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Weighted projection and optimization of coupled-channel equations

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Abstract. The conventional coupled-channel method for many-particle scattering is modified to facilitate applications to low-energy collision processes and to break-up (ionization) reactions. A new approach to the construction of coupled-channel equations is developed in terms of the weighted projections, where proper choices of the weighting function can simplify the set of coupled equations. Optimal choices of the weighting functions are discussed, and several approximations for construction of the weight functions are presented. The conventional pseudostate and mixed basis expansions are shown to be related to the weighted projection approach. The break-up (and ionization) channels can be included in the coupled-channel approach. Finally, the recently developed generalization of the Hartree–Fock (GHF) theory for scattering is shown to be a special case of the weighted projections, thus providing a partial justification of the use of amputated wavefunctions for the continuum state projection.

1. Introduction

One of the most successful approaches to treating many-particle scattering systems has been the coupled-channel method (CCM) (Breit 1946, Newton 1958, Burke and Smith 1962, Mott and Massey 1965). This includes the *R*-matrix approach (Burke 1979) which has been widely employed. It has been widely used in low-energy scattering problems in atomic, molecular and nuclear physics (Austern 1970), as well as in solid state and quantum optics calculations. Although the resulting scattering amplitudes are some of the most accurate ever produced by theory, there are many intrinsic as well as practical limitations to the theory. Some of these will be analysed in this paper in order to formulate an alternate mathematical procedure in terms of weighted projections. The new approach should be applicable to a wide range of scattering systems, to atomic, molecular, nuclear as well as to solid state and quantum optics problems. The important properties of the CCM are:

(i) The method usually works well for low-energy elastic and inelastic processes, with a small number of open channels, but it cannot be directly applied to break-up and ionization processes, where more than two clusters are present in the continua asymptotically. In the past, this problem has always been treated by the distorted-wave formalism.

(ii) The internal cluster wavefunctions in the asymptotic region must be supplied *a priori* in accurate forms. They are the integral part of the asymptotic boundary conditions needed to specify the scattering problem. For clusters with three or more particles (as in He, Li, Na atoms and ionic targets Mg^+ , O^{2+} ions, etc and He, C, O nuclei in nuclear reactions), this requirement can be met only approximately. Effects of inaccuracies in the cluster functions on the scattering solution are difficult to assess (Hahn 1968).

(iii) The non-orthogonality problem associated with the rearrangement and exchange channels can be a serious problem, and often the question of overcompleteness of mixed sets arises (Percival and Seaton 1957). Due to the possible presence of disconnected scattering kernels (Faddeev 1961, Weinberg 1963, 1964) there are convergence problems associated with perturbation series. Its formal resolution is well documented (Newton 1982), but often impractical to implement in real physical situations.

(iv) Furthermore, in the CCM, the many-particle scattering functions are expanded in some basis sets associated with the cluster systems, and the series is truncated for practical reasons. The convergence of the theory can thus be slow, as a function of the number of basis functions included in the expansion of the total wavefunction. In many cases, this depends on the basis functions chosen. The pseudostates and mixed basis sets are often employed to improve the situation.

(v) Many resonance states can occur in a certain energy range, and they must be incorporated explicitly in the basis set chosen. The problem simplifies, however, if a coarse energy resolution is desired so that the spectra can be averaged over a finite energy bin.

(vi) There are, in general, many inner-shell particles of the target core which are not seriously involved in a given reaction at low energies, although they are carried by the theory to satisfy the exclusion principle and screening. These spectator particles may sometimes be replaced by a pseudopotential or a model potential.

Evidently, (i)–(iii) are the complications intrinsic to many-particle scattering systems, while difficulties (iv)–(vi) are of a more practical nature and have been the subject of intense developments in recent years. Some of this progress, relevant to our discussion, will be summarized in section 2. Our main objective in this paper is to analyse items (i) and (iii); (ii) has been treated recently (Hahn 1996) in terms of a generalized self-consistent field (SCF) theory.

2. Coupled-channel equations for collisions

In order to describe the new approach based on the weighted projections, to be developed in section 4, we first briefly summarize the conventional coupled-channel method (CCM) for an N -particle scattering system. For simplicity, we limit the discussion here to collision channels that involve only two clusters asymptotically, $N = N_a + N_b$, for example $= 1 + (N - 1)$, and without particle rearrangements. The asymptotic channel cluster functions for the $(N - 1)$ particles are then required to characterize the open channels. The operator $P = \sum_{\alpha=1}^{\Lambda_p} |\psi_{\alpha}\rangle\langle\psi_{\alpha}|$ projects onto the open channels, in terms of the basis set $\{\psi_{\alpha}\}$. We have $P^2 = P^+ = P$. The rest of the closed-channel spectrum is grouped in the operator Q , such that $P + Q = 1$, where 1 is in the space of $N - 1$ particles. (This particular separation of the $N - 1$ particle space in which P spans only the open channels is the minimal one and most convenient for the discussion below. In general, P may in addition contain some of the closed-channel components. However, such a distinction may not be possible in practice, especially when mixed nonorthogonal functions are used.)

2.1. General coupled scattering equations

A set of coupled equations for scattering is obtained using the expansion of the total wavefunction $\Psi = P\Psi + Q\Psi$, as

$$(H - E)P\Psi = -(H - E)Q\Psi. \quad (2.1)$$

In order to reduce the number of variables ($3N$ for an N -particle system) in (2.1) to that of one particle with three variables, equation (2.1) is usually projected onto the space of $(N - 1)$ particles. The conventional procedure is to use the same set that is used in the definition of P and Q , and project (2.1) from the left, as

$$P(H - E)P\Psi = -P(H - E)Q\Psi \quad (2.2a)$$

$$Q(H - E)Q\Psi = -Q(H - E)P\Psi. \quad (2.2b)$$

We have the desired equations of the CCM in its primitive form by truncation of the P and Q spaces with a finite number of states.

In terms of the Green's function in the Q space, we can uncouple (2.2), as

$$P[F + FG^Q]P\Psi = 0 \quad (2.3)$$

where $F \equiv H - E$, and

$$G^Q = [Q(-F)Q]^{-1}. \quad (2.4)$$

The Green's function G^Q contains most of the important dynamical information on the scattering system, such as the resonance structure, polarization of the targets and distortion of the scattering states. The resulting effective 'potential' operator

$$PU^QP = PFG^QFP \quad (2.5)$$

is nonlocal and energy dependent, and in general is in matrix form, as dictated by the number of open channels spanned by P and the particular spin structure. Here, the Q space was chosen to be entirely of the closed channel space at a given total energy E , in which case this potential PU^QP is real and negative (i.e. attractive).

The P equation (2.2a) usually involves a small number of coupled equations for the open channels at a given energy E , which can be readily integrated numerically, once some form of the G^Q operator is known. Elaborate numerical codes, including the well known R-MATRIX code, are available for this purpose. Therefore, the main complication in treating the many-particle scattering problem is in estimating the Q part of the wavefunction. In this section we consider several approaches that can be used for this purpose.

We simply mention three approximations for the potential U^Q that have been frequently used in the past. (i) In the case of low-energy atomic collisions, a long-range dipole (and higher-order multipole) approximation may be introduced for $P(H - E)Q$, which then gives rise to a polarization potential and distortion of targets. (ii) A variational approximation for G^Q may be given in terms of a set of Q -space trial functions, and the resulting energy matrix for the operator $Q(H - E)Q$ diagonalized and inverted. This also gives rise to resonances. The variationally determined Q -space functions are the usual pseudostates, and the convergence of the expansion in terms of the set $\{\psi_\alpha\}$ may be improved. (iii) An adiabatic approximation for low-energy collisions is obtained by replacing G^Q by its adiabatic counterpart. This turned out to be the adiabatic state expansion, as will be discussed further in the next section.

2.2. Effective orthogonality of the projected states

In general, for identical multiparticle systems with exchange symmetries, the explicit operators P and Q are difficult to construct, even when the precise form of the ψ are available. However, in carrying out the actual scattering calculation, this requirement can be relaxed (Burke and Taylor 1966, Hahn 1970), and the orthogonality of the G^Q and P

need not be imposed. This is an important point of principle in the application of the CCM, and its proof is given below. By defining the solution $P\Psi$ as

$$P\Psi = P\Psi^P + G^P F Q\Psi \quad (2.6)$$

where

$$P(H - E)P\Psi^P = 0 \quad \text{and} \quad P(E - H)PG^P = P \quad (2.7)$$

we can write the Q equation as

$$Q[F + FG^P F]Q\Psi = -QFP\Psi^P. \quad (2.8)$$

Now, assume that an approximate Q' contains a part which overlaps with the P space, i.e. $Q' = aP + bQ$. Then, from (2.8), we immediately have for the aP projected part

$$aP[F + FG^P F](aP + bQ)\Psi' = -aPFP\Psi^P. \quad (2.9)$$

The left-hand side of (2.9) is zero by the definition of G^P , while the right-hand side also vanishes because of the property of $P\Psi^P$. Therefore, the aP component in Q' is irrelevant in so far as (2.9) is concerned. Note that the vanishing of both sides of (2.9) requires that the exact G^P and $P\Psi^P$ are available. On the other hand, the bQ part gives

$$bQ[F + FG^P F](aP + bQ)\Psi' = -bQFP\Psi^P. \quad (2.10)$$

Again the $aP\Psi'$ part in (2.10) gives zero contribution, and the bQ part becomes

$$b^2Q[F + FG^P F]Q\Psi' = -bQFP\Psi^P. \quad (2.11)$$

Now, since the aP part is not present in both (2.9) and (2.10), we may simply set $b = 1$ and we are back to $Q' = Q$; that is, equation (2.11) is identical to (2.7). This concludes the proof that, within the structure of the coupled equations (2.2), the overlap of Q' with P does not affect the final solution. The problem of overcompleteness with two or more different basis sets can be resolved by the same procedure as described above.

2.3. Rearrangement and exchange processes

The CCM method may be extended to rearrangement collisions in a mathematically consistent way by the reduced matrix equation (RME) formalism (Hahn 1982, Hahn and Watson 1972). To make the discussion transparent, we consider a three-particle collision system, $N = 3$, with rearrangement of particles (and exchange). Then

$$1 + (2 + 3)_0 \rightarrow 1 + (2 + 3)_n \quad (2.11a)$$

$$\rightarrow 2 + (1 + 3)_m \quad (2.11b)$$

$$\rightarrow 1 + 2 + 3. \quad (2.11c)$$

For this simple scattering system with the two-cluster elastic and inelastic excitation channels, the cluster function for $(2 + 3)$ and $(1 + 3)$ can be calculated accurately. On the other hand, for $N > 3$, we may have a bound cluster $(2 + 3 + 4)$, for example, and the asymptotic channel boundary conditions require that such cluster functions must be supplied prior to the scattering calculation. Such functions are, in general, difficult to obtain, however. The question of how critical is the effect of approximate cluster functions on the resulting scattering amplitudes is not so simple to assess. A fully self-consistent procedure was formulated recently, in which these cluster functions as well as the scattering functions themselves are determined simultaneously. This approach is summarized in section 5.

We follow the RME formulation, which was developed previously to circumvent the theoretical difficulties associated with the rearrangement channels. It combines the more

rigorous Faddeev theory and more practical multiple scattering theory of Watson. For simplicity, we neglect the break-up channel (2.11c) and omit the channel $3 + (1 + 2)$. Then the reduced matrix equations (sometimes called FHW equations) for this system are given by

$$M\Psi = \begin{bmatrix} H_1 + Y_1 - E & V_2 - Y_2 \\ V_1 + Y_1 & H_2 + Y_2 - E \end{bmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = 0 \quad (2.12)$$

which is a reduced form of the original matrix equation of Faddeev, in which channel 3 is collapsed. The potentials Y are arbitrary and, in general, chosen to facilitate convergence when the equations are projected; their insertion in (2.12) does not change the physics in its exact form, but any approximations to (2.12) will introduce different changes in the solution depending on the particular approximation.

The usual approach is to construct projection operators

$$P = \begin{bmatrix} P_1 & 0 \\ 0 & P_2 \end{bmatrix} \quad (2.13)$$

where P_1 and P_2 are from two different sets, associated with two distinct asymptotic channel Hamiltonians H_i . The corresponding Q operator may be defined, but with the property that $PQ = QP = 0$ and $P^2 = P^+ = P$; also $P_1Q_2 \neq 0$ and $P_1P_2 \neq 0$, etc. Thus, these operators are not all necessarily orthogonal, except in their respective asymptotic channel regions, where their overlaps vanish. We then have both the P and Q components in the wavefunction $\Psi \simeq \Psi_t = P\Psi_t + Q\Psi_t$, which are to be determined simultaneously.

3. Mixed bases expansions

Before we discuss the weighted projection method (WPM) in the next section, it is instructive to consider the use of mixed basis sets in the construction of coupled equations. As will become clear, this is a special case of the WPM. We note that the projection need not be with the set $\{\psi\}$, an alternate set $\{\psi'\}$, for example, may be used, where $P' + Q' = 1$ but $Q'P \neq 0$.

3.1. Mixed basis sets

In view of the approximations discussed in section 2, and the effective orthogonality proof, it is reasonable to generalize the wavefunction expansion for the total scattering function Ψ in terms of one or more basis sets.

(i) For example, we consider the mixing of two basis sets, $\{\psi\}$ and $\{\phi\}$ and denote them by P and Q' , respectively; in its truncated form we have

$$\Psi_t \simeq \sum_{\alpha}^{\Lambda_P} \psi_{\alpha} u_{\alpha} + \sum_{\beta}^{\Lambda_{Q'}} \phi_{\beta} w_{\beta} = P\Psi_t + Q'\Psi_t. \quad (3.1)$$

This is similar to the pseudostate expansion employed in many of the recent CCM calculations. In general, these two sets are not necessarily orthogonal to each other, although they are each complete. Therefore, the problem of overcompleteness arises. However, because of the effective orthogonality property discussed in section 2, it can be shown that, when the set of coupled equations are solved exactly numerically, the functions u and w

are arranged in such a way that this over-counting problem disappears. Thus, we have, for all $\alpha \leq \Lambda_P$ and $\beta \leq \Lambda_Q$,

$$(\psi_\alpha|[H - E]|\Psi_t) = 0 \quad (3.2a)$$

$$(\phi_\beta|[H - E]|\Psi_t) = 0 \quad (3.2b)$$

resulting in the coupled set of equations for u and w .

(ii) Alternatively, we may expand Ψ_t , in one set and the scattering equation is projected by another set, as

$$\Psi_t = \sum_{\alpha}^{\Lambda_P} \psi_\alpha u_\alpha \quad (3.3)$$

and the projection

$$(\phi_\beta|[H - E]|\Psi_t) = 0 \quad \beta = 1, 2, \dots, \Lambda_Q = \Lambda_P \quad (3.4)$$

where ϕ_β , need not be the same as ψ_α . The set (3.4) with (3.3) is the structure we study below in terms of a weighted projection. Note that (3.4) is a coupled set of Λ_P equations, rather than the set (3.2) of $(\Lambda_P + \Lambda_Q)$ coupled equations (Λ_Q can be larger than Λ_P).

3.2. Adiabatic basis

The second basis set $\{\phi\}$ in (3.4) is as yet unspecified; it could be the same set as the first as in (3.3), or arbitrarily parametrized variational functions. Excited states generated by a Hartree-Fock procedure for the Hamiltonian $Q'HQ'$ may be acceptable, where the closed-channel space is treated just like a 'bound-state' problem using the conventional HF procedure. The basis set thus generated can then be used in the diagonalization process in the evaluation of G^Q . Although this procedure is often numerically intensive, the set can provide a good first-order contribution to particular resonance states, which is otherwise difficult to guess.

We consider here the adiabatic wavefunctions for projection of (2.1). This is also closely related to the WPM, as discussed in section 5. To clarify the physical contents of this basis, we show that the adiabatic basis set may be expressed as linear combinations of the functions of the undistorted set, so that the adiabatic states represent the full polarization effect in the low-energy approximation. For this purpose, we write the scattering Hamiltonian explicitly as

$$H = K(\vec{R}) + h(\vec{r}) + V(\vec{r} - \vec{R}) \quad (3.5)$$

and the undistorted states are generated by $h\psi_n = E_n\psi_n$. We further let $P = |\psi_0\rangle\langle\psi_0|$ and $Q = 1 - P$, where 1 is in the space spanned by h , i.e. $1 = \delta(\vec{r} - \vec{r}')$. The Q space represents all the states generated by h except the $n = 0$ state. The adiabatic basis is generated by $(h + V)$, where \vec{R} is simply a parameter, as

$$(h(r) + V(r, R))\phi_m(\vec{r}, \vec{R}) = E_m^a(R)\phi_m. \quad (3.6)$$

(Note that these adiabatic states are slightly different from those used in the molecular representation, in the treatment of the core motion.)

The content of these functions may be exhibited explicitly by projecting the ϕ equation (3.6). For the ground state with $m = 0$, e.g.

$$P(h + V - E_0^a)P\phi_0 = -PVQ\phi_0 \quad (3.7a)$$

$$Q(h + V - E_0^a)Q\phi_0 = -QVP\phi_0. \quad (3.7b)$$

As in section 2, the $Q\phi_0$ is eliminated by solving (3.7b) and substituting back into (3.7a). We then obtain for (3.7a)

$$P[h + V + VG_0^{aQ}V - E_0^a]P\phi_0 = 0 \quad (3.8a)$$

where

$$G_0^{aQ} = [Q(E_0^a - h - V)Q]^{-1}. \quad (3.8b)$$

Therefore, we finally have

$$\phi_0(\vec{r}, \vec{R}) = P\phi_0 + Q\phi_0 \quad (3.9)$$

with

$$P\phi_0 = \psi_0(\vec{r})f_0^a(\vec{R}) \quad \text{and} \quad Q\phi_0(\vec{r}, \vec{R}) = G_0^{aQ}QVP\psi_0f_0^a \quad (3.10)$$

with the normalization

$$f_0^a(\vec{R})^2 [1 + \langle \psi_0 | V(G_0^{aQ})^2 V | \psi_0 \rangle] = 1. \quad (3.11)$$

The result for the adiabatic Green's function G_0^{aQ} may be compared with the exact G^Q of (2.4); we see that (i) $Q(K - E + E_0)Q$ is omitted and (ii) E_0 is replaced by E_0^a , where E_0^a is defined in terms of the adiabatic potential by $E_0^a = E_0 + U_0^a(R)$. Explicitly,

$$U_0^a = \langle PVP + PVG_0^{aQ}VP \rangle. \quad (3.12)$$

This is a nonlinear relationship for U_0^a , because G_0^{aQ} itself contains U_0^a . The pairs of functions ϕ_n and ψ_n overlap, especially at large R .

As will be seen in the next section, this pair of adiabatic functions may be a suitable candidate as weighted projections for low-energy collision processes.

3.3. Effective channel approach

In connection with the choice of a set that represents the Q space effectively, we note that the Q -space function may be approximated (Rule and Hahn 1975, 1976) by the closure property, as

$$Q\Psi = G^Q(H - E)P\Psi \simeq \Delta_t^{-1}QVP\Psi_t \equiv Q\Psi_t. \quad (3.13)$$

Except for a constant Δ , we have an approximate trial function which mixes different components of the Q space via the coupling QVP. In actual applications of (3.13), however, the theory is usually cast in a normalization-independent form, so that the constant parameter Δ_t does not appear explicitly. It can be viewed as an effective variation of this parameter for an optimal choice, thus supporting the effectiveness of the form (3.13). The function $Q\Psi_t$ was used to represent the Q space in the effective-channel approach (ECA), and was successful earlier in deriving the effective proton–nucleus scattering potential at high energies. Unlike in some of the previous theoretical analyses, this function correctly estimated (Rule and Hahn 1975) the second diffraction peak in the proton–He angular distribution at high energy, in agreement with the refined experiments at Saclay and Berkeley. As will be shown later, this form of the Q -space function has an analogous interpretation in the generalized HF theory. Incidentally, if necessary, the $Q\Psi_t$ may be further split into components that represent subspaces of Q .

4. Weighted projection method

As stressed in section 2, equation (2.1) must be projected onto the $(N - 1)$ -particle space in order to reduce the number of variables involved. In all the previous applications, however, the projection of the scattering equations was carried out invariably with the basis functions which were used in the expansion of Ψ_t . One major advantage of this approach is that the resulting set of coupled equations is symmetric and is derivable from a variational principle. Thus, for the number of basis functions included in the expansion of the scattering function Ψ_t , $\Lambda_t = \Lambda_P + \Lambda_Q$, we have the same number of coupled equations to be integrated. The partial diagonalization of the Q -space functions as in the pseudostate approach is consistent with this picture, where the coefficient functions in the diagonalization are now specified and the number of coupled equations to be solved explicitly remains at Λ_P .

However, in principle we have the option of projecting with any functions so long as the resulting scattering coefficient functions, the u and w in (3.1) for example, can be properly determined. This possible option has never been explored, and it is the main purpose of this paper to examine it within the context of the CCM. We formulate the weighted projection method (WPM) to optimize the CCM. Since this is a totally new approach for composite system scattering, there are many serious questions which must be clarified before the method can be applied with confidence. In the following we discuss some of these problems and attempt to provide some answers.

4.1. Weighted projection method

It is proposed that the projection of equation (2.1) be carried out with one or more weight functions W , such that the terms that couple the functions in P and Q disappear. That is,

$$PW^P P(H - E)P\Psi = -PW^P P(H - E)Q\Psi \simeq 0 \quad (4.1a)$$

$$QW^Q Q(H - E)Q\Psi = -QW^Q Q(H - E)P\Psi \simeq 0. \quad (4.1b)$$

Obviously, the W^P must contain the dynamical information carried by $Q\Psi$, and vice versa for W^Q . In fact, the exact W^P can be given formally such that the right-hand side of (4.1a) is zero. From equation (2.3), we have the exact W^P and W^Q ,

$$PW^P = P[1 + (H - E)G^Q] = P + P(H - E)G^Q Q \quad (4.2a)$$

$$QW^Q = Q[1 + (H - E)G^P]. \quad (4.2b)$$

Note that W^P is by definition left-projected by P , but the right-hand side mixes both the P and Q components. Explicitly, taking the Hermitian conjugate, we have the exact expression

$$W^P \psi = \psi + G^Q Q V P \psi. \quad (4.2c)$$

That is, with the exact PW^P given by (4.2a), the $Q\Psi$ component in the scattering equation is not necessary, and $P\Psi$ alone is sufficient to describe the channels contained in P . Incidentally, we note that (4.2c) is similar to (3.10) of the adiabatic basis, suggesting that for low-energy collisions a suitably constructed adiabatic function may provide the correct projection, where the weighting function is automatically included.

Similarly, we can show that adding terms in the Ψ_t , as $\Psi_t = P\Psi + \Psi'$ where Ψ' is necessarily $Q\Psi'$, is not going to change the solution. Explicitly, with the new term Ψ' , we have for the right-hand side of the PT equation,

$$\begin{aligned} \langle PW^P | H - E | Q\Psi' \rangle &= 0 \\ &= \langle P\psi | [P + VG^Q Q] (H - E) | Q\Psi' \rangle \\ &= \langle P\psi | H - E | Q\Psi' \rangle + \langle P\psi | (H - E)G^Q Q (H - E) | Q\Psi' \rangle \end{aligned}$$

by the definition of G^Q . Of course, in practice $Q\Psi'$ will be some part of the exact $Q\Psi$, but in the limit of a full Q -space function, we have the exact cancellation shown above, so that the right-hand side of the $P\Psi$ equation will approach zero in this limit. This property may be used to check the convergence of the WPM, so that the WPM is not an arbitrary procedure.

The form of the scattering equations with the weighted projection is somewhat similar to the Sturmian function expansion, where the projection is carried out and the weight function is identified with the potential that generates the basis set. However, the details and the physical content are quite different, since here W essentially mixes states that are in the original Q space.

4.2. An equivalence proof of WPM and EPM

We now show explicitly that the construction of an effective potential (EPM) of a composite system scattering for the coupled-channel approach is equivalent to the use of an effective weighting function (WPM) for the projection of a simple scattering equation. In a special case with $\Lambda_P = 1$ and $\Lambda_Q = 1$, we have $\Psi_t = \psi u + \phi w$, which gives

$$\langle \psi | F | \psi \rangle u = -\langle \psi | F | \phi \rangle w \quad (4.3a)$$

$$\langle \phi | F | \phi \rangle w = -\langle \phi | F | \psi \rangle u. \quad (4.3b)$$

These equations can be reduced to the following two different arrangements of terms:

$$\langle \psi | F + U_\phi | \psi \rangle u = 0 \quad \text{with} \quad U_\phi = -F | \psi \rangle \langle \phi | F | \phi \rangle^{-1} \langle \phi | F \quad (4.4)$$

or

$$\langle \psi | W_\phi F | \psi \rangle u = 0 \quad \text{with} \quad W_\phi = 1 - F | \phi \rangle \langle \phi | F | \phi \rangle^{-1} \langle \phi |. \quad (4.5)$$

This is a trivial regrouping of terms, but shows clearly the equivalence between the calculation of an effective (optical) potential U_ϕ , and the weighted projection with W_ϕ . They have essentially the same physical contents.

The seemingly arbitrary choice of the weight function in terms of the amputated scattering function must be corrected when an additional configuration interaction (CI) is introduced. That is, as more terms are added to Ψ_t , the theory should converge, independent of the W used. The equivalence proof given above between the WPM and the EPM shows that these two methods are complementary. In fact, a close relationship exists between them, as

$$\text{WPM} \longleftrightarrow \text{CI} \longleftrightarrow \text{EPM}$$

such that an optimal CCM must involve exploitation of both these methods. In addition, the WPM now allows the treatment of the break-up and ionization channels within the CCM. As will be discussed in the next section, the generalization of the conventional HF approach to scattering problems also require the WPM in an essential way.

4.3. Approximate construction of W^P

We list several ways by which approximate W^P may be obtained in practice.

(i) Variational principle. From equation (4.2a), we have the Hermitian conjugate

$$W^P \psi = \psi + G^Q Q V P \psi. \quad (4.6)$$

Therefore

$$P W^P \psi = \psi \quad \text{and} \quad Q W^P \psi = G^Q Q V P \psi. \quad (4.7)$$

A variational estimate of W^P should be in the G^Q , as

$$G^Q \rightarrow -|Q\Phi_t\rangle\langle Q\Phi_t|F|Q\Phi_t\rangle^{-1}\langle\Phi_t| \equiv G_t^Q. \quad (4.8)$$

For more than one $Q\Phi_t$, we have a matrix inversion of the QFQ matrix. With this variational form, we then have

$$W_t^P \psi_n = \psi_n + G_t^Q QVP\psi_n \quad (4.9)$$

for each state ψ_n in the P space.

(ii) The adiabatic approximation. As shown in section 3, we have simply an approximate projection

$$W^P \psi_n \simeq \phi_n. \quad (4.10)$$

This obviously corresponds to the use of a mixed basis expansion, in which the wavefunction Ψ is expanded in one basis set, while the projection is carried out using another set. We have no previous experience with such an approach, and many test calculations are needed to assess the reliability of (4.10).

(iii) Closure approximation. We can modify (4.2a) slightly as

$$\begin{aligned} PW_P &= P[-(H-E)G^P + (H-E)G^Q] = P[1 + (H-E)G^Q] \\ &\simeq PVP/\Delta_P + PVQ/\Delta_Q \simeq PV/\Delta_t \end{aligned} \quad (4.11)$$

where the Δ are suitable parameters defined in a closure approximation. The Δ_t is not essential when used in (4.1a), for example, especially when the right-hand side goes to zero. In this form, equation (4.11), the weight function is very much like the Q -space function used in the ECA. Obviously, with such a weighted projection, the right-hand side of the P equations may be completely eliminated, and we have essentially a simple set of open-channel equations.

Thus, the purpose of employing the weighted projection method (WPM) is to eliminate the effect of the right-hand sides in (4.1), so that the simple function $P\Psi_t$, determined by (4.1a), for example, should be sufficiently accurate.

(iv) An approximate procedure for the construction of the weight function for the GHF will be considered in section 4.5.

4.4. Rearrangement and break-up channels

The RME given in section 2 may be extended to include the WPM. Let the trial solution be simply $\Psi_t = P\Psi_t$, while the RME is to be projected from the left by the weighted operator

$$PW^P = \begin{bmatrix} PW_1^P & 0 \\ 0 & PW_2^P \end{bmatrix}. \quad (4.12)$$

This gives the desired equations for the rearrangement collisions

$$PW^P MP\Psi_t = 0. \quad (4.13)$$

The break-up reactions are described by the P which project onto the continuum. Obviously such projection operators may not be simply defined since they are no longer square-integrable. However, $\psi_1(23)W_1^P(23)$, for example, may still make the integral involved in the projected RME completely well defined. It is then a question of choosing the correct weighting operators to represent the interaction region. At present, the amputation of the continuum ψ may be the preferred projection, as discussed in the next subsection.

4.5. Weighting function for the continuum normalization

In the GHF approach, the continuum functions are used in projecting the equations for the bound-state orbitals. However, this introduces infinities because of the non-normalizability of the continuum orbital. The usual energy normalization requires a weight function of the form

$$W_{\Delta}(r) = \sin(\Delta r)/r \quad (4.14)$$

which effectively cuts off the infinitely oscillating (positive) tail, where it is assumed that $\Delta \ll k$. This is a spectral density function and essentially eliminates the short-range part of the normalization integral, so that for practical cases where the scattering functions are needed in the matrix element calculation, the above form has to be properly modified. A possible form is

$$W \simeq \tilde{\theta}(r_0 - r) + W_{\Delta}\tilde{\theta}(r - r_0) \quad (4.15)$$

where r_0 is the range of the interaction potential U_c associated with the continuum orbital. This form may further be approximated as

$$W \simeq U_c(r)/\bar{U}_c \quad (4.16)$$

where the constant \bar{U}_c often acts as a variational parameter that optimizes the effect of W . The form (4.16) was used in the recent generalization of the HF approach to scattering, where the amputated scattering function may be cast in the form of a weighted projection.

4.6. Positron–hydrogen scattering

As the first numerical test of the WPM, we applied the theory to positron–hydrogen scattering below the pick-up threshold for positronium formation. It is probably the simplest scattering system involving three particles, that is not exactly solvable. The problem has been studied

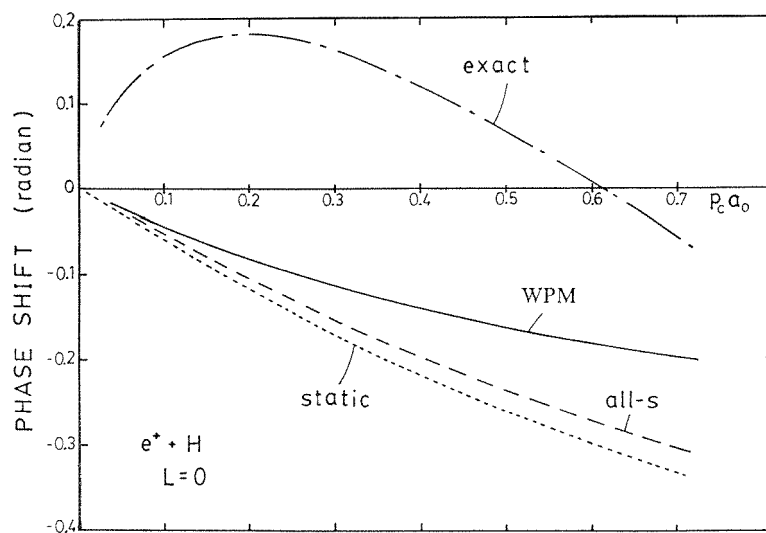


Figure 1. The positron–hydrogen scattering phase shift obtained with the simple choice (17) is compared with that obtained by the static approximation, the all-s approximation, and the exact (numerical) result. The WPM seems to improve with increasing energy.

extensively by a variety of theoretical techniques, and is a fertile ground for testing theories. For example, the usually powerful coupled-channel method was proven to have a notoriously bad convergence problem, unless a good polarization term was added. With the simple choice

$$W \simeq \langle \psi_0 | V | \psi_0 \rangle = V_{static} \quad \text{and} \quad \Psi_t = \psi_0 u_{0t} \quad (4.17)$$

however, we recover more than one half of the total correction to the static approximation. This is illustrated in figure 1. Together with other approximations for the W discussed in this section, this example shows that the WPM could be a powerful tool to improve the coupled-channel method.

5. Discussions

We have reformulated the conventional CCM by introducing the weighted projection procedure, for the purpose of optimizing the efficiency of the approach. The mixed expansion of the wavefunctions naturally leads to the partially SCF HF theory and also to the weighted projections. With a judicious choice of the weighting function, we can greatly improve the effectiveness of the CCM, and several possibilities for the forms of W are discussed. More critical is the question of whether the WPM can be made convergent. This is made plausible by the construction of W in (4.2) as they are substituted into (4.1). Finally, the fully SCF HF procedure for scattering, the generalized HF, is shown to be a special case of the weighted projection approach. There are many serious questions on the WPM and GHF which require further analyses and developments. Some of the outstanding critical problems are: (i) the convergence of the theory as more terms are added to the Ψ_t ; (ii) stability of the procedure with amputated wavefunctions; (iii) applicability of the theory to systems with more than two particles in individual clusters.

There are many processes to which the new set of equations derived in sections 4 and 5 may be applied. In particular, the break-up channels may be incorporated in a very natural way, since with the square-integrable W , all the components in the coupled scattering equations are now well defined.

The theory developed above for the lowest HF ansatz may be extended to general scattering systems. (i) More than one term may be added to Ψ which mixes the bound-state configurations. This configuration mixing is expected to make ψ approach the correct asymptotic functions. (ii) Multichannel scattering may be treated, including inelastic and rearrangement collisions. (iii) Scattering systems with more than one particle in the continuum may be treated, as in break-up and ionization reactions. The use of the weighted projection may be especially relevant there. (iv) Reactions involving two heavy particles may be analysed, where each particle may have internal cluster structures, as in heavy ion reactions and molecular collisions. We have, for the first time, a self-consistent theory that evaluates the resonance amplitudes corresponding to a two-particle one-hole state which are coupled to the continuum.

It is also of interest to adopt the theory to treat bound-state problems in which highly excited states with large spatial dimensions are involved. The conventional SCF procedure treats such particles just as any other low-lying bound particles. The amputated function provides a more compact description of such states.

Appendix A. Partially SCF Hartree–Fock theory of collisions

An alternate treatment of the problem posed by (2.1) is to solve the Q -space problem just like in the bound-state case, since the Q space is by definition closed, so that the wavefunctions are all square-integrable, but with the coupling to the P space explicitly included. The entire Q -space functions are written in HF antisymmetrized product forms and all the orbitals are to be determined self-consistently. This requires all the orbitals to be square-integrable. Similarly, the P equations are to be solved with the coupling to the Q space retained. Obviously, this is not possible for the P space, because $P\Psi$ is not square integrable. We therefore depart from full self-consistency, and assume that all the open-channel cluster functions $\{\psi_\alpha\}$ of the P space are available explicitly. Then, we have the asymptotic boundary conditions satisfied explicitly. Since we do not require the ψ to be predetermined, so that they are not SCF, the principal difficulty of the full SCF formulation of the entire scattering problem is avoided. For example, for a three-particle system with a heavy central core, with $1 + (2 + 3 + C)$ collision, we may write

$$\Psi_t = \psi(23)u(1) + \phi(23)w(1). \quad (\text{A.1})$$

For simplicity, we omitted the explicit reference to the core C , but we have to remember that the $\psi(23)$, for example, is a genuine three-particle wavefunction, which is not readily calculable. Then, the above procedure results in a set of coupled equations

$$\langle \psi | H - E | \psi \rangle u = -\langle \psi | H - E | \phi \rangle w \quad (\text{A.2a})$$

$$\langle \phi | H - E | \phi \rangle w = -\langle \phi | H - E | \psi \rangle u \quad (\text{A.2b})$$

$$\langle w | H - E | w \rangle \phi = -\langle w | H - E | u \rangle \psi \quad (\text{A.2c})$$

for the functions u , w and ϕ , all self-consistently, while ψ is assumed to be predetermined, as a part of the asymptotic boundary conditions. That is, the Hamiltonian $h(23C)$ for the cluster gives the wavefunction as $h(23C)\psi \simeq E_t\psi(23C)$, which has to be prepared separately before (A.2) is set up. It is important to note the conspicuous absence of the equation for ψ in the set (A.2). That is, ψ is not determined self-consistently. This is the continuum HF approach (CHF). The distinction between the GHF of section 5 and the present CHF is clear; it is in the treatment of ψ . As noted earlier, if we are to also determine ψ within the framework of (A.2), we have to project with function u , which is not square-integrable, and we are therefore forced into introducing the amputation.

The main difference between the present approach and the conventional CCM is also clear. That is, in the present CHF, the Q equations are solved self-consistently, as they are coupled to the P -space functions, while the P equations are to be treated exactly as in the conventional CCM.

Application of this procedure to simple three-particle scattering systems is in progress to determine the efficiency of the approach. As compared to a fully self-consistent theory summarized in section 4.5, the generalized HF, the present approach keeps the exact asymptotic channel functions as given *a priori*.

The CHF of this appendix is presented so that it may be readily compared with the GHF. Evidently, the assumption that ψ is given *a priori* makes the theory less drastically different from the conventional approaches. No difficulties of continuum normalization arise. However, from the general SCF point of view, this is not quite satisfactory, especially when cluster functions such as ψ are, in general, difficult to generate accurately. In the GHF, both ψ and ϕ may be expressed as products (or determinants) of single-particle orbital functions, and the whole set is to be determined self-consistently.

Finally, we note that the $\langle\psi|$ and $\langle\phi|$ projections in (A.2) may be replaced by their adiabatic counterpart, as $\psi \rightarrow \psi^{adiab}$ and $\phi \rightarrow \phi^{adiab}$. This is consistent with the discussion given in terms of (3.4), (3.10) and (4.2c).

References

- Austern N 1970 *Direct Nuclear Reaction Theory* (New York: Wiley)
- Bethe H A and Salpeter E E 1957 *Handbuch der Physik* ed S Flugge (Berlin: Springer)
- Burke P G 1979 *Adv. At. Mol. Phys.* **15** 471
- Burke P G and Smith K 1962 *Rev. Mod. Phys.* **34** 458
- Burke P G and Taylor A J 1966 *Proc. Phys. Soc.* **88** 549
- Breit G 1946 *Phys. Rev.* **69** 472
- Faddeev L D 1961 *Sov. Phys.-JETP* **12** 1014
- Hahn Y 1968 *Phys. Rev.* **174** 1168
- 1970 *Phys. Rev. C* **1** 12
- 1972 *Phys. Rev. A* **5** 309
- 1974 *Phys. Rev. A* **9** 2014, 2024
- 1982 *Nucl. Phys. A* **389** 1
- 1985 *Adv. At. Mol. Phys.* **21** 123
- 1996 *J. Phys. B: At. Mol. Opt. Phys.* to be published
- Hahn Y and Watson K 1972 *Phys. Rev. A* **5** 1718
- Mott N F and Massey H S W 1965 *The Theory of Atomic Collisions* (Oxford: Clarendon)
- Newton R G 1958 *Ann. Phys.* **4** 29
- 1982 *Scattering Theory of Waves and Particles* (Berlin: Springer)
- Percival I C and Seaton M J 1957 *Proc. Camb. Phil. Soc.* **53** 655
- Rule W D and Hahn Y 1975 *Phys. Rev. Lett.* **34** 332
- 1976 *Phys. Rev. C* **14** 1102
- Weinberg S 1963 *Phys. Rev.* **131** 440
- 1964 *Phys. Rev. B* **133** 232