state in fact turns out to be an agglomeration of different states. The states first had energies that were so close together that they could not be recognized as belonging to different states – indeed, they have exactly the same energy. As we shall see, that these states (seemingly) agglomerate to one single state is due to symmetry reasons.

The rotational symmetry implies that the energies of different states related by a rotation have the same energy; more pictorially, whether an electron circles around the proton with

the rotation axis in the z-direction or the y-direction gives the same energy. Turning on the magnetic field results in breaking the symmetry; then the different states that first agglomerated to form a single state are disentangled and can be observed separately in the spectrum.

But as with the increasing resolution, taking a closer look at the hydrogen atom reveals more and more structure. In a first approximation, the electron in the hydrogen atom can be treated nonrelativistically. Treating the electron relativistically, one gets a correction to the spectrum. The first order corrections of special relativity go under the name of the **first radiative corrections**.

We shall look in some detail at the hydrogen atom once we have clarified the general principles.

Symmetry and broken symmetry. The most symmetric physical systems, in particular the standard 2-body problems (the classical Kepler problem and the quantum hydrogen atom) are exactly solvable. The Helium atom is already a three-body problem and is not exactly solvable.

A physical system is called **exactly solvable** (or **integrable**, or **completely integrable**) if it has "enough" constants of motion. Equivalently, if the centralizer $C_{\mathbb{E}}(H)$ of the Hamiltonian H in the algebra $\mathbb{E}$ of observables is "large enough". The effect of having enough central elements is that the system has enough conserved quantities to explicitly solve the differential equations of the system.

A **dynamical algebra** of a classical physical system is a Lie algebra $\mathbb{L}$ that one can associate to the system such that the Hamiltonian H is contained in the Lie–Poisson algebra $C^\infty(\mathbb{L}^*)$. An extensive treatment of the role of Lie algebras in infinite-dimensional classical integrable systems (field theories in one and two space dimensions) see Roy Chowdhury [62].

In this section, we are however, only interested in the application to spectroscopy and hence concentrate on the quantum case. For a quantum mechanical system the requirement defining a **dynamical algebra** is that H is contained in the closure of the universal enveloping algebra $\mathcal{U}(\mathbb{L})$ of $\mathbb{L}$, equipped with a locally convex topology such that potentials of the form e^{-x^2} are allowed.

For example, the Heisenberg algebra $h(n)$ is the dynamical algebra of symplectic classical systems with n position degrees of freedom, and of traditional Schrödinger quantum mechanics. The hydrogen atom has additional rotational symmetry, and the special properties of the Coulomb potential imply that one can in fact find a fairly big dynamical algebra, namely $so(2,4)$, see e.g. Wybourne [296].

Now consider any Lie algebra $\mathbb{L}$ as a dynamical algebra. Call $\mathbb{E}$ the Lie–Poisson algebra associated to $\mathbb{L}$ for a classical case or the universal enveloping algebra of $\mathbb{L}$ in the quantum case. The **symmetry algebra** is the centralizer of the Hamiltonian in $\mathbb{E}$, written $C_{\mathbb{E}}(H)$. In the 'nicest' case one has $\mathbb{E} = C_{\mathbb{E}}(H)$, which means that H is a Casimir of $\mathbb{L}$. Normally, the Lie algebra $\mathbb{L}$ describes the symmetries of the (unperturbed) system and thus one would expect that the nicest case is the general case.

However, a very symmetric system is rarely studied in isolation, and realistic systems are at best perturbations of nice systems. In this case one gets broken symmetries, meaning that the Hamiltonian is only almost a Casimir. Note that it might happen that the classical theory has a symmetry, but that in the quantum version of the theory the symmetry gets broken. In case of a broken symmetry, one usually first tries to solve the symmetric problem and then perturb the solutions to get approximate solutions to the problem with broken symmetry. We will not go into details about the mathematics of perturbation theory, since this topic is amply treated in every book on quantum mechanics. But we will consider some of its qualitative implications.

Suppose we have solved a symmetric problem. Then the solutions are described as elements of some Hilbert space $\mathbb{H}$ on which $\mathbb{L}$ acts unitarily. We can decompose the Hilbert space into a direct sum of eigenspaces of the Hamiltonian; $\mathbb{H} = \oplus_\lambda \mathbb{H}_\lambda$. Let ψ be some eigenstate in $\mathbb{H}_\lambda$ of the Hamiltonian and let $f \in \mathbb{L}$, then we see

$$Hf\psi = [H, f]\psi + fH\psi = [H, f]\psi + \lambda f\psi\,.$$

Since $[f, H] = 0$ we see that $\mathbb{L}$ maps each eigenspace into itself. Thus all $\mathbb{H}_\lambda$ are $\mathbb{L}$-modules.

We call the eigenvalue λ **nondegenerate** if the dimension of $\mathbb{H}_\lambda$ is 1, and **degenerate** if it is bigger than 1. (Dimension zero means that λ is not an eigenvalue.)

If λ is degenerate, $\mathbb{H}_\lambda$ has many essentially distinct bases of eigenvectors of H. One of these is usually distinguished by the concrete representation used to describe the module; H and usually a distinguished part of $\mathbb{L}$ act diagonally. In general the perturbed Hamiltonian no longer acts diagonally on $\mathbb{H}_\lambda$, and as a result the level λ usually splits into several distinct levels. The energy level λ splits into new levels that are of the form $\lambda + \epsilon_j$ for some different but small values ϵ_j, giving rise to a fine structure. In general, a fine structure implies that either a symmetry is broken (the system reached a nonsymmetric state) or an external force that broke the symmetry explicitly has been applied.

The induced representation of $\mathbb{L}$ on $\mathbb{H}_\lambda$ is unitary. Therefore knowing the irreducible unitary representations of $\mathbb{L}$ can give information about the system under study.

23.5 The hydrogen atom

A hydrogen atom is a bound state of a proton (the nucleus) and an electron. It is most easily described by treating the much heavier nucleus as fixed (which amounts to neglecting recoil effects) and considering the electron as moving in the spherically symmetric electrostatic Coulomb field generated by the nucleus.

The electron is a spin 1/2 particle, a fermion, meaning that it is described by the spin 1/2 representation of $so(3)$ on the Hilbert space $L^2(\mathbb{R}^3, \mathbb{P}_1) \cong L^2(\mathbb{R}^3) \otimes \mathbb{P}_1$ defined in Section 2.11. Below we first discuss the orbital part of the wave functions, i.e. the $L^2(\mathbb{R}^3)$-part. Then we discuss the dynamical symmetries and how they get broken.

The orbital quantum states are labeled by integers n, l and m. The integer n takes the values $1, 2, 3, \ldots$ and the number l takes for each fixed value of n the values $0, 1, 2, \ldots, n-1$. Finally, the number m takes for each l the values $-l, -l+1, \ldots, l-1, l$. Hence the (orbital) state of an electron is described by a state

$$|n, m, l\rangle \quad \text{where} \quad n \geq 1\,, \quad 0 \leq l < n\,, \quad -l \leq m \leq l\,. \tag{23.1}$$

The **quantum number** n determines (to a first approximation) the energy of the state:

$$E_n = -\frac{13.6eV}{n^2}\,. \tag{23.2}$$

The abbreviation eV means electron Volt and is a unit for energy. The quantum number l specifies a representation of $so(3)$. Thus we can make use of the representation theory of $so(3)$ developed in Section 22.3.

The electrostatic potential of the hydrogen atom is $SO(3)$-invariant, hence it is not too surprising that $SO(3)$-representations plays a role; the orbital part of the electron wave function can be decomposed in representations of $SO(3)$. The quantum number l corresponds precisely to the irreducible representation of $so(3)$ of integral spin l, that is, precisely to the representations of $so(3)$ that lift to $SO(3)$-representations. The quantum number m labels the σ_3-eigenvectors of the representation and corresponds to the eigenvalue m. The quantum number n thus determines which $SO(3)$-representations are allowed, and the l and m then specify the representation and an eigenvector in this representation.

Now we shortly describe the relation between the quantum numbers and the orbital wave function of the electron in the hydrogen atom. We can give the hydrogen atom a coordinate system as follows. We put the proton in the center and describe the position of the electron by a radial coordinate r measuring the distance between the proton and the electron and by two angles $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$. The solutions to the Schrödinger equation for the hydrogen atom are then given by

$$\psi(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi)\,.$$

The radial part of the wave function $R_{n,l}$ is completely determined by the quantum numbers n and l and is given by

$$R_{n,l} = C_{n,l} e^{-\rho/2} \rho^l L^{2l+1}_{n-l-1}(\rho).$$

Here $C_{n,l}$ is some constant such that $R_{n,l}$ is normalized to integrate to one, the $L^p_q(\rho)$ are generalized Laguerre polynomials (one of the well-known families of special functions); ρ is the normalized radius $\rho = \frac{2r}{na_0}$, and a_0 is a constant called the **Bohr radius**. The angular part $Y_{l,m}$ of the wave function is given by

$$Y_{l,m}(\theta, \phi) = K_{l,m} P^m_l(\cos\theta) e^{im\phi}\,,$$

where the $K_{l,m}$ are normalization constants, and the P^m_l are the **associated Legendre polynomials** given by

$$P^m_l(x) = \frac{(-1)^m}{2^l l!}(1 - x^2)^{m/2} \left(\frac{d}{dx}\right)^{l+m} (x^2 - 1)^l\,.$$

Symmetries and symmetry breaking. Nonrelativistically the electron in an electromagnetic field is treated with the **Pauli equation**. The Pauli equation looks like the Schrödinger equation, but has some extra terms, describing the coupling of a spin 1/2 particle to the electromagnetic field. We now indicate why, in the case where the external electromagnetic field is switched off, the symmetry group of the Hamiltonian is $SO(4) \times SO(3)$.

The second factor in the symmetry group, the $SO(3)$, is the symmetry group that acts on the spin of the electron. That is, it acts on the $D_{1/2}$ part of $L^2(\mathbb{R}^3) \otimes D_{1/2}$.

The first factor in the symmetry group, the $SO(4)$, acts on the space-part $L^2(\mathbb{R}^3)$ of the wave function. The Hamiltonian of the hydrogen atom is rotationally invariant. Infinitesimal rotations are generated by the angular momentum $\mathbf{J} = \mathbf{r} \times \mathbf{p}$, where $\mathbf{r}$ is the radius and $\mathbf{p}$ is the linear momentum and hence the angular momentum components describe the Lie algebra $so(3)$. However, there exists an additional vector whose length is conserved: the length of the **Lenz–Runge vector**. (Some people call it the Laplace–Runge–Lenz vector, or even Laplace vector.) This leads to the bigger group $SO(4)$; see e.g. Goldstein [106].

To treat the electron relativistically one uses the Dirac equation for a spin 1/2 particle coupled to an electromagnetic field. The coupling to the electromagnetic field can be done in a quite easy way. Starting with the Dirac equation

$$(\hbar\gamma \cdot \partial + mc)\,\psi = 0$$

one simply replaces the derivatives with $\partial_\mu - iqA_\mu$ where the zeroth component of A gives the Coulomb potential and the spatial $\mathbf{A}$ components contain the magnetic field via $B = \nabla \times \mathbf{A}$; the parameter q is interpreted as the charge. We obtain

$$(\hbar\gamma \cdot \partial - iq\hbar\gamma \cdot A + mc)\,\psi = 0\,,$$

where $\gamma \cdot A = \gamma^\mu A_\mu$.

The effect of having the fully relativistic coupling terms is that there is a coupling between the spin of the electron and the orbital angular momentum of the electron. The additional coupling terms in the Hamiltonian are called **spin-orbit coupling** terms.

Due to the coupling the separate $SO(3)$ of the spin gets destroyed; without coupling there is a rotational symmetry group acting separately on the orbit and on the spin and due to the coupling, the two rotational symmetries are no longer independent. The angular momentum $\mathbf{L}$ and the spin $\mathbf{S}$ are no longer separately conserved in magnitude, but $(\mathbf{L}+\mathbf{S})^2$ is constant. The symmetry group of the relativistic hydrogen atom is therefore $SO(4)$. The spectrum that is observed is called the **fine structure spectrum**.

Going even further and treating the hydrogen atom with quantum field theory results in a further breakdown of the symmetry to the group $SO(3)$. The group $SO(4)$ is isomorphic to $SO(3) \times SO(3)$ (see Section 3.11) and corrections from quantum field theory break it down to the diagonal subgroup $SO(3)$. The observed spectrum is called the **hyperfine structure spectrum**.

23.6 Chains of subalgebras

In more realistic situations, the Hamiltonian is not invariant under the total dynamical algebra $\mathbb{E}$, the universal enveloping algebra of $\mathbb{L}$. In this case, the Hamiltonian is not in the center of $\mathbb{E}$, but we can consider the centralizer of H in $\mathbb{L}$. The centralizer of H in $\mathbb{L}$ is a subalgebra of $\mathbb{L}$, and is therefore a Lie subalgebra of $\mathbb{E}$ and we denote it by $\mathbb{L}_1$. We thus have $H \in C_{\mathbb{E}}(\mathbb{L}_1)$. The Lie subalgebra $\mathbb{L}_1$ generates a subalgebra of $\mathbb{E}$, which we denote by $\mathbb{E}_1$.

In simple applications, it often happens that the Hamiltonian H is a function $H(C_0, C_1)$ where C_0 is a Casimir of $\mathbb{L}$ (that is, it is a central element of $\mathbb{E}$) and where C_1 is a Casimir of $\mathbb{L}_1$ (in the center of $\mathbb{E}_1$). In more complicated applications we have a series of approximations to the problem, as explained for the hydrogen atom before, where relativistic and quantum field theory effects modify the Hamiltonian. In each step one modifies the Hamiltonian by adding terms with fewer and fewer symmetries, and the symmetry algebra is reduced to correspondingly smaller subalgebras. We thus have a sequence of subalgebras

$$\mathbb{L} = \mathbb{L}_0 \supseteq \mathbb{L}_1 \supseteq \ldots \supseteq \mathbb{L}_n = \hat{\mathbb{L}}\,.$$

The final subalgebra $\hat{\mathbb{L}}$ commutes with H. The generated subalgebra of $\mathbb{E}$, denoted $\hat{\mathbb{E}}$ centralizes H in $\mathbb{E}$. If the Hamiltonian is a function $H = H(C_0, \ldots, C_n)$ where C_k is a Casimir of $\mathbb{L}_k$, the scheme gives explicitly solvable problems. For example, for the nonrelativistic hydrogen atom without spin, one finds a series

$$so(4) \supset so(3) \supset so(2) \supset 1\,.$$

Of course, there are many Hamiltonians that cannot be represented as functions of a chain of Casimirs, but the above scheme covers many applications, and is a starting point for a perturbative treatment of many others.

In classical symplectic mechanics one relates the Lie algebra $\hat{\mathbb{L}}$ to so-called **action variables** and the steps to $\mathbb{L}_0$ are constructed using conjugate **angle variables**. We will not go into the details defining variables and the related techniques.

Consider the situation where $H = H(C_0, C_1)$, that is, the simple application. We write $H = H_0 + H_1$ where H_0 is only a function of C_0 and H_1 depends on C_0 and C_1. As before, we suppose we have realized the elements of $\mathbb{E}$ (and thus of $\mathbb{L}$) as operators on some Hilbert space $\mathbb{H}$. We assume that the subspaces $\mathbb{H}_\lambda$ on which the Hamiltonian $H_0 = H_0(C_0)$ acts diagonally are finite-dimensional. This is for example the case for the hydrogen atom. We furthermore split up $\mathbb{H}_\lambda$ in irreducible representations of $\mathbb{L}_0$ so that we may assume that $\mathbb{H}_\lambda$ is irreducible. Modifying H_0 to $H_0 + H_1$ means that the symmetry algebra becomes smaller; it becomes $\mathbb{L}_1$. We can restrict the representation of $\mathbb{L}_0$ on $\mathbb{H}_\lambda$ to the subalgebra $\mathbb{L}_1$ to obtain a representation of $\mathbb{L}_1$. In most cases this representation is reducible and we write the decomposition of $\mathbb{H}_\lambda$ into $\mathbb{L}_1$ irreducibles as

$$\mathbb{H}_\lambda = \bigoplus_\mu \mathbb{H}_\mu^{(1)}\,.$$

More generally, suppose we have a sequence of subalgebras $\mathbb{L}_0 \supset \mathbb{L}_1 \supset \ldots \supset \mathbb{L}_n$ and related Casimirs $C_i \in Z(U(\mathbb{L}_i))$. It follows that the C_i commute among each other; C_1 is in the center of $U(\mathbb{L}_1)$, which contains $U(\mathbb{L}_k)$ for $k \geq 2$ and hence C_1 commutes with C_2, C_3, and so on. Thus on the irreducible representations of $\mathbb{L}_1$ the Casimirs act diagonally. Hence we can assign to each representation of $\mathbb{L}_n$ appearing in the decomposition of the original representation $\mathbb{H}$ numerical values $\theta_0, \ldots, \theta_n$, corresponding to the eigenvalues of the C_i. Given a physical state v in a representation of $\mathbb{L}_n$ corresponding to the label $(\theta_0, \ldots, \theta_n)$ we see that the Hamiltonian acts as

$$H(C_0, \ldots, C_n)v = H(\theta_0, \ldots, \theta_n)v\,,$$

where on the right-hand side the Hamiltonian is an operator and on the right hand side $H(\theta_0, \ldots, \theta_n)$ is a number.

Branching rules. In a lot of favorable cases, for example when the $\mathbb{L}_i$ are simple, the decomposition of an irreducible representation of the large algebra into irreducible representations of a maximal subalgebra is known. These decompositions go under the name of **branching rules**; splitting up a representation under a subgroup or subalgebra is called **branching**.

Let us give an example of a branching rule and look at the fundamental representation of $su(3)$, that is, the 3-dimensional representation of $su(3)$ that defines the Lie algebra $su(3)$. The Lie algebra elements are faithfully represented as 3×3-matrices X that are antihermitian; $X^\dagger + X = 0$. Now we consider the Lie subalgebra $su(2)$. There are different ways we can embed $su(2)$ into $su(3)$, but it turns out that all of them are equivalent. We can always choose a basis e_1, e_2, e_3 in $\mathbb{C}^3$ such that $su(2)$ only acts nontrivially on the subspace spanned by e_1 and e_2. We thus realize $su(2)$ inside $su(3)$ as the following matrices in $su(3)$

$$\begin{pmatrix} a & b & 0 \\ c & d & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \text{where} \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in su(2)\,.$$

We see that the three-dimensional representation of $su(3)$ splits into two irreducible representations of $su(2)$, the trivial one, spanned by e_3 and the two-dimensional (fundamental) representation spanned e_1 and e_2. One writes this in shorthand as: $\mathbf{3} \to \mathbf{2} + \mathbf{1}$ under $su(2) \subset su(3)$. In the reference Slansky [255], one can find tables of branching rules.

Clebsch–Gordan coefficients. In an important special case one can relate the branching rules to the so-called Clebsch–Gordan coefficients, which are widely used in physics.

Let us explain the Clebsch–Gordan coefficients for $su(2)$. Given two representation D_l and D_k (see Section 22.3), we can form the tensor product $D_k \otimes D_l$. An $su(2)$-element x acts on $v \otimes w$ by mapping $v \otimes w$ to $x(v) \otimes w + v \otimes x(w)$, where we write $x(v)$ for the action of x on v. In general, the representation $D_k \otimes D_l$ is not irreducible, and we have

$$D_k \otimes D_l = D_{k+l} \oplus D_{k+l-2} \oplus \ldots \oplus D_{|k-l|}\,.$$

The precise decomposition of a vector $v \otimes w$, where v and w are eigenvectors of σ_3, into the irreducible components is given by the Clebsch–Gordan coefficients. For the vector in the

D_k representation with σ_3 eigenvalue m and norm one we write $|k, m\rangle$. If the representation D_K is inside the tensor product of D_{k_1} and D_{k_2}, we can decompose any vector $|K, M\rangle$ as a sum of vectors of the form $|k_1, m_1\rangle \otimes |k_2, m_2\rangle$ and the Clebsch–Gordan coefficients are then the coefficients in the decomposition

$$|K, M\rangle = \sum_{k_1, k_2 m_1, m_2} C^{KM}_{k_1 k_2 m_1 m_2} |k_1, m_1\rangle \otimes |k_2, m_2\rangle \,.$$

More generally, the Clebsch–Gordan decompositions say how the tensor product of two irreducible representations V_1 and V_2 of a compact Lie group (or its Lie algebra) decompose into irreducible representations W_i as $V_1 \otimes V_2 = \oplus_j W_j$. The Clebsch–Gordan coefficients are the numerical coefficients in the projection from one of the summands W_j to $V_1 \otimes V_2$.

Now suppose that $\mathbb{L}_0 = \mathbb{L}' \oplus \mathbb{L}'$ decomposes into two copies of the same Lie algebra $\mathbb{L}'$. An important choice of $\mathbb{L}_1$ is the diagonal Lie subalgebra given by elements of the form (a, a) with $a \in \mathbb{L}'$. Then as a Lie algebra $\mathbb{L}_1 \cong \mathbb{L}'$. The irreducible representations of $\mathbb{L}_0$ are given by tensor products of representations of $\mathbb{L}_1$. Therefore, decomposing the irreducible representations of $\mathbb{L}_0$ with respect to $\mathbb{L}_1$ amounts to giving the Clebsch–Gordan decompositions.

Much more could be said on the topic of symmetries and broken symmetries in physics. A nice overview is given in a paper by Bijker [35]. It shows how the symmetry concept organizes not only the world of atoms and molecules that we considered here, but also that of elementary particles. The isospin symmetry between protons and neutrons has a symmetry group $SU(2)$, which extends to the flavor symmetry group $SU(3)$ for the three light quarks. Applications to molecular spectra and the **interacting boson model** for modelling atomic nuclei are discussed extensively in the book by Frank & van Isacker [90].

Quantum field theory, culminating in the standard model, is also based on symmetries, namely the space-time symmetries of the Poincaré group, and a gauge group $U(2) \otimes SU(3)$ which combines the broken symmetry group $U(2) = U(1) \otimes SU(2)$ of the weak interaction (of which only a diagonal subgroup $U(1)$ encoding the electromagnetic charge is unbroken) with the unbroken color symmetry group $U(3)$ of the strong interaction.

While these topics lie far beyond the scope of this book, the interested reader will take the next step and consult deeper work of others who studies this in depth. Our journey is finished.

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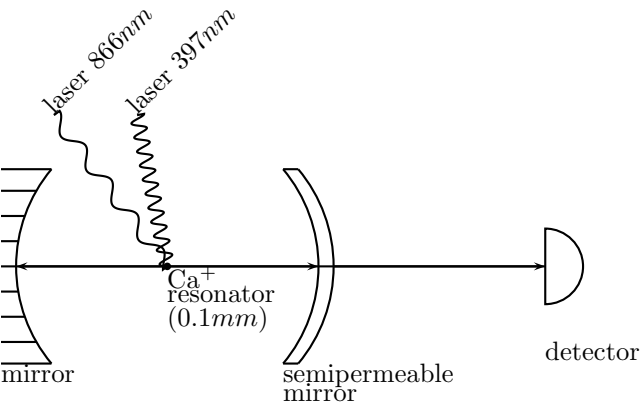
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