Channel T and K operators and the Heitler damping equation for identical-particle scattering

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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.

I. 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. In Ref. 1 (hereafter referred to as 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 Ref. 2 (referred to as B), analogous standing-wave solutions were considered for the situation of identicalparticle scattering. A generalized formal relationship between Heitler reaction matrices was derived by use of a paradigm based on unitarity of the Smatrix. The basic equation (B.24) for the paradigm was a symmetrized Heitler damping equation of the form

$$\mathcal{T} = \mathcal{K} - i\pi \mathcal{K}\delta(E - H_2)\mathcal{T}, \qquad (1)$$

where $\boldsymbol{\mathcal{T}}$ is defined by

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

and \boldsymbol{x} is analogously

$$\mathbf{K} = K(d) \pm K(e) P_{12} , \qquad (3)$$

with the (+) and (-) signs enabling treatment of bosons and fermions, respectively.

These results hold for the simplest fermion or boson systems capable of undergoing rearrangement, viz., two identical particles interacting with each other and with a center of force; the electronhydrogen system is our prototype.³ 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 **x**. Our purpose in the present paper is twofold. First, assuming distinguishable particles and using 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), 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 \mathbf{x} and K(e). This complements our more general derivation of B, based on unitarity alone. We also discuss, in Sec. IV of this paper, other forms for the direct and exchange T and Koperators, 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 (1).

Let us elaborate these points further. We consider a system of nonidentical particles in which only the elastic channel is open; i.e., the energy is below the threshold E_i 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, $E < E_i$, 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 rear-

rangement channels can be reached virtually. Furthermore, as soon $E \ge E_t$, 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 $S(E < E_t)$ is related by analytic continuation to $S(E \ge E_t)$, 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 have²

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

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 noncalculable, 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.⁶ 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. Further discussion of the general case has been given elsewhere.⁷

II. 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^{8,9} 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,

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

and

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

where $k \neq j$.

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 equation (see B for references and notation)

$$(E^{+}-H)^{-1} = (E^{+}-H_{i})^{-1} + (E^{+}-H_{i})^{-1}V_{i}(E^{+}-H)^{-1},$$
(6)

where *i* is 1 or 2 and $E^+ = E + i\epsilon$, $\epsilon \to 0^+$. We now introduce an arbitrary 2×2 channel coupling matrix W whose elements obey

$$\sum_{j} W_{ij} = 1 ; \qquad (7)$$

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

$$(E^{+}-H)^{-1} = \sum_{j} W_{ij}(E^{+}-H_{j})^{-1}[I+V_{j}(E^{+}-H)^{-1}].$$
(8)

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

$$T_{kk} = V_k + V_k \sum_{l} W_{kl} (E^+ - H_l)^{-1} [V_k + V_l (E^+ - H)^{-1} V_k]$$
(9)

and

$$T_{jk} = V_j + V_j \sum_{l} W_{jl} (E - H_l)^{-1} [V_k + V_l (E^* - H)^{-1} V_k]$$
(10)

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

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

and

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

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

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

$$=H_{i}-H_{b}, \qquad (14)$$

we have

$$(E^{+}-H_{j})^{-1}(V_{k}-V_{j}) = (E^{+}-H_{j})^{-1}(H_{j}-H_{k}).$$
(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

$$(E^{+}-H_{j})^{-1}(V_{k}-V_{j}) = (E^{+}-H_{j})^{-1}(H_{j}-E+i\epsilon-i\epsilon)$$
(16)

or

$$(E^{+}-H_{j})^{-1}(V_{k}-V_{j}) = -I + (E^{+}-H_{j})^{-1}(i\epsilon), \qquad (17)$$

when applied to initial states on the energy shell. In the limit $\epsilon \to 0^+$, we obtain^{7, 10, 11}

$$(E^{+} - H_{j})^{-1}(V_{k} - V_{j}) = -1.$$
(18)

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

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

and

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

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

$$W_{kk} = 1 - W_{kj} \tag{21}$$

and

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

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

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

and

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

$$\begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} = \begin{pmatrix} V_1 W_{11} & V_1 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix} + \begin{pmatrix} V_1 W_{11} & V_1 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix} \begin{pmatrix} G_1^+ & 0 \\ 0 & G_2^+ \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix},$$
(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

$$\begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} = \begin{pmatrix} V_1 W_{11} & V_1 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix} + \begin{pmatrix} V_1 W_{11} & V_1 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix} \begin{pmatrix} G_1^{\mu} & 0 \\ 0 & G_2^{\mu} \end{pmatrix} \begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix},$$
(26)

where $G_i^p = \operatorname{Re} G_i^+$ is the standing-wave Green's function in channel *i*.

We now investigate whether the above definition of the 2×2 matrix <u>K</u> in Eq. (26) yields a Heitler damping equation relation with <u>T</u> given by Eq. (25). To study this, we form the difference of Eqs. (25) and (26) to find

$$\begin{pmatrix} (T_{11} - K_{11}) & (T_{12} - K_{12}) \\ (T_{21} - K_{21}) & (T_{22} - K_{22}) \end{pmatrix} = \begin{pmatrix} V_1 W_{11} & V_1 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix} \begin{pmatrix} G_1^{\rho} & 0 \\ 0 & G_2^{\rho} \end{pmatrix} \begin{pmatrix} (T_{11} - K_{11}) & (T_{12} - K_{12}) \\ (T_{21} - K_{21}) & (T_{12} - K_{22}) \end{pmatrix} \\ - i\pi \begin{pmatrix} V_1 W_{11} & V_1 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix} \begin{pmatrix} \delta(E - H_1) & 0 \\ 0 & \delta(E - H_2) \end{pmatrix} \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix},$$
(27)

or in full matrix form

$$[\underline{\mathbf{I}} - \underline{\mathbf{v}}\underline{\mathbf{G}}^{p}](\underline{\mathbf{T}} - \underline{\mathbf{K}}) = -i\pi\underline{\mathbf{v}}\underline{\delta}\underline{\mathbf{T}}, \qquad (28)$$

trices <u>T</u>, <u>K</u>, <u>G</u>^{δ}, and <u> δ </u>. Now by Eq. (26), we note that

$$\underline{\mathbf{K}} = [\underline{\mathbf{I}} - \underline{\boldsymbol{\upsilon}} \underline{\mathbf{G}}^{\boldsymbol{\rho}}]^{-1} \underline{\boldsymbol{\upsilon}} , \qquad (29)$$

where comparison of the above two equations shows the obvious definitions of the elements of the ma-

so we immediately find

(30)

This is, of course, the Heitler damping equation for the case of distinguishable particles. Because <u>K</u> satisfies it, we take (26) as the definition of the appropriate K operator matrix. We discuss it in more detail in Sec. IV.

III. HEITLER DAMPING EQUATION FOR IDENTICAL PARTICLES

We now wish to specialize the results of Sec. II 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 identicalparticle scattering. Thus, our physical amplitude is \mathcal{T} , which without loss of generality, we may take as given by

$$\mathbf{T} = T_{22} \pm T_{21} P_{12} \,. \tag{31}$$

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 Sec. II, we may write (31) explicitly in terms of the channel K and T operators as

$$\mathcal{T} = K_{22} \pm K_{21} P_{12} - i\pi [K_{21}\delta(E - H_1)T_{12} + K_{22}\delta(E - H_2)T_{22}]$$

$$\mp i\pi [K_{21}\delta(E - H_1)T_{11}P_{12} + K_{22}\delta(E - H_2)T_{21}P_{12}].$$

(32)

Then using the definition of \boldsymbol{x} from B,

$$\mathbf{x} = K_{22} \pm K_{21} P_{12} , \qquad (33)$$

we may rewrite Eq. (29) as

$$\mathbf{I} = \mathbf{\mathcal{K}} - i \, \pi K_{22} \, \delta(E - H_2) \, \mathbf{\mathcal{I}} - i \, \pi K_{21} \, \delta(E - H_1) T_{12}$$

$$\mp i \, \pi K_{21} \, \delta(E - H_1) T_{11} P_{12} \, . \tag{34}$$

In the notation of B, $K(d) = K_{22}$ and $K(e) = K_{21}$. The last two terms in (34) are equal to

$$-i\pi K_{21}\delta(E-H_1)T_{12}P_{12}P_{12}\mp i\pi K_{21}\delta(E-H_1)T_{11}P_{12}$$

= $-i\pi K_{21}P_{12}\delta(E-H_2)T_{21}P_{12}\mp i\pi K_{21}P_{12}\delta(E-H_2)T_{22}$,
(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

$$-i\pi K_{21}\delta(E-H_1)T_{12}P_{12}P_{12} \mp i\pi K_{21}\delta(E-H_1)T_{11}P_{12}$$

= \pi [i\pi K_{21}P_{12}\delta(E-H_2)(T_{22} \pm T_{21}P_{12})], (36)

so Eq. (34) yields

$$\mathbf{T} = \mathbf{\mathcal{K}} - i \, \pi K_{22} \, \delta(E - H_2) \, \mathbf{T} - i \, \pi(\pm K_{21} P_{12}) \, \delta(E - H_2) \, \mathbf{T}$$
(37)

$$\mathbf{T} = \mathbf{\mathcal{K}} - i\,\pi\mathbf{\mathcal{K}}\delta(E - H_2)\,\mathbf{\mathcal{T}}\,.\tag{38}$$

It is this result which constituted the basis of the analysis in B, and it is here 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. This has been done for the general *n*-body *N*-channel case.⁷

IV. 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{T} and \mathcal{K} . For this reason, we regard Eq. (26) as an appropriate equation to use in defining K(e). As mentioned in Sec. I, 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 form for $T_{jk} = T(e)$:

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

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 . We note that if one combines Eq. (39) above with the full Green's function expressed in terms of the $(E^{+}-H_i)^{-1}$ via

$$(E^{+}-H)^{-1} = \sum_{l} \left[I + (E^{+}-H)^{-1} V_{l} \right] (E^{+}-H_{l})^{-1} W_{li},$$

then we obtain the transpose of Eq. (25) [assuming that the <u>W</u> array used is the transpose of that in Eq. (25)]. This is reasonable since T_{jk} and \hat{T}_{jk} are well known to be time-reversal partners. However, if we instead combine (8) with \hat{T}_{jk} , we then obtain [in place of Eq. (25)] the expressions

$$T_{kk} = V_k + V_k W_{kk} G_k^+ T_{kk} + V_k W_{kj} G_j^+ \hat{T}_{jk}$$
(40)

and

$$\hat{T}_{jk} = V_k + V_j W_{jk} G_k^+ T_{kk} + V_j W_{jj} G_j^+ \hat{T}_{jk} .$$
(41)

These results are immediately generalized to

$$\begin{pmatrix} T_{11} & \hat{T}_{12} \\ \hat{T}_{21} & T_{22} \end{pmatrix} = \begin{pmatrix} V_1 & V_2 \\ V_1 & V_2 \end{pmatrix} + \begin{pmatrix} V_1 W_{11} & V_2 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix} \times \begin{pmatrix} G_1^+ & 0 \\ 0 & G_2^+ \end{pmatrix} \begin{pmatrix} T_{11} & \hat{T}_{12} \\ \hat{T}_{21} & T_{22} \end{pmatrix}.$$
 (42)

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

$$\begin{pmatrix} K_{11} & \hat{K}_{12} \\ \hat{K}_{21} & K_{22} \end{pmatrix} = \begin{pmatrix} V_1 & V_2 \\ V_1 & V_2 \end{pmatrix} + \begin{pmatrix} V_1 W_{11} & V_1 W_{12} \\ V_2 W_{21} & V_2 W_{22} \end{pmatrix}$$
$$\times \begin{pmatrix} G_1^{\rho} & 0 \\ 0 & G_2^{\rho} \end{pmatrix} \begin{pmatrix} K_{11} & \hat{K}_{12} \\ \hat{K}_{11} & K_{22} \end{pmatrix}.$$
(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 convenient to use a more compact notation, similar to that of Eq. (28) in deriving our results. We rewrite (42) and (43) as

$$\hat{\mathbf{T}} = \mathbf{V} + \mathbf{U} \mathbf{G}^{\dagger} \, \hat{\mathbf{T}} \,, \tag{44}$$

and

$$\underline{\hat{K}} = \underline{V} + \underline{\tilde{U}}\underline{G}^{\rho}\underline{\hat{K}}$$
(45)

$$= \underline{\mathbf{V}} + \underline{\mathbf{v}}\underline{\mathbf{G}}^{+}\underline{\hat{\mathbf{K}}} + i\pi\underline{\mathbf{v}}\underline{\delta}\underline{\hat{\mathbf{K}}} .$$
(46)

Subtracting (46) from (44) leads to

$$\underline{\hat{\mathbf{T}}} - \underline{\hat{\mathbf{K}}} = \underline{\boldsymbol{\upsilon}} \underline{\mathbf{G}}^{*} (\underline{\hat{\mathbf{T}}} - \underline{\hat{\mathbf{K}}}) - i\pi \underline{\boldsymbol{\upsilon}} \underline{\delta} \underline{\hat{\mathbf{K}}}$$
(47)

or

$$\underline{\hat{\mathbf{T}}} - \underline{\hat{\mathbf{K}}} = -i\pi(\underline{\mathbf{G}}^+)^{-1}[(\underline{\mathbf{G}}^+)^{-1} - \underline{\underline{\mathbf{\upsilon}}}]^{-1}\underline{\underline{\mathbf{\upsilon}}}\underline{\delta}\underline{\mathbf{K}}.$$
(48)

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

$$\underline{\widehat{\mathbf{T}}} = (\underline{\mathbf{G}}^+)^{-1} [(\underline{\mathbf{G}}^+)^{-1} - \underline{\underline{\mathbf{v}}}]^{-1} \underline{\mathbf{V}}.$$
(49)

Hence, $\underline{\hat{T}} - \underline{\hat{K}} \neq -i\pi\underline{\hat{T}}\underline{\hat{O}}\underline{\hat{K}}$, 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

$$\frac{\hat{\mathbf{T}}}{\mathbf{T}} - \frac{\hat{\mathbf{K}}}{\mathbf{E}} = -i\pi \frac{\hat{\mathbf{T}}}{\mathbf{D}} \frac{\hat{\mathbf{K}}}{\mathbf{E}} - i\pi (\underline{\mathbf{G}}^{+})^{-1} [(\underline{\mathbf{G}}^{+})^{-1} - \underline{\underline{v}}]^{-1} \\ \times \begin{pmatrix} V_{2} & 0 \\ 0 & V_{1} \end{pmatrix} \underline{\mathbf{W}} \underline{\delta} \frac{\hat{\mathbf{K}}}{\mathbf{E}};$$
(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 <u>K</u> nor <u>K</u> has explicit solutions open to easy interpretation, due to G_i^p not having a Lippmann-Schwinger iteration,¹ we cannot determine if they agree, for example, on the energy shell. We are thus forced to conclude that <u>K</u> is not an appropriate K matrix operator to use with <u>T</u> of Eq. (41); we have not as yet found any other K matrix operator to use with this particular form of <u>T</u> in order to obtain an equation of the form (30) [however, see our comments below Eq. (66)].

Another approach to formulating an appropriate K(e) is as follows. Lippmann¹¹ has shown that the rearrangement state vector $|\psi_{\vec{k},\vec{k}}^{+}\rangle$ obeys

$$\left|\psi_{\vec{k},R}^{+}\right\rangle = \left|\Phi_{\vec{k}}(2)\right\rangle + G_{1}^{+}(V_{2} - V_{1})\left|\Phi_{\vec{k}}(2)\right\rangle + G_{1}^{+}V_{1}\left|\psi_{\vec{k},R}^{+}\right\rangle$$
(51)

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

$$T_{12} \left| \Phi_{\vec{k}}(2) \right\rangle = V_1 \left| \psi_{\vec{k},R}^{\dagger} \right\rangle; \tag{52}$$

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

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

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

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

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

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

$$\left|\psi_{\vec{k},R}^{2}\right\rangle = \left|\Phi_{\vec{k}}(2)\right\rangle + G_{1}^{b}(V_{2} - V_{1})\left|\Phi_{\vec{k}}(2)\right\rangle + G_{1}^{b}V_{1}\left|\psi_{\vec{k},R}^{0}\right\rangle.$$
(55)

Just as only the last term on the right-hand side of (51) contributes when $|\psi_{k,R}^{\pm}\rangle$ is projected onto a bound state of 2, so does only the last term on the right-hand side of (55) contribute when $|\psi_{k,R}^{0}\rangle$ 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 spinorbit and tensor forces), as expected for a standing wave.

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

$$K_{12}^{R} \left| \Phi_{k}^{+}(2) \right\rangle = V_{1} \left| \psi_{k}^{0} \right\rangle, \qquad (56)$$

should be an appropriate K operator. Let us examine this. Multiplication of both sides of (55) by V_1 leads to

$$K_{12}^{R} = V_{1} + V_{1}G_{1}^{p}(V_{2} - V_{1}) + V_{1}G_{1}^{p}K_{12}^{R}.$$
 (57)

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

$$K_{21}^{R} = V_{2} + V_{2}G_{2}^{\flat}(V_{1} - V_{2}) + V_{2}G_{2}^{\flat}K_{21}^{R}$$
(58)

and

$$T_{21} = V_2 + V_2 G_2^+ (V_1 - V_2) + V_2 G_2^+ T_{21}.$$
 (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

$$[1 - G_2^+ V_2](T_{21} - K_{21}^R) = -i\pi V_2 \delta(E - H_2)[(V_2 - V_1) + K_{21}^R].$$
(60)

Using $T_{22} = [1 - G_2^+ V_2]^{-1} V_2$, the uncoupled equation for T_{22} , (60) can be solved to give

$$T_{21} = K_{21}^R - i\pi T_{22}\delta(E - H_2) [(V_2 - V_1) + K_{21}^R].$$
(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 $\underline{\hat{T}}$ and $\underline{\hat{K}}$ 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

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

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

$$\hat{T}_{jk} = V_k + V_j G_j^+ \hat{T}_{jk} \,. \tag{63}$$

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

$$\hat{K}_{jk} = V_k + V_j G_j^p \hat{K}_{jk} . \tag{64}$$

A calculation similar to those of the preceding now gives⁹

$$\hat{T}_{jk} = \hat{K}_{jk} - i\pi (1 - G_j^* V_j)^{-1} V_j \delta(E - H_j) \hat{K}_{jk}$$

= $\hat{K}_{jk} - i\pi T_{jj} \delta(E - H_j) \hat{K}_{jk} ,$ (65)

a nondamping equation because of the T_{ij} . Using

 $\hat{\mathbf{T}} = T_{jj} - \hat{T}_{jk}P_{jk}$ and $\hat{\mathbf{K}} = K_{jj} - K_{jk}P_{kj}$, we again find a result like (62):

$$\widehat{\mathbf{f}} = \widehat{\mathbf{k}} - i\pi T_{jj}\delta(E - H_j)\widehat{\mathbf{k}}.$$
(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.

One possible conclusion to be drawn from these results is that (25) is the only equation from which a simple damping relation can be derived. As we have shown elsewhere, however, there is another procedure which can be followed.⁷ This involves \hat{T}_{jk} , W_{ij} , and the *left-hand* version of Eq. (6), viz.,

$$(E^{+}-H)^{-1} = (E-H_{i})^{-1} + (E^{+}-H)^{-1}V_{i}(E^{+}-H_{i})^{-1}.$$
(67)

By following through the analysis given in Sec. II, we find equations involving the transpose of the operators $V_j W_{jk}$; i.e., $W_{jk} V_k$. Equations for K operators are then easily found which yield a damping equation exactly like Eq. (30). The extension to the identical-particle case follows in the same manner as in Sec. III. These results have been discussed elsewhere⁷ for the general n-body case, and we do not detail them here. It is important, however, to stress one point, common to both the equations for \hat{T}_{jk} referred to above and Eq. (25), but not associated with any of the equations of this section that failed to yield a damping equation. This is the presence of the matrix v in both the Born term and the kernel of Eq. (25). Apart from the equation for \hat{T}_{jk} noted just above, no formulation of coupled equations for rearrangement T operators other than (25) (or the extensions to the N-channel case⁷) with which we are familiar have this property: that the kernel of the equation has the Born term as a factor. It is this property that ultimately gives rise to the damping equation, and is, therefore, the main reason we have for proposing our method as a satisfactory means for treating rearrangement scattering problems.

V. 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 many 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 and extensions of this approach are discussed elsewhere,⁷ where, in particular, we examine in some detail the role played by the parameters W_{ij} , whose choice is dictated by the requirement that the resulting integral equations have a connected, iterated kernel.^{7, 12} Such a discussion is beyond the scope of the present article, whose purpose is to establish that (1) follows from (new) equations for T and K, and also to show that some of the plausible equations for K(e) that one might think of using to derive (1) are not, in fact, suitable.

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calculation for the n-body case has been discussed elsewhere (see Ref. 5).

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