

# Effective Schrödinger equations for nonlocal and/or dissipative systems

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## **Abstract.**

The projection formalism for calculating effective Hamiltonians and resonances is generalized to the nonlocal and/or nonhermitian case, so that it is applicable to the reduction of relativistic systems (Bethe-Salpeter equations), and to dissipative systems modeled by an optical potential.

It is also shown how to recover *all* solutions of the time-independent Schrödinger equation in terms of solutions of the effective Schrödinger equation in the reduced state space and a Schrödinger equation in a reference state space.

For practical calculations, it is important that the resulting formulas can be used without computing any projection operators. This leads to a modified coupled reaction channel/resonating group method framework for the calculation of multichannel scattering information.

**Keywords:** Feshbach projection, effective Hamiltonian, nonlocal Schrödinger equation, Bethe-Salpeter equation, coupled reaction channels, resonating group method, dissipative quantum system, optical potential, form factor, doorway operator, time-independent perturbation theory, backward error analysis, multichannel scattering

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# 1 Introduction

In many applications, a quantum system of interest is part of a much bigger system, and the latter's state influences the system state. If the big system is represented by solutions of a Schrödinger equation in a big state space, it is desirable to find an effective Schrödinger equation in a small state space that describes how the small system of interest is affected by the embedding into the big system. Under certain conditions, a Schrödinger equation in the big state space can indeed be reduced to an effective Schrödinger equation in the small state space, in such a way that the interesting part of any solution of the full Schrödinger equation satisfies exactly the effective Schrödinger equation.

Much effort has gone into solving this reduction problem, and in a sense it is well understood [1, 6, 13, 17, 28]. Exact expressions for the effective Hamiltonian can be given. In its exact form, the effective Hamiltonian is energy dependent and usually acquires a nonhermitian part; its eigenvalues describe the bound states and resonances of the reduced system. There are approximation schemes that compute the effective Hamiltonian (at least in principle) to arbitrary accuracy.

Less known (but proved here) is that certain solutions of the full Schrödinger equation can be reconstructed from solutions of the effective Schrödinger equation, using little more than what is already available from the reduction process.

The reduction is usually done for bound state calculations by the variational principle discussed in every textbook on quantum mechanics. For resonance calculations, the reduction may be done within the FESHBACH [7, 9] projection formalism (for an exposition see, e.g., KUKULIN et al. [17, Chapter 4]). In both cases, the reduced state space is finite-dimensional. For the calculation of scattering states, the reduction may be done by means of coupled reaction channel equations, also called the resonating group method; a nice exposition is given in WILDERMUTH & TANG [28]. In this case, the reduced state space is a direct sum of finitely many function spaces, one for each energetically admissible arrangement of particles into clusters, with states parameterized by coordinates or momenta of cluster centers only.

The coupled reaction channel equations are numerically easy to handle, but the approximations involved in their derivation make an assessment of their accuracy difficult. On the other hand, the projection formalism gives in principle exact results, limited in accuracy only by the approximations made in the calculation of the effective Hamiltonian. However, this involves projection operators, which are clumsy to use if an orthogonal basis is not easily available.

Moreover, if the full Hamiltonian is already nonhermitian, or if the Hamilto-

nian is energy-dependent (such as in relativistic calculations; cf. [8, 14, 15, 16, 12, 18, 19, 22, 26]), the standard derivation of the effective Hamiltonian is no longer valid. In the following, we shall remedy both defects.

The paper is organized as follows. We first extend the projection formalism such that it applies to the reduction of nonlocal systems and of dissipative systems modeled by an optical potential. Thus we work throughout with complex symmetric Hamiltonians, introduced in Section 2, and generalize in Sections 3 and 4 the traditional Feshbach projection approach to this more general situation. We then show in Section 5 that the formalism in fact allows to recover *all* solutions of the time-independent Schrödinger equation in terms of solutions of two Schrödinger equations, one in the reduced state space and the other in a reference state space. The resulting formulas are closely related to those of time-independent perturbation theory.

For practical calculations, the resulting formalism is revised in Section 6 so that it can be used without computing any projection operators. Section 7 shows how the use of doorway operators gives flexible approximation schemes for the exact formulas derived in Section 6. A backward error analysis discussed in Section 8 allows the estimation of the reliability of approximate solutions of Schrödinger equations obtained by this or any other method.

Specific choices of the embedding map lead in Section 9 to a modified coupled reaction channel/resonating group method framework for the calculation of multichannel scattering information, in which solutions of the full Schrödinger equation can be obtained from solutions of coupled reaction channel equations for the effective Hamiltonian. In principle it is capable of arbitrarily accurate approximations to the full dynamics, and shares this feature with the two Hilbert space method of CHANDLER & GIBSON [3, 4], which partly inspired the present investigations.

The theory is presented in a fully rigorous manner, allowing for unbounded operators by using in place of Hilbert spaces a pair of dual topological vector spaces. The most useful results are in Sections 6, 7, and 9.

The reader interested in the results but not in mathematical rigor may omit all references to spaces and topology, may think of all spaces as finite-dimensional and of operators as matrices, and may skip all proofs. In particular, of Section 2 introducing the basic terminology, only (1)–(3) are essential, and most of Sections 3–5 can be skimmed.

## 2 Symmetric operators

$\text{Lin}(\mathbb{V}, \mathbb{W})$  denotes the space of continuous linear mappings between two topological vector spaces  $\mathbb{V}$  and  $\mathbb{W}$ ,  $\mathbb{V}^* = \text{Lin}(\mathbb{V}, \mathbb{C})$  denotes the dual space of

continuous, complex-valued linear functionals on  $\mathbb{V}$ , and  $\text{Lin } \mathbb{V} = \text{Lin}(\mathbb{V}, \mathbb{V})$  denotes the algebra of continuous linear transformations of  $\mathbb{V}$ .

In the following,  $\mathbb{H}$  is a complex topological vector space with a definite, continuous symmetric bilinear form, providing a natural embedding of  $\mathbb{H}$  into the dual space  $\mathbb{H}^*$ . We refer to  $\mathbb{H}^*$  as a **state space**, and to the  $\psi \in \mathbb{H}^*$  as **states**. We write the pairing and the bilinear inner product as

$$\varphi^T \psi = \psi^T \varphi \quad \text{for } \varphi \in \mathbb{H}, \psi \in \mathbb{H}^*.$$

The notation is chosen such that it looks as closely as possible like standard finite-dimensional linear algebra.

We say that a sequence (or net)  $\psi_l \in \mathbb{H}^*$  **converges weakly** to  $\psi \in \mathbb{H}^*$ , and write  $\psi_l \rightharpoonup \psi$ , if

$$\lim_{l \rightarrow \infty} \varphi^T \psi_l = \varphi^T \psi \quad \forall \varphi \in \mathbb{H}.$$

We extend the bilinear inner product to arbitrary pairs  $(\varphi, \psi) \in \mathbb{H}^* \times \mathbb{H}^*$  for which

$$\varphi^T \psi = \lim_{l \rightarrow \infty} \varphi_l^T \psi_l$$

is defined and independent of the weakly converging sequences (or nets)  $\varphi_l \rightharpoonup \varphi$ ,  $\psi_l \rightharpoonup \psi$  of  $\varphi_l, \psi_l \in \mathbb{H}$ . (In the applications, this allows to form the inner product of state vectors corresponding to bound states and resonances but not that of scattering states.)

Complex conjugation is denoted by a bar, and, with the notation  $\psi^* = \bar{\psi}^T$ , the Hermitian inner product on  $\mathbb{H}$  is

$$\langle \varphi | \psi \rangle = \varphi^* \psi \quad \text{for } \varphi, \psi \in \mathbb{H}.$$

The associated Euclidean norm is

$$\|\psi\| = \sqrt{\psi^* \psi},$$

and  $\bar{\mathbb{H}}$  is the closure of  $\mathbb{H}$  in  $\mathbb{H}^*$  with respect to the Euclidean norm. Thus  $\mathbb{H} \subseteq \bar{\mathbb{H}} \subseteq \mathbb{H}^*$ , and  $\bar{\mathbb{H}}$  is a Hilbert space.

In the applications,  $\mathbb{H}$  is a space of sufficiently nice functions (namely arbitrarily often differentiable, with compact support) on some finite- or infinite-dimensional manifold, the inner product of two functions is some integral of their pointwise product induced by a nonnegative measure on the manifold, and  $\mathbb{H} \subseteq \bar{\mathbb{H}} \subseteq \mathbb{H}^*$  is a Gelfand triple (or rigged Hilbert space). (For these concepts, see GELFAND & VILENKIN [10], MAURIN [21]. For an exposition in physicists' terms see KUKULIN [17, Appendix A]; cf. also BÖHM [2].)

The **transpose** of a linear operator  $A \in \text{Lin}(\mathbb{H}, \mathbb{H}^*)$  is the linear operator  $A^T \in \text{Lin}(\mathbb{H}, \mathbb{H}^*)$  defined by

$$(A^T \varphi)^T \psi = \varphi^T A \psi \quad \text{for } \varphi, \psi \in \mathbb{H},$$

$A^* = \bar{A}^T$  defines the **adjoint** of  $A$ , and

$$\operatorname{Re} A = \frac{1}{2}(A + A^*), \quad \operatorname{Im} A = \frac{1}{2i}(A - A^*)$$

define the **real** and **imaginary part** of  $A$ . Clearly,  $(AB)^T = B^T A^T$  and  $(AB)^* = B^* A^*$ . The operator  $A \in \operatorname{Lin} \mathbb{H}$  is called **symmetric** if  $A^T = A$  on  $\mathbb{H}$ , **Hermitian** if  $A^* = A$  on  $\mathbb{H}$ , and **positive semidefinite** if

$$\psi^* A \psi \geq 0 \quad \text{for all } \psi \in \mathbb{H}.$$

In particular,  $A$  is Hermitian if and only if  $\operatorname{Im} A = 0$ . We extend symmetric operators  $A \in \operatorname{Lin} \mathbb{H}$  to  $\operatorname{Lin} \mathbb{H}^*$  by defining  $A\psi \in \mathbb{H}^*$  for  $\psi \in \mathbb{H}^*$  by

$$\varphi^T A \psi = (A\varphi)^T \psi \quad \forall \varphi \in \mathbb{H}.$$

In the following,  $L \in \operatorname{Lin} \mathbb{H}$  is always a symmetric operator such that

$$\operatorname{Im} L \text{ is positive semidefinite.} \tag{1}$$

(In particular, this includes the case where  $L$  is Hermitian since then  $\operatorname{Im} L = 0$ .)

Since  $\psi^* L \psi = \psi^*(\operatorname{Re} L)\psi + i\psi^*(\operatorname{Im} L)\psi$  and both  $\psi^*(\operatorname{Re} L)\psi$  and  $\psi^*(\operatorname{Im} L)\psi$  are real, (1) is equivalent to

$$\operatorname{Im} \psi^* L \psi \geq 0 \quad \text{for all } \psi \in \mathbb{H}. \tag{2}$$

In particular, the spectrum of  $L$  is in the complex upper half plane. If  $L$  has a spectral resolution then, since  $|\lambda + i\varepsilon| \geq \varepsilon$  for  $\operatorname{Im} \lambda \geq 0$ , we conclude that  $(L + i\varepsilon)^{-1}$  exists for all  $\varepsilon > 0$  as a bounded operator on  $\bar{\mathbb{H}}$  with spectral norm

$$\|(L + i\varepsilon)^{-1}\| \leq \varepsilon^{-1} \quad \text{for all } \varepsilon > 0.$$

The traditional situation is the one where  $L = E - H$  with a complex energy  $E$  satisfying  $\operatorname{Im} E \geq 0$  and a **Hamiltonian**  $H = H_s - \frac{i}{2}\Gamma$ . Here  $H_s, \Gamma \in \operatorname{Lin} \mathbb{H}$  are symmetric and Hermitian, and  $\Gamma$  is positive semidefinite. In the most important case of a conservative system,  $\Gamma = 0$  and  $H$  is Hermitian. However, care is taken that all our results hold in the nonhermitian case, corresponding to dissipative systems with an optical potential that contributes to  $\Gamma$ .

The use of  $L$  helps to avoid a multitude of expressions involving  $E - H$  or  $E - H + i\varepsilon$ . Since the (time-independent) **Schrödinger equation**  $H\psi = E\psi$  takes the simple form

$$L\psi = 0, \tag{3}$$

this makes the formal manipulations independent of energy and free of references to the Hamiltonian  $H$ , and thus much more readable. (Of course, in actual calculations,  $E$  and  $H$  reappear.)

More generally, (3) also covers nonlocal problems with a nonlinear dependence of  $L$  on  $E$ , and therefore can be used for the Bethe-Salpeter equations arising in bound state and resonance calculations for relativistic systems [14, 15, 18, 19, 26].

### 3 Reduction of the state space

Let  $\mathbb{H}$  and  $\mathbb{H}_{\text{eff}}$  be topological vector spaces with a definite, continuous bilinear inner product, related by the **embedding map**  $P$ , an injective, closed linear operator from  $\mathbb{H}_{\text{eff}}^*$  to  $\mathbb{H}^*$  satisfying  $\bar{P} = P$  and

$$P\psi_{\text{eff}} \in \mathbb{H} \quad \text{for all } \psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}.$$

We want to relate a Schrödinger equation  $L\psi = 0$  in the full state space  $\mathbb{H}^*$  to an effective Schrödinger equation  $L_{\text{eff}}\psi_{\text{eff}} = 0$  in the reduced state space  $\mathbb{H}_{\text{eff}}^*$ .

$P^* = P^T$  maps  $\mathbb{H}^*$  to  $\mathbb{H}_{\text{eff}}^*$  and  $\mathbb{H}$  to  $\mathbb{H}_{\text{eff}}$ . Moreover,  $P^*P : \mathbb{H}_{\text{eff}}^* \rightarrow \mathbb{H}_{\text{eff}}^*$  is invertible since  $P$  is closed and injective. The **pseudo inverse**

$$P^I := (P^*P)^{-1}P^* \tag{4}$$

maps  $\mathbb{H}^*$  to  $\mathbb{H}_{\text{eff}}^*$  and possesses the properties

$$(PP^I)^T = PP^I, \quad P^T PP^I = P^T, \quad P^I P = 1. \tag{5}$$

This implies that

$$Q := 1 - PP^I = 1 - (P^I)^T P^T \in \text{Lin } \mathbb{H}^* \tag{6}$$

satisfies

$$P^I Q = P^T Q = 0, \quad QP = 0, \quad Q^2 = Q^T = Q. \tag{7}$$

and hence is the orthogonal projection to the orthogonal complement of the range of  $P$ .

A  **$Q$ -resolvent** of a symmetric operator  $L \in \text{Lin } \mathbb{H}$  is a symmetric operator  $G \in \text{Lin } \mathbb{H}$  satisfying

$$GP = 0, \quad GLQ = Q. \tag{8}$$

Since  $GQ = G(1 - PP^I) = G$ , the symmetry of  $G$  implies

$$QG = G = GQ, \quad QLG = Q = GLQ. \tag{9}$$

Formally,  $G = Q(QLQ)^{-1}Q$ , but  $(QLQ)^{-1}$  is only defined on the range  $Q\mathbb{H}^*$  of  $Q$ .

The following discussion generalizes the Feshbach projection formalism which is obtained in the special case where  $L = E - H$  and  $H$  is Hermitian and  $G$  is the ordinary resolvent of  $QHQ$  in  $Q\mathbb{H}^*$  (cf. the development in KUKULIN et al. [17, Chapter 4]; in their notation,  $G = G_Q(z)$  is called the ‘orthogonalized resolvent’).

#### 3.1 Proposition.

(i) If  $L$  has a  $Q$ -resolvent  $G$ , it is uniquely determined, the operator

$$L_{\text{eff}} := P^T LP - P^T LGLP = P^T(L - LGL)P = P^T L(P - GLP) \tag{10}$$

is symmetric, and  $\text{Im } L_{\text{eff}}$  is positive semidefinite.

(ii) For arbitrary  $\psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}^*$ , the vector

$$\psi = (P - GLP)\psi_{\text{eff}} \in \mathbb{H}^* \quad (11)$$

satisfies

$$P^T L\psi = L_{\text{eff}}\psi_{\text{eff}}, \quad QL\psi = 0, \quad \psi_{\text{eff}} = P^I\psi. \quad (12)$$

*Proof.* If (9) holds with  $G'$  in place of  $G$  then

$$G' = G'Q = G'QLG = G'LG = G'LQG = QG = G,$$

giving uniqueness. The vector (11) satisfies

$$QL\psi = QL(P - GLP)\psi_{\text{eff}} = (Q - QLG)LP\psi_{\text{eff}} = 0,$$

$$P^T L\psi = P^T L(P - GLP)\psi_{\text{eff}} = L_{\text{eff}}\psi_{\text{eff}},$$

and, since  $P^I G = P^I QG = 0$ ,

$$P^I\psi = P^I(P - GLP)\psi_{\text{eff}} = P^I P\psi_{\text{eff}} = \psi_{\text{eff}}.$$

This proves (ii). Since  $\bar{P} = P$ , we have

$$\begin{aligned} \psi^* L\psi &= \psi^* ((P^I)^T P^T + Q)L\psi = \psi^* (P^I)^T L_{\text{eff}}\psi_{\text{eff}} \\ &= \psi^* (P^I)^* L_{\text{eff}}\psi_{\text{eff}} = \psi_{\text{eff}}^* L_{\text{eff}}\psi_{\text{eff}}. \end{aligned}$$

Thus, for arbitrary  $\psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}^*$ , we have  $\text{Im } \psi_{\text{eff}}^* L_{\text{eff}}\psi_{\text{eff}} = \text{Im } \psi^* L\psi \geq 0$ . This proves (i).  $\square$

The second term

$$\Delta := P^T LGLP \quad (13)$$

in the definition of  $L_{\text{eff}}$  is called the **optical potential** induced by the reduction process. (The name is explained in TAYLOR [27, p.385].)

In the special case where  $P^T P = 1$  and  $L = E - H$ ,  $G = G(E)$  and hence the optical potential  $\Delta(E) = P^T (E - H)G(E)(E - H)P$  is energy-dependent (and nonlocal) and we have  $L_{\text{eff}} = E - H_{\text{eff}}(E)$  with the **effective Hamiltonian**

$$H_{\text{eff}}(E) = P^T H P + \Delta(E).$$

Thus the optical potential causes energy shifts in the eigenvalues of the **projected Hamiltonian**  $P^T H P$ . We also note that the reduced Schrödinger equation is generally a *nonlinear* eigenvalue problem

$$H_{\text{eff}}(E)\psi = E\psi.$$

Frequently, the energy-dependence is ignored; however, nonlinear eigenvalue problems for nonlocal Schrödinger equations arising from Bethe-Salpeter

equations for relativistic problems were actually solved, e.g., [14, 15, 18, 19, 26].

Note that the resonating group method (WILDERMUTH & TANG [28]) works with coupled reaction channel equations derived from a projected Hamiltonian and hence misses the optical potential; an energy-independent term is added instead on a phenomenological basis [28, Chapter 8.2]. An alternative exact method is derived below.

We return to the general case.

**3.2 Proposition.** *The following identities hold:*

$$L_{\text{eff}}P^I = P^T(1 - LG)L, \quad (P^I)^T L_{\text{eff}} = L(P - GLP), \quad (14)$$

and, if  $L$  and  $L_{\text{eff}}$  are invertible,

$$P^T L^{-1} P = P^T P L_{\text{eff}}^{-1} P^T P. \quad (15)$$

*Proof.* Since  $(L - LGL)Q = L(Q - GLQ) = 0$ , we have

$$L_{\text{eff}}P^I = P^T(L - LGL)PP^I = P^T(L - LGL)(1 - Q) = P^T(L - LGL).$$

This gives the first equation in (14), and the transpose gives the second equation. For invertible  $L$ ,  $L_{\text{eff}}$ , we conclude from (14) and  $GP = GQP = 0$  that

$$L_{\text{eff}}P^I L^{-1} P = P^T(1 - LG)P = P^T P,$$

hence  $P^T P L_{\text{eff}}^{-1} P^T P = P^T P P^I L^{-1} P = P^T L^{-1} P$ .  $\square$

(15) implies that for invertible  $L$  and  $L_{\text{eff}}$ , the part of  $L^{-1}$  accessible from  $\mathbb{H}_{\text{eff}}^*$  can be computed from the knowledge of  $L_{\text{eff}}$  alone. Similarly, our next result says that, if  $L$  has a  $Q$ -resolvent, all solutions of the Schrödinger equation  $L\psi = 0$  can be computed from solutions of the reduced Schrödinger equation  $L_{\text{eff}}\psi_{\text{eff}} = 0$  and a knowledge of the **correction operator**

$$R = GLP \quad (16)$$

occurring in (10) and (11).

**3.3 Theorem.** *Suppose that  $L$  has a  $Q$ -resolvent  $G$ .*

(i) *For any  $\psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}^*$  with  $L_{\text{eff}}\psi_{\text{eff}} = 0$ , the vector  $\psi \in \mathbb{H}^*$  defined by (11) satisfies  $L\psi = 0$  and*

$$\psi_{\text{eff}} = P^I \psi \in \mathbb{H}_{\text{eff}}^*. \quad (17)$$

(ii) *For any  $\psi \in \mathbb{H}^*$  with  $L\psi = 0$ , the vector (17) satisfies  $L_{\text{eff}}\psi_{\text{eff}} = 0$ , and we can reconstruct  $\psi$  from (11).*

*Proof.* (i) Multiplication of the second equation of (14) with  $\psi_{\text{eff}}$  gives

$$0 = (P^I)^T L_{\text{eff}} \psi_{\text{eff}} = L(P - GLP) \psi_{\text{eff}} = L\psi,$$

and (17) follows from Proposition 3.1(ii).

(ii) Multiplication of the first equation of (14) with  $\psi$  gives

$$L_{\text{eff}} \psi_{\text{eff}} = L_{\text{eff}} P^I \psi = P^T (1 - LG) L \psi = 0.$$

Since  $P\psi_{\text{eff}} = PP^I \psi = (1 - Q)\psi = \psi - Q\psi$ , (11) follows from

$$\begin{aligned} (1 - GL)\psi &= (1 - GL)\psi - (Q - GLQ)\psi = (1 - GL)(1 - Q)\psi \\ &= (1 - GL)P\psi_{\text{eff}} = (P - GLP)\psi_{\text{eff}} \end{aligned}$$

since

$$GL\psi = 0. \tag{18}$$

□

Note that, while  $L_{\text{eff}} \psi_{\text{eff}} = 0$  looks like a Schrödinger equation, this is generally a **nonlinear** eigenvalue problem. Indeed, if  $L = L(E) = E - H$  then  $L_{\text{eff}}(E)$  is generally a nonlinear analytic function of  $E$ , and the **effective Hamiltonian**

$$H_{\text{eff}}(E) := E - L_{\text{eff}}(E)$$

has a nonlinear dependence on the energy.

In many cases of interest, the  $Q$ -resolvent does not exist for the Hamiltonian  $H$  of interest. But frequently the  $Q$ -resolvents  $G_\varepsilon$  for the perturbed Hamiltonians  $H - i\varepsilon$  corresponding to  $L_\varepsilon = L + i\varepsilon$  exist for all  $\varepsilon > 0$ , and are given by

$$G_\varepsilon = Q(QLQ + i\varepsilon)^{-1}Q.$$

If the limit

$$R := \lim_{\varepsilon \downarrow 0} G_\varepsilon L_\varepsilon P \tag{19}$$

exists, most of the preceding proof still goes through, with  $R$  in place of  $GLP$  and  $R^T$  in place of  $P^T LG$ , and the effective Hamiltonian (usually) acquires a nonhermitian part.

The only exception is the second half of statement (ii), which must be modified. (This is most conspicuously seen when  $P = 0$ , where  $L_{\text{eff}} = 0$  and the reduced Schrödinger equation provides no information at all.) Inspection of the proof shows that (18) fails. Thus, if  $\psi \in \mathbb{H}^*$  satisfies  $L\psi = 0$ , the expression

$$\psi^\perp := \psi - (P - R)\psi_{\text{eff}} \tag{20}$$

need not vanish (as predicted by (11) under the stronger assumptions), but only the much weaker equation  $P^T \psi^\perp = 0$  follows. Thus the reduction does

no longer allow one to recover *all* solutions of  $L\psi = 0$ . By Theorem 3.3(i),  $\psi^\perp$  is also a solution of the Schrödinger equation in  $\mathbb{H}^*$ , and since  $P^T\psi = 0$  implies  $\psi_{\text{eff}} = 0$  and hence  $\psi^\perp = \psi$  we have

$$\{\psi^\perp \mid L\psi = 0\} = \{\psi \mid L\psi = 0, P^T\psi = 0\}.$$

We discuss later (Theorem 5.2) how to access this missing part.

## 4 Perturbation theory

The computation of the  $Q$ -resolvent is traditionally done using perturbation theory. It is assumed that the inhomogeneous Schrödinger equation for a related reference problem is explicitly solvable, and the problem of interest is considered as a perturbation of the reference Schrödinger equation.

We therefore assume that we have a symmetric operator  $L_{\text{ref}} \in \text{Lin } \mathbb{H}$  satisfying

$$L_{\text{ref}}Q = QL_{\text{ref}}; \quad (21)$$

this commutation relation can always be achieved by taking an arbitrary symmetric approximation  $L_0$  to  $L$  and putting

$$L_{\text{ref}} = L_0 - (1 - Q)L_0Q - QL_0(1 - Q). \quad (22)$$

Let  $G$  be a  $Q$ -resolvent of  $L$  and put

$$V = L_{\text{ref}} - L, \quad T = V + VGV, \quad \Omega := 1 + GV. \quad (23)$$

$V$  is called the **interaction**,  $T$  the ( $Q$ -version of the) **transition operator** or **T-matrix**, and  $\Omega$  the ( $Q$ -version of the) **Möller operator**. This terminology is justified by the close formal relations of the properties of  $T$  and  $\Omega$ , derived below, with those of the T-matrix and the Möller operators of standard scattering theory. Indeed, for  $P = 0$ ,  $Q = 1$  (which is uninteresting from the point of view of effective Schrödinger equations), the results reduce to those of standard perturbation theory.

**4.1 Proposition.** *If (21) holds then*

$$\Omega P = (1 - GL)P, \quad \Omega^T P = P, \quad (24)$$

$$T = V\Omega = \Omega^T V, \quad (25)$$

$$P^T L \Omega P = L_{\text{eff}} = P^T (L_{\text{ref}} - T) P. \quad (26)$$

*Proof.* Since

$$GL_{\text{ref}}P = GQL_{\text{ref}}P = GL_{\text{ref}}QP = 0$$

we have

$$GLP = GL_{\text{ref}}P - GVP = -GVP,$$

$$P^T L G = (GLP)^T = -(GVP)^T = -P^T V G,$$

hence

$$\Omega P = P + GVP = (1 - GL)P.$$

Together with  $\Omega^T P = (1 + VG)P = (1 + VGQ)P = P$ , this gives (24). (25) follows directly from (23). Since

$$\begin{aligned} P^T L \Omega P &= P^T L(1 - GL)P = L_{\text{eff}} \\ &= P^T L P - P^T L G L P = P^T L P + P^T L G V P \\ &= P^T (L_{\text{ref}} - V)P - P^T V G V P = P^T (L_{\text{ref}} - T)P, \end{aligned}$$

(26) follows.  $\square$

**4.2 Proposition.** *If  $\Omega$  is invertible then*

$$G_{\text{ref}} = \Omega^{-1} G \tag{27}$$

is a  $Q$ -resolvent of  $L_{\text{ref}}$ , and

$$\Omega = (1 - W)^{-1}, \quad \text{where } W = G_{\text{ref}} V. \tag{28}$$

*Proof.*

$$\Omega(1 - W) = \Omega - \Omega G_{\text{ref}} V = \Omega - G V = 1,$$

gives (28). Since  $G_{\text{ref}} P = \Omega^{-1} G P = 0$  and

$$G_{\text{ref}} L_{\text{ref}} Q = G_{\text{ref}} L Q + G_{\text{ref}} V Q = \Omega^{-1} G L Q + W Q = (1 - W) Q + W Q = Q,$$

$G_{\text{ref}}$  is a  $Q$ -resolvent of  $L_{\text{ref}}$ .  $\square$

**4.3 Theorem.** *Suppose that  $G_{\text{ref}}$  is a  $Q$ -resolvent of a symmetric operator  $L_{\text{ref}}$  satisfying (21), and suppose that  $\Omega$  with (28) exists. Then  $G = \Omega G_{\text{ref}}$  is a  $Q$ -resolvent of  $L = L_{\text{ref}} - V$ , and with*

$$T = V + V G V, \tag{29}$$

(23)–(27) hold. Moreover, we have

$$\Omega = 1 + W \Omega = 1 + \Omega W, \tag{30}$$

$$T = V + T W = V + W^T T, \tag{31}$$

$$G = G_{\text{ref}} + W G = G_{\text{ref}} + G W^T. \tag{32}$$

*Proof.* (30) follows directly from  $\Omega(1 - W) = (1 - W)\Omega = 1$  and implies  $\Omega = 1 + \Omega G_{\text{ref}} V = 1 + G V$ , hence (23). Since  $G P = \Omega G_{\text{ref}} P = 0$  and

$$G L Q = G L_{\text{ref}} Q - G V Q = \Omega G_{\text{ref}} L_{\text{ref}} Q - G V Q = \Omega Q - G V Q = Q,$$

$G$  is a  $Q$ -resolvent of  $L$ . Thus Proposition 4.1 applies, and gives (24)–(26). (27) is obvious. The first equality in (31) follows from (25) and (30), and the second follows by transposing the first equation. The first equation in (32) follows from

$$WG = G_{\text{ref}}VG = G_{\text{ref}}QVQG = G_{\text{ref}}(QL_{\text{ref}}Q - QLQ)G = G - G_{\text{ref}},$$

and the second follows again by transposing the first equation.  $\square$

Inserting the definition (28) of  $W$  into (32) gives the ( $Q$ -version of the) **Dyson equation**

$$G = G_{\text{ref}} + G_{\text{ref}}VG = G_{\text{ref}} + GV^TG_{\text{ref}}. \quad (33)$$

If the spectral norm of  $W = G_{\text{ref}}V$  is smaller than one, (30)–(32) can be used to calculate iteratively the Möller operator  $\Omega$ , the transition operator  $T$  and the  $Q$ -resolvent  $G$ . To lowest order, we get

$$\Omega \approx 1 + G_{\text{ref}}V, \quad T \approx V, \quad G \approx G_{\text{ref}} + G_{\text{ref}}VG_{\text{ref}}.$$

When  $\mathbb{H}_{\text{eff}} = \{0\}$ , this is the **Born approximation**, and when  $\mathbb{H}_{\text{eff}}$  is finite-dimensional, this is a version of the **distorted wave Born approximation** (see, e.g., NEWTON [24, Section 9.1]). In the Born approximation, we simply get

$$L_{\text{eff}} \approx P^T(L_{\text{ref}} - V)P = P^TLP;$$

in second order,

$$L_{\text{eff}} \approx P^TLP - P^TVG_{\text{ref}}VP, \quad (34)$$

giving the approximation  $\Delta \approx P^TVG_{\text{ref}}VP$  for the optical potential (13). Further iteration gives the **Born series**

$$T = V + VG_{\text{ref}}V + VG_{\text{ref}}VG_{\text{ref}}V + \dots,$$

giving the exact optical potential

$$\Delta = P^TVG_{\text{ref}}VP + P^TVG_{\text{ref}}VG_{\text{ref}}VP + \dots$$

Thus we have recovered a generalized version of traditional perturbation theory. For  $\mathbb{H}_{\text{eff}} = \{0\}$ ,  $P = 0$ ,  $Q = 1$ , the equations obtained above reduce to those of standard perturbative scattering theory; the missing part – that one gets the scattering solutions of the Schrödinger equations – follows in the next section. Of course, from the point of view of effective Schrödinger equations, the case  $P = 0$  is completely uninteresting; however, it is instructive in that it shows that the methods used to solve scattering problems apply with small modifications to the problem of finding effective Hamiltonians.

Similarly, if  $\mathbb{H}_{\text{eff}}$  is the eigenspace of  $H_{\text{ref}}$  corresponding to a bound state of the reference system and  $P$  the orthogonal projector to this space, we get

the situation leading (in the Born approximation) to Fermi's Golden Rule; cf. KUKULIN et al. [17, Section 4.4]. For a nondegenerate bound state,  $\mathbb{H}_{\text{eff}}$  is one-dimensional, and again the point of view of effective Schrödinger equations is empty. For degenerate bound states, however, we recover a nontrivial low-dimensional eigenvalue problem as effective Schrödinger equation.

## 5 Solving the Schrödinger equation

We are now ready to express all solutions of the Schrödinger equation in terms of the solutions of a reduced Schrödinger equation and special solutions of a reference Schrödinger equation.

**5.1 Proposition.** *If*

$$\psi_{\text{eff}} = P^I \psi, \quad \psi_{\text{ref}} = Q(1 - W)\psi \quad (35)$$

then

$$P^T \psi_{\text{ref}} = 0, \quad \psi = \Omega(P\psi_{\text{eff}} + Q\psi_{\text{ref}}). \quad (36)$$

If (36) holds then

$$L_{\text{eff}}\psi_{\text{eff}} = P^T \Omega^T L\psi, \quad (37)$$

$$L_{\text{ref}}\psi_{\text{ref}} = QL\psi, \quad (38)$$

$$L\psi = (P^I)^T L_{\text{eff}}\psi_{\text{eff}} + L_{\text{ref}}\psi_{\text{ref}} - (1 - Q)\Omega^T L_{\text{ref}}\psi_{\text{ref}}. \quad (39)$$

*Proof.* Since

$$QW = QG_{\text{ref}}V = G_{\text{ref}}V = W,$$

(35) implies

$$\begin{aligned} Q\psi_{\text{ref}} &= Q(1 - W)\psi = (Q - W)\psi \\ &= (1 - PP^I - W)\psi = (1 - W)\psi - P\psi_{\text{eff}}, \end{aligned}$$

hence

$$\begin{aligned} \Omega(P\psi_{\text{eff}} + Q\psi_{\text{ref}}) &= \Omega(1 - W)\psi = \psi, \\ P^T \psi_{\text{ref}} &= P^T Q(1 - W)\psi = 0. \end{aligned}$$

This gives (36). Now suppose that (36) holds. By (24),

$$P^T \Omega^T L = (\Omega P)^T L = P^T (1 - LG)L = P^T L(1 - GL), \quad (40)$$

and

$$P^T \Omega^T LQ = P^T L(Q - GLQ) = 0. \quad (41)$$

Since  $(1 - QW)\Omega = (1 - W)\Omega = 1$ , this implies

$$P^T \Omega^T L\Omega = P^T \Omega^T L(1 - QW)\Omega = P^T \Omega^T L. \quad (42)$$

Using (36), (42), (41), and (40), we find

$$\begin{aligned} P^T \Omega^T L \psi &= P^T \Omega^T L \Omega (P \psi_{\text{eff}} + Q \psi_{\text{ref}}) = P^T \Omega^T L (P \psi_{\text{eff}} + Q \psi_{\text{ref}}) \\ &= P^T \Omega^T L P \psi_{\text{eff}} = P^T L (1 - GL) P \psi_{\text{eff}} = L_{\text{eff}} \psi_{\text{eff}}, \end{aligned}$$

giving (37). Since  $QL_{\text{ref}}W = QL_{\text{ref}}G_{\text{ref}}V = QV$ , we have

$$QL\Omega = (QL_{\text{ref}} - QV)\Omega = QL_{\text{ref}}(1 - W)\Omega = QL_{\text{ref}} = L_{\text{ref}}Q,$$

hence

$$\begin{aligned} QL\psi &= QL\Omega(P\psi_{\text{eff}} + Q\psi_{\text{ref}}) = L_{\text{ref}}Q(P\psi_{\text{eff}} + Q\psi_{\text{ref}}) \\ &= L_{\text{ref}}Q\psi_{\text{ref}} = L_{\text{ref}}\psi_{\text{ref}}, \end{aligned}$$

by (35), giving (38). Finally,  $X := 1 - (1 - Q)\Omega^T$  satisfies

$$XP = P - (1 - Q)\Omega^T P = P - (1 - Q)P = QP = 0$$

by (24), hence

$$XQL = X(1 - PP^I)L = XL = (1 - (1 - Q)\Omega^T)L = L - (P^I)^T P^T \Omega^T L,$$

so that

$$L\psi = ((P^I)^T P^T \Omega^T + XQ)L\psi = (P^I)^T L_{\text{eff}}\psi_{\text{eff}} + XL_{\text{ref}}\psi_{\text{ref}}$$

by (37) and (38). □

Since the formulas in Proposition 5.1 and  $L_{\text{eff}} = P^T L \Omega P$  do not involve  $G$ , we can take limits and obtain:

**5.2 Theorem.** *Let  $G_{\text{ref},\varepsilon}$  be a  $Q$ -resolvent of  $L_{\text{ref},\varepsilon}$  with  $\lim_{\varepsilon \downarrow 0} L_{\text{ref},\varepsilon} = L_{\text{ref}}$ . Suppose that*

$$W := \lim_{\varepsilon \downarrow 0} G_{\text{ref},\varepsilon} V \quad \text{and} \quad \Omega = (1 - W)^{-1}$$

*exist. If*

$$\psi_{\text{eff}} = P^I \psi, \quad \psi_{\text{ref}} = Q(1 - W)\psi$$

*then*

$$P^T \psi_{\text{ref}} = 0, \quad \psi = \Omega(P\psi_{\text{eff}} + Q\psi_{\text{ref}}).$$

*Moreover, with  $L_{\text{eff}} := P^T L \Omega P$ , we have*

$$L\psi = 0 \quad \Leftrightarrow \quad L_{\text{eff}}\psi_{\text{eff}} = 0, \quad L_{\text{ref}}\psi_{\text{ref}} = 0.$$

## 6 State space reduction without projections

Projection operators and the associated  $Q$ -resolvents are clumsy to use if an orthogonal basis is not easily available. We therefore revise the above formalism so that it can be used without computing any projection operators

or  $Q$ -resolvents. Additional flexibility is gained by using in place of the reference operator  $L_{\text{ref}} \in \text{Lin } \mathbb{H}$  an appropriate operator  $P_0 : \mathbb{H}_0^* \rightarrow \mathbb{H}^*$  from the dual of a reference space  $\mathbb{H}_0$ . For exact solutions, this reference space must be at least as big as  $\mathbb{H}$ ; however, in Section 7, we choose  $\mathbb{H}_0$  to be a smaller space in which numerical calculations are tractable, and obtain practical approximation schemes for the correction operator and the effective Hamiltonian. (This is related to the two Hilbert space method of CHANDLER & GIBSON [3, 4], and indeed was inspired by their work.)

As before,  $L \in \text{Lin } \mathbb{H}$  is assumed to be symmetric, and  $P : \mathbb{H}_{\text{eff}}^* \rightarrow \mathbb{H}^*$  is assumed to be a closed injective linear mapping satisfying  $\bar{P} = P$  and

$$P\psi_{\text{eff}} \in \mathbb{H} \quad \text{for all } \psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}.$$

Let  $P_0 : \mathbb{H}_0^* \rightarrow \mathbb{H}^*$  be a closed, surjective linear mapping satisfying

$$P_0\psi_0 \in \mathbb{H} \quad \text{for all } \psi_0 \in \mathbb{H}_0.$$

Then  $P_0^T$  maps  $\mathbb{H}^*$  to  $\mathbb{H}_0^*$  and  $\mathbb{H}$  to  $\mathbb{H}_0$ . Moreover,  $P_0P_0^T : \mathbb{H}^* \rightarrow \mathbb{H}^*$  is invertible since  $P_0$  is closed and surjective.

The pseudo inverse  $P^I$  of the injective  $P$  satisfies as before

$$P^I = (P^T P)^{-1} P^T, \quad P^I P = 1, \quad P^T P P^I = P^T$$

but the pseudo inverse  $P_0^I$  of the surjective  $P_0$  satisfies

$$P_0^I = P_0^T (P_0 P_0^T)^{-1}, \quad P_0 P_0^I = 1, \quad P_0^I P_0 P_0^T = P_0^T.$$

**6.1 Proposition.** *If there are linear mappings  $R : \mathbb{H}_{\text{eff}}^* \rightarrow \mathbb{H}^*$  and  $L' : \mathbb{H}_{\text{eff}}^* \rightarrow \mathbb{H}_{\text{eff}}^*$  such that*

$$R\psi_{\text{eff}} \in \mathbb{H} \quad \text{for all } \psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}; \quad L'\psi_0 \in \mathbb{H}_{\text{eff}} \quad \text{for all } \psi_0 \in \mathbb{H}_{\text{eff}}$$

and

$$P_0^T L R + P_0^T P L' = P_0^T L P, \quad P^T R = 0, \tag{43}$$

then

$$L_{\text{eff}} := P^T L P - R^T L R \in \text{Lin } \mathbb{H} \tag{44}$$

is a symmetric operator satisfying

$$L_{\text{eff}} = P^T L (P - R), \quad (P^I)^T L_{\text{eff}} = L (P - R). \tag{45}$$

Moreover, if  $L$  and  $L_{\text{eff}}$  are invertible then

$$P^T L^{-1} P = P^T P L_{\text{eff}}^{-1} P^T P. \tag{46}$$

*Proof.* Symmetry is obvious. Multiplication of (43) with  $Q(P^I)^T$  gives

$$Q L P = Q L R + Q P L' = Q L R.$$

Now

$$\begin{aligned} R^T L R &= R^T L(Q + (P^I)^T P^T) R = R^T L Q R \\ &= (Q L R)^T R = (Q L P)^T R = P^T L Q R = P^T L R \end{aligned}$$

since  $Q R = (1 - (P^I)^T P^T) R = R$ , hence

$$L_{\text{eff}} = P^T L P - R^T L R = P^T L P - P^T L R = P^T L(P - R).$$

This is the first half of (45). By multiplication with  $(P^I)^T$ , we find

$$\begin{aligned} (P^I)^T L_{\text{eff}} &= (P^I)^T P^T L(P - R) = (1 - Q)L(P - R) \\ &= L(P - R) - Q L P + Q L R = L(P - R) \end{aligned}$$

giving the second half of (45). If  $L$  and  $L_{\text{eff}}$  are invertible then (45) implies

$$P^T L^{-1} (P^I)^T L_{\text{eff}} = P^T (P - R) = P^T P,$$

hence

$$P^T P L_{\text{eff}}^{-1} P^T P = P^T L^{-1} (P^I)^T P^T P = P^T L^{-1} P,$$

giving (46).  $\square$

It is not difficult to see that  $R$  and  $L_{\text{eff}}$  from Section 3 are an instance of this construction, with  $\mathbb{H}_0 = \mathbb{H}$  and  $P_0 = 1$ .

## 6.2 Proposition.

(i) For arbitrary  $\psi \in \mathbb{H}^*$ , the vectors

$$\psi_{\text{eff}} = P^I \psi \in \mathbb{H}_{\text{eff}}^*, \quad \psi_0 = P_0^I (\psi - (P - R)\psi_{\text{eff}}) \in \mathbb{H}_0^* \quad (47)$$

satisfy

$$P^T P_0 \psi_0 = 0, \quad \psi = (P - R)\psi_{\text{eff}} + P_0 \psi_0. \quad (48)$$

(ii) If (48) holds for some  $\psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}^*$ ,  $\psi_0 \in \mathbb{H}_0^*$  then

$$L_{\text{eff}} \psi_{\text{eff}} = (P - R)^T L \psi, \quad (49)$$

$$P_0^T L P_0 \psi_0 = (P_0 - (P - R)P^I P_0)^T L \psi, \quad (50)$$

$$L \psi = (P^I)^T L_{\text{eff}} \psi_{\text{eff}} + (P_0^I)^T (P_0^T L P_0 \psi_0). \quad (51)$$

*Proof.* (i) follows from

$$P_0 \psi_0 = P_0 P_0^I (\psi - (P - R)\psi_{\text{eff}}) = \psi - (P - R)\psi_{\text{eff}},$$

$$\begin{aligned} P^T P_0 \psi_0 &= P^T \psi - P^T (P - R)\psi_{\text{eff}} = P^T \psi - P^T P \psi_{\text{eff}} \\ &= P^T \psi - P^T P P^I \psi = 0. \end{aligned}$$

(ii) Since by (43)

$$\begin{aligned} R^T L \psi &= R^T L P_0 \psi_0 = (P_0^T L R)^T \psi_0 = (P_0^T L P - P_0^T P L)^T \psi_0 \\ &= P^T L P_0 \psi_0 - L^T P^T P_0 \psi_0 = P^T L P_0 \psi_0, \end{aligned}$$

(49) follows from (45) and (48):

$$\begin{aligned} L_{\text{eff}}\psi_{\text{eff}} &= P^T L(P - R)\psi_{\text{eff}} = P^T L(\psi - P_0\psi_0) \\ &= P^T L\psi - P^T L P_0\psi_0 = P^T L\psi - R^T L\psi = (P - R)^T L\psi. \end{aligned}$$

(50) holds since by (48), (45) and (49),

$$\begin{aligned} P_0^T L P_0\psi_0 &= P_0^T L\psi - P_0^T L(P - R)\psi_{\text{eff}} = P_0^T L\psi - P_0^T (P^I)^T L_{\text{eff}}\psi_{\text{eff}} \\ &= P_0^T L\psi - P_0^T (P^I)^T (P - R)^T L\psi \\ &= (P_0 - (P - R)P^I P_0)^T L\psi. \end{aligned}$$

(51) holds since by (47) and (45),

$$\begin{aligned} (P_0^I)^T P_0^T L P_0\psi_0 &= L P_0\psi_0 = L P_0 P_0^I (\psi - (P - R)\psi_{\text{eff}}) \\ &= L(\psi - (P - R)\psi_{\text{eff}}) = L\psi - (P^I)^T L_{\text{eff}}\psi_{\text{eff}}. \end{aligned}$$

□

We now have the following projector-free and  $Q$ -resolvent-free version of Theorem 5.2, constructing all solutions of the Schrödinger equation  $L\psi = 0$  in terms of two simpler Schrödinger equations.

### 6.3 Theorem.

(i) If  $\text{Im } L$  is positive semidefinite then  $\text{Im } L_{\text{eff}}$  is positive semidefinite. If also  $\bar{P}_0 = P_0$  then also  $\text{Im } P_0^T L P_0$  is positive semidefinite.

(ii) For arbitrary  $\psi \in \mathbb{H}^*$ ,  $\psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}^*$ ,  $\psi_0 \in \mathbb{H}_0^*$  satisfying (47) or (48),

$$L\psi = 0 \quad \Leftrightarrow \quad L_{\text{eff}}\psi_{\text{eff}} = 0, \quad P_0^T L P_0\psi_0 = 0.$$

In particular, to find all solutions of  $L\psi = 0$ , it suffices to solve the two problems

$$\begin{aligned} L_{\text{eff}}\psi_{\text{eff}} &= 0, \\ P_0^T L P_0\psi_0 &= 0, \quad P^T P_0\psi_0 = 0. \end{aligned}$$

*Proof.* (i) For arbitrary  $\psi_{\text{eff}} \in \mathbb{H}_{\text{eff}}^*$ , we define  $\psi$  by (48) with  $\psi_0 = 0$ . Then  $P^T \psi = P^T (P - R)\psi_{\text{eff}} = P^T P\psi_{\text{eff}}$ , hence  $\psi_{\text{eff}} = P^I \psi$ . Now (51) gives

$$L\psi = (P^I)^T L_{\text{eff}}\psi_{\text{eff}},$$

and since  $(P^I)^* = (P^I)^T$ , we get

$$\psi^* L\psi = \psi^* (P^I)^T L_{\text{eff}}\psi_{\text{eff}} = (P^I \psi)^* L_{\text{eff}}\psi_{\text{eff}} = \psi_{\text{eff}}^* L_{\text{eff}}\psi_{\text{eff}}.$$

Hence  $\psi_{\text{eff}}^* (\text{Im } L_{\text{eff}})\psi_{\text{eff}} = \psi^* (\text{Im } L)\psi \geq 0$ , and  $\text{Im } L_{\text{eff}}$  is positive semidefinite. If also  $\bar{P}_0 = P_0$  then  $P_0^* = P_0^T$  and  $\text{Im } P_0^T L P_0$  is positive semidefinite since

$$\psi_0^* (\text{Im } P_0^T L P_0)\psi_0 = (P_0\psi_0)^* (\text{Im } L)(P_0\psi_0) \geq 0.$$

(ii) The forward implication follows directly from (49) and (50), the reverse implication from (51). □

**6.4 Remark.** If  $\psi_0 = 0$  then  $\varphi^T \psi = \varphi_{\text{eff}}^T (P^T P + R^T R) \psi_{\text{eff}}$ , so that

$$G_{\text{eff}} = P^T P + R^T R$$

is the **effective metric** induced on  $\mathbb{H}_{\text{eff}}$ . Note that it is generally not the original metric in  $\mathbb{H}_{\text{eff}}$ , not even when  $P$  is an orthogonal projection.

## 7 Form factors

In this section we show how to obtain efficiently approximations to the correction operator  $R$ . This leads in Section 9 to a modified coupled reaction channel/resonating group method framework for the calculation of multi-channel scattering information.

We emphasize that the formulas derived in this section no longer involve a pseudo inverse. In particular, they can be used even when  $P$  is not injective and  $P_0$  is not surjective. (However, since the assumptions under which the formulas are derived are then violated, they lose some information and hence give only approximate effective Hamiltonians.)

**7.1 Theorem.** *Let*

$$L_0 := P_0^T L P_0, \quad P_1 := P^T P_0, \quad U := P_0^T L P - P_0^T P \tilde{L} \quad (52)$$

with a symmetric  $\tilde{L} \in \text{Lin } \mathbb{H}_{\text{eff}}$  (and hence in  $\text{Lin } \mathbb{H}_{\text{eff}}^*$ ), and write

$$\hat{L}_\varepsilon := \begin{pmatrix} L_\varepsilon & P_1^T \\ P_1 & -i\varepsilon \end{pmatrix} \in \text{Lin}(\mathbb{H}_0 \oplus \mathbb{H}_{\text{eff}}) \quad \text{with } L_\varepsilon = L_0 + i\varepsilon.$$

(i) *If the strong limit*

$$\lim_{\varepsilon \downarrow 0} \hat{L}_\varepsilon^{-1} \begin{pmatrix} U \\ 0 \end{pmatrix} = \begin{pmatrix} F_0 \\ F_1 \end{pmatrix} \quad (53)$$

exists then (43) is solved by

$$R = P_0 F_0, \quad L' = \tilde{L} + F_1. \quad (54)$$

(ii) *Relation (53) holds with*

$$F_0 = \lim_{\varepsilon \downarrow 0} F_{0\varepsilon}, \quad F_1 = \lim_{\varepsilon \downarrow 0} F_{1\varepsilon}, \quad (55)$$

where

$$F_{1\varepsilon} = (P_1 L_\varepsilon^{-1} P_1^T + i\varepsilon)^{-1} P_1 L_\varepsilon^{-1} U, \quad F_{0\varepsilon} = L_\varepsilon^{-1} (U - P_1^T F_{1\varepsilon}), \quad (56)$$

if these limits exist.

*Proof.* (i) follows from

$$\begin{aligned}
\begin{pmatrix} P_0^T LR + P_0^T PL' \\ P^T R \end{pmatrix} &= \begin{pmatrix} P_0^T LP_0 F_0 + P_0^T P F_1 + P_0^T P \tilde{L} \\ P^T P_0 F_0 \end{pmatrix} \\
&= \hat{L}_0 \begin{pmatrix} F_0 \\ F_1 \end{pmatrix} + \begin{pmatrix} P_0^T P \tilde{L} \\ 0 \end{pmatrix} \\
&= \lim_{\varepsilon \downarrow 0} \hat{L}_0 \hat{L}_\varepsilon^{-1} \begin{pmatrix} U \\ 0 \end{pmatrix} + \begin{pmatrix} P_0^T P \tilde{L} \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} U \\ 0 \end{pmatrix} + \begin{pmatrix} P_0^T P \tilde{L} \\ 0 \end{pmatrix} = \begin{pmatrix} P_0^T LP \\ 0 \end{pmatrix}
\end{aligned}$$

by looking at the upper and the lower part separately. (ii) follows from the equation

$$\hat{L}_\varepsilon \begin{pmatrix} F_{0\varepsilon} \\ F_{1\varepsilon} \end{pmatrix} = \begin{pmatrix} U \\ 0 \end{pmatrix},$$

which is easily verified by substitution.  $\square$

In principle,  $\tilde{L}$  in (52) may be chosen arbitrarily. However, for numerical calculations it may be advisable to choose  $\tilde{L}$  in such a way that  $U$  (which replaces the interaction  $V$  in the projection approach) becomes small in some sense. This has the beneficial consequence that then the numerical approximation errors have a much smaller effect on the calculated solution.

In practice it is impossible to compute the exact correction operator and hence the exact effective Hamiltonian, since these tend to be exceedingly complicated. One therefore exploits physical intuition to select a space  $\mathbb{H}_0$  of manageable complexity whose dual contains the **doorway states** believed to mediate the interaction of the reduced system and the unmodelled environment.  $\mathbb{H}_0^*$  is embedded into  $\mathbb{H}^*$  by means of a **doorway operator**  $P_0$  that is now no longer surjective. Fortunately, the formulas (43) and (44) defining  $R$  and  $L_{\text{eff}}$  do not depend on pseudo inverses, and hence make also sense in this case. (43) and (44) now only yield approximate solutions for the correction operator and an approximate effective Hamiltonian. However, these approximations become better and better as the range of  $P_0$  covers a bigger and bigger part of  $\mathbb{H}$ .

The situation is fully analogous to numerical discretization schemes that are necessary to solve all but the simplest partial differential equations; the only difference is that in the present context it frequently makes sense to consider approximations in manageable function spaces, so that one does not discretize completely.

A proper choice of the doorway operator  $P_0$  makes the computations more tractable. At the same time, it limits the formal complexity of the optical potential

$$\Delta = R^T LR = F_0^T (P_0^T LP_0) F_0, \quad (57)$$

the second term in  $L_{\text{eff}}$ . As one can see,  $P_0$  specifies the allowed form of the optical potential while the **form factor**  $F_0$  specifies the coefficients in the optical potential, and thus introduces energy-dependent **running coupling constants**.

The art in applying the reduction technique consists in finding embeddings  $P$  that ‘dress’ the subsystem of interest in a sufficiently accurate way, a doorway operator  $P_0$  embedding the relevant doorway states, and an operator  $\tilde{L}$  such that  $U$  is small, and the limit (53) exists and can be approximated efficiently.

Setting  $P_0 = 0$  gives  $R = 0$ ,  $\Delta = 0$ , and hence the trivial approximation

$$L_{\text{eff}} \approx P^T L P. \quad (58)$$

This simply amounts to discarding the interaction of the subsystem with the rest of the system. The choice  $\mathbb{H}_0 = \mathbb{H}$ ,  $P_0 = P$  is not better since then  $P^T P F_0 = P^T P_0 F_0 = P^T R = 0$  by (43), and hence  $F_0 = 0$ ,  $R = 0$ . This is not surprising since we expect that the doorway operator  $P_0$  should incorporate *additional* information about doorway states not yet represented in the subsystem but significantly interacting with it.

If  $\mathbb{H}_0$  and  $\mathbb{H}_{\text{eff}}$  are finite-dimensional then (52) defines finite-dimensional matrices, and the computation of the form factor amounts to solving the matrix equation

$$\begin{pmatrix} L_0 & P_1^T \\ P_1 & 0 \end{pmatrix} \begin{pmatrix} F_0 \\ F_1 \end{pmatrix} = \begin{pmatrix} U \\ 0 \end{pmatrix} \quad (59)$$

with a complex symmetric (and for  $L = L^*$ ,  $\bar{P}_0 = P_0$  Hermitian) coefficient matrix. (59) can be solved efficiently by sparse matrix methods (cf. DUFF et al. [25, 5]) if suitable localized basis functions are used to construct  $P$  and  $P_0$ .

In practice, it may be useful to employ in combination with discretization methods a complex absorbing potential in place of the  $+i\varepsilon$ . In particular, if one proceeds as in NEUMAIER & MANDELSHTAM [23] one gets a quadratic eigenvalue problem that can handle all energies in a certain range simultaneously using harmonic inversion (MANDELSHTAM & TAYLOR [20]).

If  $\mathbb{H}_{\text{eff}}$  is finite-dimensional but  $\mathbb{H}_0$  is a function space then  $L_0$  is a differential or integral operator on  $\mathbb{H}_0$ . By solving suitable differential or integral equations we can find the vector-valued functions

$$B_0 := \lim_{\varepsilon \downarrow 0} L_\varepsilon^{-1} P_0^T L P, \quad B_1 := \lim_{\varepsilon \downarrow 0} L_\varepsilon^{-1} P_0^T P.$$

and the complex symmetric matrix

$$G_1 := P_1 B_1 = \lim_{\varepsilon \downarrow 0} (P_1 L_\varepsilon^{-1} P_1^T + i\varepsilon).$$

Noting that  $L' = F_1$  if  $\tilde{L} = 0$ , the formula (55) for the form factor becomes

$$F_0 = B_0 - B_1 L', \quad \text{where } L' = G_1^{-1} P_1 B_0.$$

## 8 The quality of approximate state vectors

In practice, it is usually impossible to find exact solutions of a Schrödinger equation  $L\psi = 0$ . On the other hand, in real applications,  $L$  is never precisely known either. Hence it makes sense to assess the quality of an approximate state vector  $\psi$  by trying to modify  $L$  a little to an operator  $\tilde{L}$  that satisfies  $\tilde{L}\psi = 0$  exactly. If the modification  $\tilde{L} - L$  is within the accuracy to which  $L$  is known, we are confident that  $\psi$  is a good approximation to the true but unknown  $L$ .

This way of assessing the quality of an approximate solution of a problem is widely used in numerical analysis (see, e.g., WILKINSON [29]) and is known under the name of **backward error analysis**. Here we give a backward error analysis for the equation  $L\psi = 0$ , and deduce guidelines for quality assessment of approximate state vectors.

**8.1 Theorem.** *Let  $L \in \text{Lin } \mathbb{H}$  be symmetric. Then, for arbitrary  $\psi \in \mathbb{H}^*$  with finite  $\psi^T\psi \neq 0$ , the modified operator*

$$\hat{L} = \left(1 - \frac{\psi\psi^T}{\psi^T\psi}\right)L\left(1 - \frac{\psi\psi^T}{\psi^T\psi}\right). \quad (60)$$

satisfies  $\hat{L}\psi = 0$  and

$$\text{tr}(\hat{L} - L)^2 = \tau_L(\psi), \quad (61)$$

where

$$\tau_L(\psi) := 2\frac{(L\psi)^T(L\psi)}{\psi^T\psi} - \left(\frac{\psi^T L\psi}{\psi^T\psi}\right)^2. \quad (62)$$

*Proof.* Since the formulas are invariant under scaling  $\psi$  we may assume that  $\psi$  is normalized to norm 1. Then

$$\psi^T\psi = 1, \quad \psi^T L\psi =: \lambda, \quad \psi^T L^2\psi =: \mu,$$

with real  $\lambda, \mu$ . The operator

$$\Delta := L - \hat{L} = \psi\psi^T L + L\psi\psi^T - \lambda\psi\psi^T$$

satisfies  $\Delta\psi = L\psi$ , hence  $\hat{L}\psi = 0$ . Since

$$\Delta L\psi = \lambda L\psi + (\mu - \lambda^2)\psi,$$

we find

$$\Delta^2 = L\psi\psi^T L + (\mu - \lambda^2)\psi\psi^T.$$

$\Delta^2$  maps  $\mathbb{H}$  to the two-dimensional space spanned by  $\psi$  and  $L\psi$ , hence is trace class. Using the formula  $\text{tr } \varphi\psi^T = \psi^T\varphi$ , we find

$$\text{tr } \Delta^2 = \mu + (\mu - \lambda^2) = 2\mu - \lambda^2 = \tau_L(\psi),$$

giving (61). □

In the conservative case where  $\text{Im } L = 0$ , and hence  $L$  is Hermitian, it is possible to show that the choice (60) is best possible. Note that a state vector  $\psi \in \mathbb{H}^*$  with  $\bar{\psi} = \psi$  and finite  $\psi^T \psi$  is now in the Hilbert space  $\bar{\mathbb{H}}$ .

**8.2 Theorem.** *Let  $L \in \text{Lin } \mathbb{H}$  be Hermitian, and suppose that  $\psi \in \bar{\mathbb{H}} \setminus \{0\}$  satisfies  $\bar{\psi} = \psi$  and  $L\psi \in \bar{\mathbb{H}}$ .*

(i) *Any symmetric and Hermitian  $\tilde{L} \in \text{Lin } \mathbb{H}$  with  $\tilde{L}\psi = 0$  satisfies*

$$\text{tr}(\tilde{L} - L)^2 \geq \tau_L(\psi). \quad (63)$$

*Equality in (63) is achieved precisely when  $\tilde{L} = \hat{L}$ .*

(ii) *We always have*

$$0 \leq \frac{(L\psi)^T L\psi}{\psi^T \psi} \leq \tau_L(\psi) \leq 2 \frac{(L\psi)^T L\psi}{\psi^T \psi}. \quad (64)$$

*In particular,  $\tau_L(\psi) = 0$  if and only if  $L\psi = 0$ .*

*Proof.* By the preceding theorem,  $\tilde{L} = \hat{L}$  gives equality in (63), and is a good choice since  $\hat{L}\psi = 0$ . Hence suppose that  $\tilde{L} \neq \hat{L}$ . Without loss of generality,  $(\tilde{L} - L)^2$  is trace class (otherwise the trace is infinity and (63) is trivially satisfied). Since  $(\tilde{L} - \hat{L})\psi = \tilde{L}\psi - \hat{L}\psi = 0$  we have

$$\begin{aligned} \text{tr}(L - \hat{L})(\tilde{L} - \hat{L}) &= \text{tr} \Delta(\tilde{L} - \hat{L}) \\ &= \psi^T L(\tilde{L} - \hat{L})\psi + \psi^T (\tilde{L} - \hat{L})L\psi - \lambda \psi^T (\tilde{L} - \hat{L})\psi = 0. \end{aligned}$$

Therefore

$$\begin{aligned} \text{tr}(\tilde{L} - L)^2 - \tau_L(\psi) &= \text{tr}(\tilde{L} - L)^2 - \text{tr}(\hat{L} - L)^2 \\ &= \text{tr}(\tilde{L} + \hat{L} - 2L)(\tilde{L} - \hat{L}) \\ &= \text{tr}(\tilde{L} - \hat{L})^2 - 2 \text{tr}(L - \hat{L})(\tilde{L} - \hat{L}) \\ &= \text{tr}(\tilde{L} - \hat{L})^2 > 0 \end{aligned}$$

since  $\tilde{L} \neq \hat{L}$ . Therefore, (63) holds for  $\tilde{L} \neq \hat{L}$  with strict inequality. This proves (i). Since  $\bar{\psi} = \psi$ , the second term in (61) is nonnegative. This gives the upper bound in (64) and implies the final assertion. The lower bound follows from the Cauchy-Schwarz inequality  $(\psi^T L\psi)^2 \leq \psi^T \psi \cdot (L\psi)^T L\psi$ . □

(60) is the orthogonal projection of  $L$  to the orthogonal complement of  $\psi$ , and  $\sqrt{\tau_L(\psi)}$  measures, in a sense, its deviation from  $L$ . Therefore,  $\tau_L(\psi)$  (or its square root) serves as a useful measure for the quality of an approximate solution  $\psi$  of the Schrödinger equation with Hermitian  $L$ .

In the nonhermitian case, it seems possible that  $\tau_L(\psi) = 0$  even if  $L\psi \neq 0$ . (A finite-dimensional example is  $L = \begin{pmatrix} \alpha & i \\ i & 0 \end{pmatrix}$ ,  $\psi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  which has  $L^2 = 0$  and  $\tau_L(\psi) = 0$  for  $\alpha = \sqrt{2}$ , and for  $\alpha = 1$  even  $\tau_L(\psi) < 0$ .) Thus, unless  $L^* = L$ , the measure  $\tau_L(\psi)$  might be sometimes too optimistic. However, in practice  $L$  is nearly Hermitian and the use of  $\tau_L(\psi)$  should cause no problems.

## 9 Multichannel scattering

We now apply the above to the multichannel approach discussed below. A projection approach to multichannel scattering leading to effective Hamiltonians is discussed, e.g., in NEWTON [24, Section 16.6], but the equations derived there appear not to be suitable to numerical approximation. A more useful formulation is given by the present equations from Theorem 7.1, with  $P$  and  $P_0$  as given below.

An **arrangement** is a partition  $A$  of the system of particles into clusters  $i \in A$ , with correct assignment of distinguishability. At a fixed energy  $E$ , those arrangements are relevant that contain **channels** defined by cluster bound states with energies  $E_i$  such that

$$\sum_{i \in A} E_i \leq E + \Delta E$$

where  $\Delta E$  is zero or a small quantity. These open or nearly open channels are assumed to correspond approximately to states in a  $n_A$ -dimensional space

$$\mathbb{H}_{A0} \subseteq \bigotimes_{i \in A} \mathbb{H}_i$$

with basis functions

$$\varphi_{Ak}(x) = \prod_{i \in A} \varphi_{iik}(x_i), \quad (65)$$

where  $x_i$  is the vector of coordinates of particles in cluster  $i$ , and the  $\varphi_{il}(x_i)$  are translation invariant basis functions from the cluster Hilbert space  $\mathbb{H}_i$ , used in all possible combinations in (65). The motion of the clusters is described by a space  $\mathbb{H}_A$  of functions of a system of relative coordinates  $r_A$  between the cluster centers.

Consider, for example, a 3-particle reaction  $XY + Z \rightleftharpoons X + YZ$ . Then  $\mathbb{H}_{XY+Z,0}$  consists of products of approximate bound states  $\psi_{XY}$  and the ground state  $\psi_Z$ ;  $\mathbb{H}_{X+YZ,0}$  consists of products of the ground state  $\psi_X$  and approximate bound states  $\psi_{YZ}$ , and  $\mathbb{H}_{XYZ,0}$  consists of sufficiently many states localized in the transition region to resolve the resonances of interest. Usually, one would keep the arrangements  $(XY, Z)$  and  $(X, YZ)$  in the reduced description, and use the states belonging to the arrangement  $(XYZ)$  as doorway states for the transition regime.

Let  $\mathcal{C}$  be the set of arrangements considered relevant for the reduced description. The reduced **multichannel state space** is then the dual of the space

$$\mathbb{H}_{\text{eff}} = \bigoplus_{A \in \mathcal{C}_{\text{eff}}} \mathbb{H}_A^{n_A}$$

or the properly symmetrized subspace in case of indistinguishable clusters. The inner product in  $\mathbb{H}_{\text{eff}}$  is given by

$$\varphi_{\text{eff}}^T \psi_{\text{eff}} = \sum_{A \in \mathcal{C}_{\text{eff}}} \int dr_A \varphi_A(r_A)^T \psi_A(r_A).$$

The embedding map  $P : \mathbb{H}_{\text{eff}}^* \rightarrow \mathbb{H}^*$  is given by

$$P\psi_{\text{eff}} = \sum_{A \in \mathcal{C}_{\text{eff}}} P_A \psi_A,$$

where the  $k$ th component of  $P_A : (\mathbb{H}_A^{n_A})^* \rightarrow \mathbb{H}^*$  maps a function of  $r_A$  to the  $k$ th basis vector of  $\mathbb{H}_A$  modified to have the corresponding dependence on the center of mass  $r_A(x)$  of the cluster coordinates  $x$ ,

$$(P_A \psi_A)_k(x) = \psi_A(r_A(x)) \varphi_{Ak}(x).$$

The transpose  $P^T : \mathbb{H}^* \rightarrow \mathbb{H}_{\text{eff}}^*$  is given by

$$(P^T \psi)_A = P_A^T \psi \quad \text{for all } A \in \mathcal{C}_{\text{eff}}.$$

By construction,  $P^T L P$  is a direct sum of contributions of the form

$$P_A^T L P_A = L_A - H_A,$$

where  $H_A$  is the free Hamiltonian for the motion of the cluster centers and  $L_A$  is a symmetric  $n_A \times n_A$ -matrix. In a basis of cluster eigenstates with energies  $E_i$ ,  $L_A$  is the diagonal matrix formed by the energy differences  $E - E_i$ .

The construction of  $(\mathbb{H}_0, P_0)$  is completely analogous, using a larger set of arrangements and/or channels that contain the doorway states.

Thus the calculations have the same complexity as those for the coupled reaction channel equations (or resonating group method), as described, e.g., by WILDERMUTH & TANG [28]). However, the present scheme is more flexible in that it can incorporate information from doorway states. In principle, by increasing the size of the doorway state space, it is capable of arbitrarily accurate approximations to the full dynamics, and shares this feature with the two Hilbert space method of CHANDLER & GIBSON [3, 4] and with a technique by GOLDFLAM & KOWALSKI [11].

To solve the reduced Schrödinger equation (and, if a similar construction is used for the doorway operator, the equations for the form factor), the whole arsenal of methods developed in the applications is available. Binary

arrangements can be handled by Lippmann-Schwinger equations (see, e.g., WILDERMUTH & TANG [28], ADHIKARI & KOWALSKI [1, Chapter 3]), and 3-cluster arrangements by the FADDEEV [6] connected kernel approach (see, e.g., GLÖCKLE [13, Chapter 3], KUKULIN et al. [17], ADHIKARI & KOWALSKI [1, Chapter 7]).

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