On Channel T and K Operators and the Heitler Damping
Equation for Identical Particle Scattering

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Abstract

Coupled integral equations linking the direct and exchange (rearrangement) K operators are proposed in analogy to similar ones linking the direct and exchange T operators derived in this paper. It is shown that these pairs of coupled equations lead to the damping equation which was used in previous work on identical particle scattering and which expresses the unitarity condition. Other formulations of integral equations for the K operator are also discussed.

1. Introduction

In earlier articles [1,2] we have considered several types of standing wave solutions to the Schrödinger equation describing potential well scattering and to the inhomogeneous differential equation for identical particle scattering.¹ In A it was shown that different standing wave solutions were obtained depending on how one introduced the reaction matrix. These solutions were shown to be associated with different principal value Green's functions and the precise formal relationship was derived. Then in B, analogous standing wave solutions were considered for the situation of identical particle scattering. A generalized formal relationship between Heitler reaction matrices was derived by use of a paradigm based on unitarity of the S matrix. The basic equation (B.24) for the paradigm was a symmetrized Heitler damping equation of the form

$$\mathcal{T} = \mathcal{K}^{-1} \mathcal{K} \delta(E - E_2) \mathcal{T} \quad (1)$$

where $\mathcal{T}$ is defined by

$$\mathcal{T} = T(d) \pm T(e) P_{12} \quad (2)$$

and $\mathcal{K}$ is analogously

$$\mathcal{K} = K(d) \pm K(e) P_{12} \quad (3)$$

with the + and - sign enabling treatment of Bosons and Fermions.

¹ We refer to references [1] and [2] as A and B, and their equations as (A.1), (B.1) etc.

These results hold for the simplest fermion or boson system capable of undergoing rearrangement, viz., two identical particles interacting with each other and with a center of force; the electron-hydrogen system is our prototype². In terms of the particle labels 1 and 2, $T(d)$ and $K(d)$ correspond to particle 2 incident on and emergent from a target containing particle 1 in a bound state, while $T(e)$ and $K(e)$ refer to the exchange process in which 2 is incident and 1 is emergent. P_{12} is the two-particle transposition operator and H_2 is the unperturbed Hamiltonian for 2 incident on a bound state of 1.

In B, no attempt was made to display the integral equations actually obeyed by $K(e)$ and χ . Our purpose in the present paper is two-fold. First, assuming distinguishable particles and using the coupled equations obeyed by $T(d)$ and $T(e)$ herein derived, we generalize the usual integral equation for $K(d)$ to a coupled set of integral equations for $K(d)$ and $K(e)$. This new matrix equation is then shown, in conjunction with the one for $T(d)$ and $T(e)$,

² The results we obtain for the two-particle case are generalizable to the N-body case, as long as only two-body final states are considered. This follows from the fact that in the latter case, as we have shown [3], the direct and exchange amplitudes differ essentially only by the labels of two-particles. Hence, the many-body amplitudes can be written as effective three-body amplitudes, with only two of the particle labels occurring. In forming properly symmetrized amplitudes for identical particles, however, there are normalization factors not occurring in the three-body case; these, of course, must be included.

to obey a damping equation in matrix form. Second, now assuming identical particles, these latter results are shown to lead to Eq. (1), thus providing a direct derivation of (1) based on specific equations for χ and $K(e)$. This complements our more general derivation of B , based on unitarity alone. We also discuss, in the last section of this paper, other forms for the direct and exchange T and K operators, using them to argue that the sets derived below, Eqs. (25) and (26) are the only ones, so far as we are aware, that lead to the damping equation, Eq. (1).

Let us elaborate these points further. We consider a system of non-identical particles in which only the elastic channel is open; i.e., the energy is below the threshold E_c for either inelastic scattering or rearrangement collisions. Then the S matrix is simply related to a real phase shift in each partial wave and therefore the operator $K(d)$ must exist. Naturally, a direct scattering transition operator $T(d)$ exists as well. For this domain of energy, $E < E_c$, the problem resembles that of potential well scattering in that only one channel is open. However, this resemblance is superficial because in the problem at hand inelastic and rearrangement channels can be reached virtually. Furthermore, as soon as $E \geq E_c$, one or both of these other kinds of channels become open and $K(d)$ alone cannot be used to specify even the elastic portion of S . Since $S(E < E_c)$ is related by analytic continuation to $S(E \geq E_c)$ this implies that rearrangement and inelastic channels will influence $K(d)$ no matter which domain of energy is being considered. Put another way, this means that for any composite system $K(e)$ will be reflected in $T(d)$ and vice-versa, and similarly for $K(d)$ and $T(e)$. It should be no surprise, therefore, that our results are expressed in terms of

equations coupling the direct and rearrangement (exchange) T and K operators.

An important reason for using coupled equations is that this permits problems associated with the continuum for particles initially in bound states to be circumvented. This is particularly useful in attempting calculations involving rearrangements. Consider elastic scattering of particle 2 from a bound state of 1. Writing $T(2)$ for $T(d)$, we have [2]

$$T(2) = V_2 + V_2 (E^+ - H)^{-1} V_2$$

or equivalently

$$T(2) = V_2 + V_2 (E^+ - H_2)^{-1} T(2),$$

where

$$V_2 = H - H_2.$$

The rearrangement channels (2 in, 1 out) are evidently in $(E^+ - H)^{-1}$, which is generally non-calculable, or in the continuum states of 1 present in $(E^+ - H_2)^{-1}$, and this portion of $(E^+ - H_2)^{-1}$ is equally difficult to calculate. However, by relating $T(d)$ and $T(e)$ via coupled equations in which both $(E^+ - H_2)^{-1}$ and $(E^+ - H_1)^{-1}$ appear, bound states of 2 (occurring in a rearrangement) can be automatically taken into account in $(E^+ - H_1)^{-1}$ in a simple way, thus finessing the problem of expressing them using the continuum portion of $(E^+ - H_2)^{-1}$. Similar remarks obviously hold for $K(d)$ and $K(e)$.

The case of identical particles (indistinguishability of 1 and 2) is even more to the point, for here, no matter what value of E is considered, rearrangement channels are always open. Hence, a coupled equation approach would seem beneficial ab initio. Indeed, using coupled equations of the kind we propose

herein, and retaining only the ground state of the H atom, reasonably accurate results for $e^- + H$ scattering, comparable to those obtained from much more complicated calculations, have been recently determined [4]. This, coupled with the direct derivation of Eq. (1), leads us to believe that our coupled equation formulation of the K operator problem is the most appropriate one available.

2. Coupled Channel Operator Equations

We now turn to a discussion of coupled integral equations for the direct and exchange T matrices, $T(d)$ and $T(e)$. As is well known, there are two distinct definitions of this latter operator [5,6] and they will, in general, not lead to the same equations for analogous channel K operators. In the present section, we shall use the equations

$$T_{kk} = V_k + V_k (E^+ - H)^{-1} V_k \quad (4)$$

and

$$T_{jk} = V_j + V_j (E^+ - H)^{-1} V_k, \quad (5)$$

where k

We shall discuss the alternative definition later in this paper. The full, interacting Green's operator $(E^+ - H)^{-1}$ may be written in terms of the noninteracting Green's operator $(E^+ - H_i)^{-1}$ by the usual equation³

$$(E^+ - H)^{-1} = (E^+ - H_i)^{-1} + (E^+ - H_i)^{-1} V_i (E^+ - H)^{-1}, \quad (6)$$

where i is 1 or 2 and $E^+ = E + i\epsilon, \epsilon \rightarrow 0^+$. We now introduce an arbitrary channel coupling matrix W_{ij} whose elements obey

$$\sum_j W_{ij} = 1; \quad (7)$$

³ We follow the notation of B, to which the reader is referred for details.

combining Eqs. (6) and (7) leads to

$$(E^+ - H)^{-1} = \Sigma W_{ij} (E^+ - H_j)^{-1} [I + V_j (E^+ - H)^{-1}]. \quad (8)$$

Using Eq. (8) in (4) and (5) leads to

$$T_{kk} = V_k \Sigma W_{k\ell} (E^+ - H_\ell)^{-1} [V_k + V_\ell (E^+ - H)^{-1} V_k], \quad (9)$$

and

$$T_{jk} = V_j + V_j \Sigma W_{j\ell} (E^+ - H_\ell)^{-1} [V_k + V_\ell (E^+ - H)^{-1} V_k]. \quad (10)$$

By the definitions of T_{kk} and T_{jk} , Eqs. (4) and (5), the above expressions lead to

$$T_{kk} + V_k + V_k W_{kk} (E^+ - H_k)^{-1} T_{kk} + V_k W_{kj} (E^+ - H_j)^{-1} (T_{jk} - V_j + V_k) \quad (11)$$

and

$$T_{jk} = V_j + V_j W_{jk} (E^+ - H_k)^{-1} T_{kk} + V_j W_{jj} (E^+ - H_j)^{-1} (T_{jk} - V_j + V_k), \quad (12)$$

which are coupled equations for T_{kk} and T_{jk} .

Let us focus on the quantity $(E^+ - H_j)^{-1} (V_k - V_j)$ appearing in the above two equations. By the identity

$$V_k - V_j = H - V_j - (H - V_k) \quad (13)$$

$$= H_j - H_k, \quad (14)$$

we have

$$(E^+ - H_j)^{-1} (V_k - V_j) = (E^+ - H_j)^{-1} (H_j - H_k). \quad (15)$$

We now assume that all matrix elements will be taken between initial and final two-body bound states; i.e., that no three-body final states occur.

With these restrictions, we may rewrite Eq. (15) as

$$(E^+ - H_j)^{-1} (V_k - V_j) = (E^+ - H_j)^{-1} (H_j - E + i\epsilon - i\epsilon) \quad (16)$$

or

$$(E^+ - H_j)^{-1} (V_k - V_j) = -I + (E^+ - H_j)^{-1} (i\epsilon) \quad (17)$$

when applied to initial states on the energy shell. In the limit $\epsilon \rightarrow 0^+$, we obtain [7,8]

$$(E^+ - H_j)^{-1} (V_k - V_j) = -I \quad (18)$$

again with the above restriction on the type of states to which the operator is to be applied.

Using this result, Eqs. (11) and (12) may be rewritten as

$$T_{kk} = V_k (1 - W_{kj}) + V_k W_{kk} (E^+ - H_k)^{-1} T_{kk} + V_k W_{kj} (E^+ - H_j) T_{jk} \quad (19)$$

and

$$T_{jk} = V_j (1 - W_{jj}) + V_j W_{jk} (E^+ - H_k)^{-1} T_{kk} + V_j W_{jj} (E^+ - H_j) T_{jk}. \quad (20)$$

Now for the present two-channel rearrangement problem, we note that Eq. (7) leads to

$$W_{kk} = 1 - W_{kj} \quad (21)$$

and

$$W_{jk} = 1 - W_{jj}, \quad (22)$$

so that Eqs. (19) and (20) become

$$T_{kk} = V_k W_{kk} + V_k W_{kk} (E^+ - H_k)^{-1} T_{kk} + V_k W_{kj} (E^+ - H_j) T_{jk}, \quad (23)$$

and

$$T_{jk} = V_j W_{jk} + V_j W_{jk} (E^+ - H_k)^{-1} T_{kk} + V_j W_{jj} (E^+ - H_j) T_{jk}. \quad (24)$$

These are the coupled equations for T_{kk} and T_{jk} , which for particle 2 incident on particle 1 in a bound state are the channel T operators T_{22} and T_{12} . Note that there is no coupling to either T_{11} or T_{21} , though these latter two operators are themselves coupled by equations obtained by interchanging k and j

in Eqs. (23) and (24). Either pair can be used to describe scattering of identical particles since the overall amplitude is independent of which particle labels are used.

Treating the pairs (T_{11}, T_{21}) and (T_{22}, T_{12}) as elements of a column vector, we may combine these two pairs of coupled equations into one matrix equation:

$$\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = \begin{pmatrix} V_{1W_{11}} & V_{1W_{12}} \\ V_{2W_{21}} & V_{2W_{22}} \end{pmatrix} + \begin{pmatrix} V_{1W_{11}} & V_{1W_{12}} \\ V_{2W_{21}} & V_{2W_{22}} \end{pmatrix} \begin{pmatrix} G_1^+ & 0 \\ 0 & G_2^+ \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}, \quad (25)$$

with $G_i^+ = (E^+ - H_i)^{-1}$.

This is our basic equation for the channel T operators. By analogy, we define the equations for the channel K operators as

$$\begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} = \begin{pmatrix} V_{1W_{11}} & V_{1W_{12}} \\ V_{2W_{21}} & V_{2W_{22}} \end{pmatrix} + \begin{pmatrix} V_{1W_{11}} & V_{1W_{12}} \\ V_{2W_{21}} & V_{2W_{22}} \end{pmatrix} \begin{pmatrix} G_1^P & 0 \\ 0 & G_2^P \end{pmatrix} \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix}, \quad (26)$$

where $G_i^P = \text{Re } G_i^+$ is the standing wave Green's function in channel i.

We now investigate whether the above definition of the 2x2 matrix $\underline{K}$ in equation (26) yields a Heitler damping equation relation with $\underline{T}$ given by Eq. (25).

To study this, we form the difference of Eqs. (25) and (26) to find

$$\begin{pmatrix} (T_{11} - K_{11}) & (T_{12} - K_{12}) \\ (T_{21} - K_{21}) & (T_{22} - K_{22}) \end{pmatrix} = \begin{pmatrix} V_{1W_{11}} & V_{1W_{12}} \\ V_{2W_{21}} & V_{2W_{22}} \end{pmatrix} \begin{pmatrix} G_1^P & 0 \\ 0 & G_2^P \end{pmatrix} \begin{pmatrix} (T_{11} - K_{11}) & (T_{12} - K_{12}) \\ (T_{21} - K_{21}) & (T_{22} - K_{22}) \end{pmatrix} \\ - i\pi \begin{pmatrix} V_{1W_{11}} & V_{1W_{12}} \\ V_{2W_{21}} & V_{2W_{22}} \end{pmatrix} \begin{pmatrix} \delta(E - H_1) & 0 \\ 0 & \delta(E - H_2) \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix}, \quad (27)$$

or in full matrix form

$$[\underline{I} - \underline{V} \underline{G}^P] (\underline{T} - \underline{K}) = -i\pi \underline{V} \underline{\delta} \underline{T}, \quad (28)$$

where comparison of the above two equations shows the obvious definitions of the elements of the matrices $\underline{T}$, $\underline{K}$, $\underline{G}^P$ and $\underline{\delta}$. Now by equation (26), we note that

$$\underline{K} = [\underline{I} - \underline{V}^P \underline{G}^P]^{-1} \underline{V}^P, \quad (29)$$

so we immediately find

$$\underline{T} = \underline{K} - i\pi \underline{K} \underline{\delta} \underline{T}. \quad (30)$$

This is, of course, the Heitler damping equation for the case of distinguishable particles. Because $\underline{K}$ satisfies it, we take (26) as the definition of the appropriate K operator matrix. We discuss it in more detail in section 4.

3. Heitler Damping Equation for Identical Particles

We now wish to specialize the results of the preceding section to the problem of scattering of identical particles. We take the point of view that we may take amplitudes for distinguishable particles and symmetrize them in order to obtain the amplitude for identical particle scattering. Thus, our physical amplitude is $\mathcal{T}$, which without loss of generality, we may take as given by

$$\mathcal{T} = T_{22} \pm T_{21} P_{12}. \quad (31)$$

Matrix elements are to be taken between initial and final states where 2 is free and 1 is bound, as in B, so that in the notation of B, $T(d) = T_{22}$ and $T(e) = T_{21}$.

Using Eq. (30) derived in the preceding section, we may write (31) explicitly in terms of the channel K and T operators as

$$\begin{aligned} \mathcal{T} = & K_{22} \pm K_{21} P_{12} - i\pi [K_{21} \delta(E - H_1) T_{12} + K_{22} \delta(E - H_2) T_{22}] \\ & \pm i\pi [K_{21} \delta(E - H_1) T_{11} P_{12} + K_{22} \delta(E - H_2) T_{21} P_{12}]. \end{aligned} \quad (32)$$

Then using the definition of χ from B,

$$\chi = K_{22} \pm K_{21} P_{12} . \quad (33)$$

we may rewrite Eq. (29) as

$$\begin{aligned} \mathcal{J} = & \chi - i\pi K_{22} \delta(E - H_2) \\ & - i\pi K_{21} \delta(E - H_1) T_{12} \bar{P}_{12} \mp i\pi K_{21} \delta(E - H_1) T_{11} P_{12} . \end{aligned} \quad (34)$$

In the notation of B, $K(d) = K_{22}$ and $K(e) = K_{21}$.

The last two terms in (34) are equal to

$$\begin{aligned} & -i\pi K_{21} \delta(E - H_1) T_{12} P_{12} P_{12} \bar{P}_{12} \mp i\pi K_{21} \delta(E - H_1) T_{11} P_{12} \\ & = -i\pi K_{21} P_{12} \delta(E - H_2) T_{21} P_{12} \bar{P}_{12} \mp i\pi K_{21} P_{12} \delta(E - H_2) T_{22} , \end{aligned} \quad (35)$$

by use of the properties $P_{ij}^2 = 1$, $T_{ij} = P_{ij} T_{ji} P_{ij}$, etc. This can be rearranged to yield the result

$$\begin{aligned} & -i\pi K_{21} \delta(E - H_1) T_{12} P_{12} P_{12} \bar{P}_{12} \mp i\pi K_{21} \delta(E - H_1) T_{11} P_{12} \\ & = \mp [i\pi K_{21} P_{12} \delta(E - H_2) (T_{22} \pm T_{21} P_{12})] , \end{aligned} \quad (36)$$

so Eq. (34) yields

$$\begin{aligned} \mathcal{J} = & \chi - i\pi K_{22} \delta(E - H_2) \mathcal{J} \\ & - i\pi (\pm K_{21} P_{12}) \delta(E - H_2) \mathcal{J} \end{aligned} \quad (37)$$

or

$$= \chi - i\pi \chi \delta(E - H_2) \mathcal{J} . \quad (38)$$

It is this result which constituted the basis of the analysis in B, and it here is shown to follow from a coupled equation definition of the channel K operators for the various rearrangements. It is important to note the restrictions applying in its derivation. First, it is assumed that initial and final physical

states are restricted to those not involving three free particles. In addition, matrix elements are to be taken only with initial and final states on the energy shell. Otherwise, the form of the equations for the T_{jk} elements need no longer be given by Eqs. (23) and (24) and a more careful analysis of Eq. (15) must be carried out, although we can define (38) as well as (23) and (24) as one of the infinitely many off-shell extensions of our on-shell results. For the case where three free particle channels are present, it is likely that more powerful methods must be employed (e.g., one probably must start with the Faddeev-type equations [5,7]). This is beyond the scope of the present study.

4. Comments on Other Definitions for $K(e)$.

We have seen that coupled equations for $K(e) = K_{21}$ and $K(d) = K_{22}$, Eq. (26), lead to the proper damping equation relating $\mathcal{J}$ and $\mathcal{X}$. For this reason, we regard Eq. (26) as an appropriate equation to use in defining $K(e)$. As mentioned in section 1, there are other ways by which equations for $K(e)$ can be introduced, and we now consider some of them.

We start with the alternate form⁴ for $T_{jk} = T(e)$:

$$\hat{T}_{jk} = V_k + V_j G^+ V_k, \quad (39)$$

where $G^+ = (E^+ - H)^{-1}$ is the full outgoing wave Green's function. This equation differs from (5) in that the first interaction on the right hand side is V_k , not V_j .

While use of the expansion (6) in (5) (plus Eq. (7)) leads to an integral

⁴In Lovelace's notation [5], T_{jk} corresponds to U_{jk}^+ and $\hat{T}_{jk}$ corresponds to U_{jk}^- .

equation for T_{jk} that involves the difference $v_k - v_j$, use of (6) and (7) in $\hat{T}_{jk}$ and T_{kk} leads instead to

$$T_{kk} = v_k + v_k w_{kk} G_k^+ T_{kk} + v_k w_{kj} G_j^+ \hat{T}_{jk} \quad (40)$$

and

$$\hat{T}_{jk} = v_k + v_j w_{jk} G^+ T_{kk} + v_j w_{jj} G_j^+ \hat{T}_{jk}. \quad (41)$$

These results are immediately generalized to

$$\begin{pmatrix} T_{11} & \hat{T}_{12} \\ \hat{T}_{21} & T_{22} \end{pmatrix} = \begin{pmatrix} v_1 & v_2 \\ v_1 & v_2 \end{pmatrix} + \begin{pmatrix} v_1 w_{11} & v_2 w_{12} \\ v_2 w_{21} & v_2 w_{22} \end{pmatrix} \begin{pmatrix} G_1^+ & 0 \\ 0 & G_2^+ \end{pmatrix} \begin{pmatrix} \hat{T}_{11} & \hat{T}_{12} \\ \hat{T}_{21} & T_{22} \end{pmatrix}. \quad (42)$$

The first alternate form for $\underline{K}$ we consider in this section is obtained by replacing G_1^+ by G_1^P :

$$\begin{pmatrix} K_{11} & \hat{K}_{12} \\ \hat{K}_{21} & K_{22} \end{pmatrix} = \begin{pmatrix} v_1 & v_2 \\ v_1 & v_2 \end{pmatrix} + \begin{pmatrix} v_1 w_{11} & v_1 w_{12} \\ v_2 w_{21} & v_2 w_{22} \end{pmatrix} \begin{pmatrix} G_1^P & 0 \\ 0 & G_2^P \end{pmatrix} \begin{pmatrix} K_{11} & \hat{K}_{12} \\ \hat{K}_{21} & K_{22} \end{pmatrix}. \quad (43)$$

Equation (43) defines an Hermitian set of K operators. However, the T 's and K 's of Eqs. (42) and (43) are not related via a damping equation. It is simpler to use a more compact notation, similar to that of Eq. (28) in deriving our results. We rewrite (42) and (43) as

$$\hat{\underline{T}} = \underline{v} + \underline{v} G^+ \hat{\underline{T}} \quad (44)$$

and

$$\hat{\underline{K}} = \underline{v} + \underline{v} G^P \hat{\underline{K}}. \quad (45)$$

$$= \underline{v} + \underline{v} G^+ \hat{\underline{K}} + 1\pi \underline{v} \delta \hat{\underline{K}}. \quad (46)$$

Subtracting (46) from (44) leads to

$$\hat{\underline{T}} - \hat{\underline{K}} = \underline{v} G^+ (\hat{\underline{T}} - \hat{\underline{K}}) - 1\pi \underline{v} \delta \hat{\underline{K}} \quad (47)$$

or,

$$\hat{T} - \hat{K} = -i\pi (\hat{G}^+)^{-1} [(\hat{G}^+)^{-1} - \hat{V}]^{-1} \hat{V} \hat{K} \quad (48)$$

If the product $(\hat{G}^+)^{-1} [(\hat{G}^+)^{-1} - \hat{V}]^{-1} \hat{V}$ were equal to $\hat{T}$, then Eq. (48) would be the damping equation relating $\hat{T}$ and $\hat{K}$. It is easily seen from (44) however, that the explicit solution for $\hat{T}$ is

$$\hat{T} = (\hat{G}^+)^{-1} [(\hat{G}^+)^{-1} - \hat{V}]^{-1} \hat{V}. \quad (49)$$

Hence, $\hat{T} - \hat{K} \neq -i\pi \hat{T} \hat{K}$, and we have our first example of a Hermitian set of K operators which do not lead to a damping equation. Hence, the set $\hat{K}$ is not appropriate. In further detail, we can easily see that

$$\begin{aligned} \hat{T} - \hat{K} = & -i\pi \hat{T} \hat{K} - i\pi (\hat{G}^+)^{-1} [(\hat{G}^+)^{-1} - \hat{V}]^{-1} \\ & \times \begin{pmatrix} v_2 & 0 \\ 0 & v_1 \end{pmatrix} \hat{W} \hat{K}; \end{aligned} \quad (50)$$

the second term on the right hand side does not vanish.

Now we know that T_{jk} and $\hat{T}_{jk}$ are both valid forms for the rearrangement transition operator, and that they agree on the energy shell. Since neither $\hat{K}$ nor $\hat{K}$ have explicit solutions open to easy interpretation, due to G_1^P not having a Lippmann-Schwinger iteration, we cannot determine if they agree, for example, on the energy shell. We are forced to conclude that $\hat{K}$ is not an appropriate K matrix operator to use with $\hat{T}$, and we have not as yet found any other K matrix operator to use with $\hat{T}$ in order to obtain an equation of the form (30).

Another approach to formulating an appropriate $K(e)$ is as follows.

Lippmann [8] has shown that the rearrangement state vector $|\psi_{k,R}^+\rangle$ obeys

$$|\psi_{\underline{k},R}^+ \rangle = |\phi_{\underline{k}}(2) \rangle + G_1^+ (V_2 - V_1) |\phi_{\underline{k}}(2) \rangle + G_1^+ V_1 |\psi_{\underline{k},R}^+ \rangle, \quad (51)$$

where $|\phi_{\underline{k}}(2) \rangle$ is a product of a bound state for particle 1 and a plane wave state of momentum $\underline{k}$ for particle 2. The notation is that of B. The rearrangement (exchange) T(e)-operator T_{12} is defined by

$$T_{12} |\phi_{\underline{k}}(2) \rangle = V_1 |\psi_{\underline{k},R}^+ \rangle; \quad (52)$$

multiplication of (51) by V_1 leads to the following integral equation for T_{12} :

$$T_{12} = V_1 + V_1 G_1^+ (V_2 - V_1) + V_1 G_1^+ T_{12}. \quad (53)$$

A formal solution to T_{12} is easily obtained as

$$T_{12} = V_1 + V_1 G^+ V_2, \quad (54)$$

which is identical to Eq. (5), and thus justifies using the notation T_{12} in (52).

Let us now define a rearrangement standing wave solution $|\psi_{\underline{k},R}^0 \rangle$ to the Schrödinger equation analogous to (51):

$$|\psi_{\underline{k},R}^0 \rangle = |\phi_{\underline{k}}(2) \rangle + G_1^0 (V_2 - V_1) |\phi_{\underline{k}}(2) \rangle + G_1^0 V_1 |\psi_{\underline{k},R}^0 \rangle \quad (55)$$

Just as only the last term on the right hand side of (51) contributes when $|\psi_{\underline{k},R}^+$ is projected onto a bound state of 2, so does only the last term on the right hand side of (55) contribute when $|\psi_{\underline{k},R}^0 \rangle$ is projected onto a bound state of 2. In this case, the dependence on the spatial coordinates of 1 in the l th partial wave is $n_l(r_1)$, where n_l is the l th spherical Neumann function [we are here ignoring spin-orbit and tensor forces], as expected for a standing wave.

If $|\psi_{k,R}^0\rangle$ is an appropriate standing wave solution, then the "natural" K(e) operator associated with it, K_{12}^R , defined by

$$K_{12}^R |\psi_k^0(2)\rangle = v_1 |\psi_{k,R}^0\rangle, \quad (56)$$

should be an appropriate K operator. Let us examine this. Multiplication of both sides of (55) by v_1 leads to

$$K_{12}^R = v_1 + v_1 G_1^P (v_2 - v_1) + v_1 G_1^P K_{12}^R. \quad (57)$$

Similarly, K_{21}^R and T_{21} obey

$$K_{21}^R = v_2 + v_2 G_2^P (v_1 - v_2) + v_2 G_2^P K_{21}^R, \quad (58)$$

and

$$T_{21} = v_2 + v_2 G_2^+ (v_1 - v_2) + v_2 G_2^+ T_{21}. \quad (59)$$

Neither the pair T_{12} and K_{12}^R nor the pair T_{21} and K_{21}^R are related by damping equations.

We prove this latter statement for the pair T_{21} and K_{21}^R . Subtraction leads to

$$[1 - G_2^+ v_2] (T_{21} - K_{21}^R) = -iv_2 \delta(E - H_2) [(v_2 - v_1) + K_{21}^R]. \quad (60)$$

Using $T_{22} = [1 - G_2^+ v_2]^{-1} v_2$ the uncoupled equation for T_{22} , (60) can be solved to give

$$T_{21} = K_{21}^R - iv_2 T_{22} \delta(E - H_2) [(v_2 - v_1) + K_{21}^R]. \quad (61)$$

Equation (61) fails to be a damping equation for two reasons, the more important being the appearance of T_{22} , rather than T_{21} on the right hand side. The other is the factor $(v_2 - v_1)$; this vanishes when E is below the three-

body breakup threshold E_3 , but even in such a case, $T_{22} \neq T_{21}$.

It is clear that $T(e)$ and $K(e)$ need not be related via a damping equation since unitarity does not apply to the pure rearrangement part of the amplitude. Nevertheless, $\underline{T}$ and $\underline{K}$ do obey a damping equation, and they ultimately lead to Eq. (1), while $\hat{T}$ and $\hat{K}$ do not. We can ask if (61), combined with the usual damping equation for T_{22} and K_{22} might lead to Eq. (1). The answer is no, since even if $E < E_3$, we get

$$\mathcal{T} = \chi^R - i\pi T_{22} \delta(E - H_2) \chi^R \quad (62)$$

where $\chi^R = K_{22} \pm K_{21}^R P_{12}$ and $\mathcal{T}$ is defined by Eq. (31). That is, instead of (1), we have an equation in which T_{22} rather than $\mathcal{T} = T_{22} \pm T_{21} P_{12}$ occurs on the right hand side. Thus, only Eq. (26) has so far lead to the damping equation (1) for the symmetrized operators.

Yet a different approach is possible. We could consider the case where $w_{jk} = 0$, $w_{jj} = 1$ in (7); then $\hat{T}_{jk}$ obeys

$$\hat{T}_{jk} = v_k + v_j G_j^+ \hat{T}_{jk} \quad (63)$$

Analogously, $\hat{K}_{jk}$ is defined as

$$\hat{K}_{jk} = v_k + v_j G_j^P \hat{K}_{jk} \quad (64)$$

A calculation similar to those of the preceding now gives [6]

$$\begin{aligned} \hat{T}_{jk} &= \hat{K}_{jk} - i\pi (1 - G_j^+ v_j)^{-1} v_j \delta(E - H_j) \hat{K}_{jk} \\ &= \hat{K}_{jk} - i\pi T_{jj} \delta(E - H_j) \hat{K}_{jk} \end{aligned} \quad (65)$$

a non-damping equation because of the T_{jj} . Using $\hat{J} = T_{jj} - \hat{T}_{jk} P_{jk}$ and $\hat{K} = K_{jj} - K_{jk} P_{kj}$, we again find a result like (62):

$$\hat{J} = \hat{K}^{-1} T_{jj} \delta(E - H_j) \hat{K}. \quad (66)$$

In this instance, also, we fail to produce Eq. (1), the sine qua non of our results. Furthermore, we are unable to show that Eqs. (38) and (65) are equivalent, so that (65) does not seem to be an equation to be used in the identical particle case.

Since none of the above methods lead to Eq. (1), we could try to work backwards from (1) to a relation between $T(e) = T_{21}$ and $K(e) = K_{21}$, and thence to an equation involving only reaction operators. It is no surprise, in light of the preceding results, that no result other than that embodied in Eq. (26) seems to occur. Using equations for the transition operators other than (25) leads to equations for the K's which are not Hermitian, or at least in which the non-Hermitian portions cannot, apparently, be eliminated. We regard these results as a strong, if not nearly conclusive, indication that Eq. (26) is the only appropriate equation to use as an integral equation for K operators involving rearrangement. Indeed, that $K(d)$ and $K(e)$ must be coupled follows from Eq. (1) and the damping equations relating $T(d)$ and $K(d)$.

A further point is that when approximations are made, the choice of which integral equation for K is to be approximated can be very important. The equality of Born approximation matrix elements of the potential does not mean that any higher order approximations, in, say, Eqs. (64) and (26) will be the

same. Results based on use of an equation like (64) may be of doubtful validity. Computations based on Eqs. (26) and (38) are being carried out and will be reported elsewhere.

5. Summary

The results of this work are new coupled integral equations for channel T and K operators for collisions in which rearrangements are possible. These have been shown to lead to a Heitler damping equation relating these operators and for the special case of identical particles, to the symmetrized form of damping equation obtained earlier by general arguments. Further, it is shown that other common definitions of K operators do not lead to the expected damping equations. This has implications regarding which form of definition of K operators should be used in approximate calculations. Other aspects of this approach to rearrangement scattering will be reported in a subsequent paper.

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References

1. D.J. Kouri and F.S. Levin, On Standing Wave Solutions to the Schrodinger Equation, to be published in Annals of Physics
2. D.J. Kouri and F.S. Levin, On Standing Wave Solutions to the Inhomogeneous Equation for Identical Particle Scattering, to be published in Annals of Physics
3. F.S. Levin, Nuclear Phys. 46 (1963), 275
4. M. Craigie, D. Secrest and D.J. Kouri, to be published
5. C. Lovelace, Phys. Rev. 135 (1964), B1225; K.M. Watson and J. Nuttall, Topics in Several Particle Dynamics, Holden-Day, San Francisco, 1967
6. W. Tobocman and M.A. Nagarajan, Phys. Rev. 163 (1967), 1011 [see Phys. Rev 179 (1969), 1230 and 187 (1969), 1744 for an addendum and an erratum, respectively]
7. L. Faddeev, Soviet Physics - JETP 12 (1961), 1014
8. B.A. Lippmann, Phys. Rev. 102 (1956), 204