A Resolution of Some Orthogonality and Expansion-Set Problems
in Many-Body Scattering Theory

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Abstract

A modification to the coupled channel equations for many-body scattering is introduced, based on the evaluation of the discontinuity equation for the matrix of transition operators. The resulting (modified) equations are shown to be in a form which resolves some problems associated with continuum states in an analysis of rearrangement collisions using the eigenstate expansion method.

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A standard method for analyzing many-body scattering problems has been to expand the scattering state $|\Psi\rangle$ by means of a complete set of states, say $\{|\varphi_\alpha\rangle\}$, often chosen to be the states of the target. Examples of this occur for $e^- + H$ scattering [1], (d,p) reactions [2], and the optical model for elastic [3] and collective inelastic [4] scattering. Two of the interesting and heretofore only partially answered questions arising in this context concern the role played by the continuum states of $\{|\varphi_\alpha\rangle\}$. These may be stated as: (1) how do the continuum states enter the description of a rearrangement scattering process (or in two other, equivalent forms -- can one use bound states from several expansion sets corresponding to different arrangements of particles, or, how does one generally choose an optimal expansion basis); and, (2) how does the non-orthogonality of different expansion sets affect the analysis?

The former question, though difficult to answer by means of a numerical calculation because the continuum is involved, is nevertheless important. For instance, if we label the electrons in the $e^- + H$ case by 1 and 2, and let $\{|\varphi_\alpha(1)\rangle\}$ be the complete set of hydrogenic states of 1, then it is clearly of interest to know if exchange scattering (2 in, 1 out) is better described by the continuum states of $\{|\varphi_\alpha(1)\rangle\}$, the bound states of $\{|\varphi_\alpha(2)\rangle\}$, or if both sets are required. It is well known that a non-negligible fraction of the polarizability of the H-atom comes from the continuum [5], but how and in what form it enters the scattering problem is not well known. Or, in the case of (d,p) stripping, the states of the deuteron and the states of the captured nucleon both provide useful expansion sets. Members of one set are not orthogonal to those of the other. The former seems more useful for describing elastic deuteron scattering (and the deuteron optical potential),

while the latter set seems best suited to discuss spectroscopic factors (and elastic proton scattering). It is easy to see that continuum states of one of these two sets are needed to describe bound states of the other. No simple way of describing both (d,d) and (d,p) reactions, each of which influences the other, is known [6], nor is a description utilizing both sets of states, but overcoming the non-orthogonality problem [7], at hand.

A major step toward resolving some of these problems was provided several years ago by the work of Hahn [8]. His result is that, even though members of different expansion sets are not orthogonal, the projection of $|\Psi\rangle$ onto members of one expansion set is orthogonal to the further projection onto members of a different set. This result follows from the equations obeyed by the projected states and is thus an effective orthogonality, which, as shown by Hahn [8] also holds for approximate calculations.

In this note we show that a further step can be taken in the resolution of these problems. Our result is stated in the context of the coupled channel, integral equation formulation of the many-body scattering problem we have discussed recently [9]. It is a modification of these equations, based on unitarity considerations, which limits the expansion bases in each arrangement channel to only the internal bound states of the subsystems forming that channel (except for the channel corresponding to complete breakup where there is no such limitation). Thus, rearrangement scattering problems can be analyzed, using the formulation of ref. [9], by keeping only internal bound states in each channel, plus the complete set of breakup states. Because the coupled channel formulation is a matrix one, different arrangement channel quantities occur in different row and/or columns in the relevant matrices, and non-orthogonality problems are not encountered. Hence the two questions raised above are resolved.

To derive our result, we consider an n-body, N-channel scattering system, for which the Hamiltonian H may be split in N ways into a channel Hamiltonian H_j (describing internal states of, and plane wave relative motions between, the subsystems in the channel j) and a channel perturbation V_j :

$H = H_j + V_j$, $1 \leq j \leq N$. The n free-particle channel is denoted $j = 0$.

The operators of the coupled channel formulation whose matrix elements give the amplitudes for transitions between states $|\phi_E(k)\rangle$ in channel k with energy E and $\langle\phi_E(j)|$ in channel j are denoted $T_{jk}(z)$, where z is a complex energy parameter. Physical values occur at $z = E + i\epsilon$, $\epsilon \rightarrow 0^+$. In matrix form, the equation for $T(z)$ is [9]

$$T(z) = \mathcal{V} + \mathcal{V} \mathcal{G}(z) T(z), \quad (1)$$

where $\mathcal{V}_{ij} = V_i W_{ij}$ and $\mathcal{G}_{ij}(z) = \delta_{ij} G_j(z) \equiv \delta_{ij} (z - H_j)^{-1}$ is the matrix of channel resolvent operators. The quantity W is the channel coupling array whose elements W_{lk} determine which channels are explicitly coupled together; they are normalized by $\sum_i W_{il} = 1 = \sum_i W_{li}$. The index l is free; a discussion of how to choose the elements W_{lk} is given elsewhere [9] and is not germane to the present development.

The formal solution to (1) is

$$T(z) = \mathcal{V} + \mathcal{V} \mathcal{Y}(z) \mathcal{V}, \quad (2)$$

where

$$\mathcal{Y}(z) = [\mathcal{G}^{-1}(z) - \mathcal{V}]^{-1} \quad (3)$$

and obeys, e.g., $\mathcal{Y}(z) = \mathcal{G}(z)[1 + \mathcal{V} \mathcal{Y}(z)]$. Since $\mathcal{G}(z)$ is Hermitian analytic [10], i.e., $\mathcal{G}^*(z) = \mathcal{G}(z^*)$, then it follows from (3) and the reality of $\mathcal{V}$ that $\mathcal{Y}^*(z) = \mathcal{Y}(z^*)$, and then from (2) that $T^*(z) = T(z^*)$.

We now ask, assuming all possible arrangement channels are included in the set $\{j\}$, is the set of equations (1) - (3) correct; i.e., does this set lead to the proper unitarity relation? The answer is no, and we now outline the reasons for this.

We have recently shown [11] that the discontinuity relation that must be obeyed by $T(E + i0)$ is

$$\begin{aligned} DT(E + i0) &\equiv T(E + i0) - T(E - i0) = 2i \operatorname{Im} T(E + i0) \\ &= -2\pi i T(E + i0) \tilde{\Delta}(E) T(E - i0) \quad , \end{aligned} \quad (4)$$

where $\tilde{\Delta}(E)$ is a matrix of on-shell projection operators whose elements are given by

$$\tilde{\Delta}_{ij}(E) = \delta_{ij} \delta(E - H_j) P(j) \quad , \quad (5)$$

with $P(j)$ being the projection operator onto the internal bound states in channel j . This is the relation discussed by Weyers [11]; it reduces to Lovelace's expression [12] for the case $n = 3$.

To show that $T(E + i0)$ as given by (1) or (2) with $z = E + i\varepsilon$, $\varepsilon \rightarrow 0^+$, does not obey (4), we form $DT(z)$ using (2). It is easily seen that

$$\begin{aligned} DT(z) &= \mathcal{V} [D \mathcal{G}(z)] \mathcal{V} \\ &= T(z) [D \mathcal{G}(z)] T(z^*) \quad . \end{aligned} \quad (6)$$

Thus, in order to find $DT(E + i0)$, we must examine the difference $\mathcal{G}_{ij}(E + i\varepsilon) - \mathcal{G}_{ij}(E - i\varepsilon)$ across the right hand cuts, and then take limit $\varepsilon \rightarrow 0^+$.

If we simply assume that $D \mathcal{G}_{ij}(z) \equiv 2i \operatorname{Im} \mathcal{G}_{ij}(z) = 2i [\operatorname{Im} G_j(z)] \delta_{ij}$, then from (6), we find [11]

$$\operatorname{Im} T(E + i0) = -\pi T(E + i0) \Delta(E) T(E - i0) \quad , \quad (7)$$

where $\Delta_{ij}(E) = \delta_{ij} \delta(E - H_j)$. The difference between (4) and (7) is that all possible internal eigenstates of each H_j are included in (7) and especially the breakup states of the subsystems forming the channel, unlike (4), in which these breakup states are explicitly excluded.

This difference is significant. The right hand cuts in a non-relativistic n -body theory such as this one begin at the thresholds for the internal bound states in all possible channels. A cut that might arise from a 2-body breakup

state of a subsystem in an m -body channel will also appear as a cut (or a set of cuts) corresponding to internal bound states in an $(m+1)$ -body channel [11], and similarly for 3-body, 4-body, and up to $(n-1)$ -body breakup states. Since each cut contributes to the discontinuity only once, it is thus sufficient to count only the contributions arising from the internal bound states, as long as the free, n -particle channel ($j=0$) is included. This result is well known for the case $n=3$, as shown by Lovelace [12]: continuum (breakup) 2-body states (plus a free third particle) gave the same contribution to the discontinuity as do the 3-particle free states; only the latter contribution is to be included [11, 12].

The foregoing remarks clearly indicate that (7) violates unitarity, since in (7) there will be multiple counting of the contributions from many of the cuts. In order to obtain the correct unitarity (discontinuity) relation (4), the basic equation (1) must be modified. The modification is relatively simple to obtain. We must regard $G_{ij}(z)$ as an operator function of the complex variable z whose real and imaginary parts are to be determined by examining the behavior of $D G(z)$ across the right hand cuts. That is, we cannot assume that the element $G_{ij}(z)$ has an imaginary part given by $\delta_{ij} \text{Im } G_j(z)$ as would be the case if we were considering $G_j(z)$ in isolation, i.e., not as part of the set $\{G_j(z)\}$ which form $G(z)$. In other words, the analytic properties of $G_{ij}(z)$, and $G_j(z)$ when considered in isolation, are not the same.

Taking account of our earlier comments about the need to avoid multiple counting of the contributions from any cut, we find that

$$D G_{ij}(z) = 2i \text{Im } G_{ij}(z) = 2i \delta_{ij} [\text{Im } G_j(z)] P(j) \quad (8)$$

This is the only relation consistent with, and derivable from, the cut structure of $M(z)$.

Equation (8) gives the correct imaginary part of $G_{ij}(z)$. To find the correct real part, we use Cauchy's theorem for $G_{ij}(z)$, writing

$$G_{ij}(z) = \frac{1}{2\pi i} \int_C \frac{G_{ij}(\xi) d\xi}{\xi - z}, \quad (9)$$

where C is the contour of the figure. The only singularities of $G(z)$ are the cuts on the real axis: there are no bound state poles, since $H_j = H - V_j$ has no interactions that could bind the n -particle system. Standard methods [10] for evaluating the integral in (9) then lead to

$$\text{Re } G_{ij}(z) = \delta_{ij} [\text{Re } G_j(z)] P(j), \quad (10)$$

the analog of (8).

With (8) and (10), we now see that $G(z)$ is to be replaced by $\tilde{G}(z)$, where $\tilde{G}_{ij}(z) = G_{ij}(z)P(j)$. Hence the equations for $T(z)$ and $\mathcal{Y}(z)$ are to be replaced by

$$\begin{aligned} T(z) &= \mathcal{V} + \mathcal{V} \tilde{G}(z) T(z) \\ &= \mathcal{V} + \mathcal{V} \tilde{\mathcal{Y}}(z) \mathcal{V}, \end{aligned} \quad (11)$$

and

$$\tilde{\mathcal{Y}}(z) = [\tilde{G}^{-1}(z) - \mathcal{V}]^{-1}. \quad (12)$$

These modified equations guarantee that $T(z)$ obeys the correct unitarity relation (4).

Similar modifications also hold for the K -operator matrix equations of our previous work [9]. We now find

$$K(E) = \mathcal{V} + \mathcal{V} \text{Re } \tilde{G}(E + i0) K(E), \quad (13)$$

so that the damping equation [9] relating $T(E + i0)$ and $K(E)$ becomes

$$T(E + i0) = K(E) - i\pi K(E) \tilde{\Delta}(E) T(E + i0), \quad (14)$$

consistent with the unitarity relation (4).

These results establish our remarks above on the appearance of only bound states in the expansion sets occurring in the theory, due to the presence of

$P(j)$ in $\tilde{G}_{ij}(z)$. [For the n -body breakup channel, $j = 0$, $P(0) = 1$, and all relative motion states enter.] It should be evident that the presence of the $P(j)$ carries over to the differential equation formulation of the scattering problem as well. In this case the important quantity is the matrix of Møller wave operators Ω , which lead to the vector of scattering states $|\Psi_E\rangle$. In component form we have [9] $|\Psi_E(j)\rangle = \Omega_{jk} |\Phi_E(k)\rangle$ [note that the $|\Phi_E(k)\rangle$ will contain only bound internal states]. The matrix Ω is defined by $T = \mathcal{V} \Omega$, so that from (11) we find

$$\Omega = 1 + \tilde{G} \mathcal{V} \Omega \quad (15)$$

From (15) it is straightforward to establish the set of coupled differential equations

$$(E - H_j) |\Psi_E(j)\rangle = P(j) \mathcal{V}_j \sum_1 W_{1j} |\Psi_E(1)\rangle \quad (16)$$

with $\langle \Phi_E(j) | \Psi_E(j) \rangle = 0$ if $\langle \Phi_E(j) |$ contains unbound (breakup) internal states in channel j . Reference to the initial state $|\Phi_E(k)\rangle$ is suppressed in (16), though it does appear in the boundary condition equation:

$$|\Psi_E(j)\rangle = \delta_{jk} |\Phi_E(k)\rangle + \tilde{G}_j (E + i0) \sum_1 \mathcal{V}_1 W_{1j} |\Psi_E(1)\rangle \quad (17)$$

The set of coupled equations (16) [and (17)] are an interesting realization of the results implied by Nahn's effective orthogonality condition [8]. A simple example illustrating their content is provided by the (d,p) reaction on a structureless core. There are four arrangement channels: (d,d) , (d,p) , (d,n) , and (d,np) . According to (11) and/or (16), the following sets are to be used, respectively, for the preceding four channels: the deuteron ground state, the set of neutron-core bound states, the set of proton-core bound states, and the free neutron and proton states. Notice that, even though the free n and p states are a complete set, we must still include the bound states in the other three channels in order to satisfy the unitarity relations. If the n and p free states are ignored, then (17) reduces to three coupled equations

for the three scattering states $|\psi_{\mathbf{p}}(j)\rangle$ corresponding to elastic deuteron scattering, and (d,p) and (d,n) stripping into bound states. These results are reminiscent of the coupled channel (d,d) and (d,p) equations of Pawitscher [6], although the two sets of equations are neither very similar nor physically interchangeable. Notice that an entirely different structure results if the reaction is $\underline{p}$ incident on a bound $\underline{n}$. If exact calculations were done in the two cases, then the (p,d) and (d,p) amplitudes would necessarily be equal by time reversal invariance. A detailed discussion of this model (d,p) problem and choices for W will be given elsewhere.

We close with two comments: first, the modification $G \rightarrow \tilde{G}$ has enabled us to resolve the continuum state problems noted at the beginning of this article (and the matrix formulation bypasses the non-orthogonality problems); and second, we have seen how and why the structure of a resolvent operator when considered in isolation must be modified when it is considered as part of a larger operator, in this case $G(z)$, which is itself formed from the set of all resolvents, $\{G_j(z)\}$.

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Figure Caption

The contour C used in the Cauchy theorem evaluation of $g_{ij}(z)$.
The limits $R \rightarrow \infty$ and $n \rightarrow 0$ are to be taken in evaluating the integral of eq. (9);
the heavy lines represent the right hand cuts.