K operators and unitary approximations for the three-body problem

D. J. Kouri*
Departments of Chemistry and Physics, University of Houston, Houston, Texas 77004

F. S. Levin†
Physics Department, University of Surrey, Guildford, Surrey GU2 5XH, England

W. Sandhas
Physikalisches Institut, Universitat Bonn, Bonn, Germany

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The method of channel coupling arrays is used as a means to introduce unitary approximations for the three-body problem. First, the transition operators defined by the channel coupling array equations are shown to obey the correct (on-shell) discontinuity equations. Next, K (reaction) operators are defined by using principal value Green's functions in the channel coupling array equations. These operators are then shown to be related to the transition operators by a damping equation which leads to the correct discontinuity relation. This development provides the basis for introducing unitary approximations, since any set of K operators having zero discontinuity will yield, through the damping equation, a set of transition operators having the proper singularity structure. The use of the channel coupling array method achieves this result without the need for introducing an intermediate hierarchy of operators, as in other approaches.

[NUCLEAR REACTIONS Channel coupling array theory, K operators, unitary approximations, three-body problem.]

I. INTRODUCTION

The derivation of K (reaction) operators for the nonrelativistic three-body problem ($n=3$ case) has been a topic of recent theoretical investigations, both as an intrinsically interesting problem in its own right and also as a source for introducing unitary approximations.[1-4] As in the two-body problem ($n=2$ case), the goal has been to derive a set of nonsingular equations defining the K operators and then show that these operators are related to the transition (T) operators by a (matrix) form of damping equation.[5] This latter equation, by construction, contains the effects of the singularity structure of the three-body problem, i.e., the various two-body and three-body thresholds and their associated cuts in the complex energy plane. Since the defining equations lead to K operators with zero discontinuity across these latter cuts, the damping equation is easily shown to lead to the usual three-body discontinuity (unitarity) relation[6] for the transition operators. Furthermore, use in the damping equation of any approximate set of K operators having zero discontinuity across the cuts will also lead to the discontinuity relation, so that it is trivial to introduce unitary approximations.

Unlike the $n=2$ case there is no unique way to introduce K operators when $n=3$ (or $n>3$). That is, while the K operators are uniquely linked to the T operator, there are, as noted for example by Amado,[7] an infinite number of ways of defining T operators, and hence an infinite number of ways of defining K operators, all equally valid. The derivations noted above are a few realizations of the possibilities for obtaining unitary approximations. Our purpose in this paper is to introduce an alternate approach to the derivation of K operators, one which we believe has the advantages of both generality and ease of applicability. The approach used here is based on a previous application to the three-body problem[8] of the channel coupling array method for many-body scattering.[9] The use of this method to introduce K operators was noted sometime ago[10]; general discussions for, as well as specific application to, two-channel systems have already been published.[11]

Since this present work deals with unitarity approximations, we remark here on two different problems that have arisen in this connection in the past. One of them is the occurrence of nonunitary approximate amplitudes resulting from certain ways of formulating the channel coupling array equations. The results of Baer and Kouri, noted in Ref. 11, are an example of this. A detailed explanation of these results, based on K operators and the damping equation, is given by Kouri, Levin, Craigie, and Secrest.[11] It is important to note, however, that nonunitary results are to be expected only in *approximate* calculations: exact solutions of the Baer-Kouri equations, like those of Kouri-Levin, will be unitary. We also note that an advantage of the Kouri-Levin formulation used

herein is that it yields approximate amplitudes which will be unitary, as discussed theoretically by Kouri, Levin, Craigie, and Secrest[11] and demonstrated explicitly for the e^-+H scattering system by Kouri, Craigie, and Secrest, and Kouri, Levin, Craigie, and Secrest.[9] The other problem remarked on above concerns the failure of the $G_l \to \tilde{G}_l$ transformation, which was pointed out by Benoist-Gueutal.[12] As this is not connected with the preceding discussion, we postpone comments on it until Sec. III A below.

In the papers of Ref. 11 restriction to the two-channel case was imposed by considering either an idealized system or a specific three-body system in which not all arrangement channels[13] were taken into account. The present paper considers the general $n=3$ case, for which the maximum number N of channels is $N=4$. That is, we assume that the system is composed of three distinguishable particles labeled 1, 2, and 3, which may form two-body bound states in three ways and which may also exist in the usual three-body breakup (unbound) mode.

Our goals are first, to derive the discontinuity relations for the transition operators of the channel coupling theory and second to introduce K operators and show how they can be used for formulating unitary approximations via a matrix damping relation. Since derivations of the basic equations have been given elsewhere,[8,9] we only summarize their general form here. This is done in the next section, where we review the notation and discuss other definitions of the transition operators. The main results are derived in Sec. III, where the relevant discontinuity, K operator, and damping equations are presented. A brief discussion of approximations is also included. In general, the channel coupling array approach gives rise to an infinite number of sets of coupled equations describing the three-body (or the N-body) problem. We have found four sets (i.e., four classes of the channel coupling array W) for which the iterated kernels of the coupled equations are connected. These are given in detail in the Appendix, and a number of connections with other operators, etc., are also stated there rather than in the main text of the paper. This is done so as to permit the direct derivation of our main (and general) results in Sec. III. Specific details of the T operator equations, etc., as given in the Appendix, can thus be studied separately from the results of Sec. III.

II. COUPLED CHANNEL T OPERATOR EQUATIONS

A. Notation

The notation has been stated before[8] and is only summarized here. We consider a nonrelativistic, three-body scattering system having four possible arrangement channels: three two-body channels and one three-body or breakup channel, labeled by the letters j, k, l, etc., $0 \le j \le 3$, where $j=0$ means the breakup channel. The various particles are assumed distinguishable, so that a two-body arrangement channel corresponds to a specific grouping of labeled particles into a single particle plus a two-body bound state. Such groupings, plus the breakup channel, lead to the notion of asymptotic states, defined by Ekstein.[14] The assumed existence of such asymptotic states means that the Hamiltonian H may be partitioned into a channel Hamiltonian H_k and a channel perturbation V_k in four ways:

$$H = H_k + V_k, \quad 0 \le k \le 3. \tag{1}$$

Here H_k describes the internal states of the fragments or clusters forming channel k plus their relative plane wave motion, and V_k is the interaction between various fragments in channel k. The V_k are assumed to go to zero rapidly enough to permit asymptotic states to be defined.[14] They also are assumed to be sufficiently well behaved to permit the kernels of the relevant integral equations, or some iterate of the kernels, to be compact.[6,15]

The eigenstates of H_k with energy E, the channel states, are denoted by $|\Phi_E(k)\rangle$. They obey

$$H_k|\Phi_E(k)\rangle = E|\Phi_E(k)\rangle, \tag{2}$$

and are products of bound states (or spin states) of the fragments forming the channel and plane wave relative motion states.

There are two forms for the on-shell transition operators (the notation of Lovelace[6] is used here):

$$U_{jk}^{(+)}(\pm) = V_j + V_j G(\pm) V_k \tag{3}$$

and

$$U_{jk}^{(-)}(\pm) = V_k + V_j G(\pm) V_k, \tag{4}$$

where the full Green's function $G(\pm)$ is defined by

$$G(\pm) = \lim_{\epsilon \to 0^+} G(E \pm i\epsilon) \tag{5}$$

and

$$G(E \pm i\epsilon) = (E \pm i\epsilon - H)^{-1}. \tag{6}$$

The analogous channel Green's functions $G_k(\pm)$ are

$$G_k(\pm) = \lim_{\epsilon \to 0^+} G_k(E \pm i\epsilon) \tag{7}$$

with

$$G_k(E \pm i\epsilon) = (E \pm i\epsilon - H_k)^{-1}. \tag{8}$$

The G and G_k are related by the resolvent equations

$$G = G_k + G_k V_k G = G_k + G V_k G_k, \tag{9}$$

where the same energy dependence is assumed for

G and G_k.

The amplitude A_{jk} for transitions from a state $|\Phi_E(k)\rangle$ in channel k to a state $|\Phi_E(j)\rangle$ in channel j is given by

$$A_{jk} = \langle \Phi_E(j) | U_{jk}^{(+)}(+) | \Phi_E(k) \rangle = \langle \Phi_E(j) | U_{jk}^{(-)}(+) | \Phi_E(k) \rangle .$$

This pair of equations is a statement of the well known result that on-shell matrix elements of $U_{jk}^{(+)}(+)$ and $U_{jk}^{(-)}(+)$ are identical.

We will restrict ourselves in this article to the case of pair interactions only.[16] Then the full Hamiltonian is given by

$$H = H_0 + V_{12} + V_{13} + V_{23} \tag{10}$$

$$\equiv H_0 + V. \tag{11}$$

Here H_0 is the sum of kinetic energy operators and V, the full interaction, is also the interaction in the breakup channel labeled by $k=0$.

In terms of the superscript pair label (j), defined by[6]

$$V^{(j)} = V_{kl} \tag{12}$$

and

$$V^{(0)} = 0, \tag{13}$$

the channel Hamiltonian is

$$H_k = H_0 + V^{(k)}. \tag{14}$$

The channel interaction, or interaction between the fragments, is given by

$$V_k = V - V^{(k)}; \tag{15}$$

consequently,

$$V_k = \sum_{n=0}^{3} \bar{\delta}_{kn} V^{(n)} = \sum_{n=1}^{3} \bar{\delta}_{kn} V^{(n)}, \tag{16}$$

where $\bar{\delta}_{kn} = 1 - \delta_{kn}$. Equations (14) and (15) obviously hold for the breakup case $k=0$ as well as for the three two-body channels $k=1$, 2, and 3. We also note that only in the present case of $n=3$ does specification of the label of a single particle suffice to define the two-body channel.

B. Channel coupling array operators

The derivation of the coupled equations for the transition operators was originally given[9,10] for the case of an arbitrary number n of distinguishable particles and their associated arrangement channels. In the present case $n=3$, and the number N of arrangement channels we shall finally consider is either $N=3$ or $N=4$. We shall leave the value of N unspecified; details are given in the Appendix. If we use the pair indexes j, k, and l to label channels, then in matrix form the channel coupling array equations for the transition operators $T_{jk}(z)$ are

$$T(z) = \mathcal{U} + \mathcal{U}\mathcal{G}(z)T(z), \tag{17}$$

where $T(z)$, $\mathcal{U}$, and $\mathcal{G}(z)$ are $N \times N$ matrices in channel index space with elements given by

$$[T(z)]_{jk} = T_{jk}(z),$$

$$(\mathcal{U})_{jk} = V_j W_{lk}, \tag{18}$$

and

$$[\mathcal{G}(z)]_{jk} = \delta_{jk} G_k(z).$$

In this equation, z is a complex energy parameter whose physical value is $z = E + i0$; V_j is the channel interaction of Eqs. (15) or (16); W_{lk} is an element of the channel coupling array W; and $G_k(z)$ is the kth resolvent operator given by $G_k(z) = (z - H_k)^{-1}$, an obvious generalization of Eq. (8). The elements W_{mn} are real and are initially restricted only by the normalization condition[9]

$$\sum_n W_{mn} = 1, \quad \text{all } m. \tag{19}$$

Notice that the subscript l on W_{lk} in Eq. (18) is free to be chosen at our convenience. For $N=3$, we have found[8] two independent choices of l leading to three sets of the coupled equations (17) with connected, iterated kernels, while for $N=4$, we have found only one such choice. These are given in the appendix, where some of their properties are discussed, including the connection with the Alt, Grassberger, and Sandhas (AGS) equations[17] for the $N=3$ case and the role of the breakup channel.

The operator $T_{jk}(E+i0)$ defined by Eq. (17) has on-shell matrix elements identical to those of $U_{jk}^{(\pm)}(E+i0)$ when the initial channel k is a two-body channel. In this case, the transition amplitude A_{jk} is also given by

$$A_{jk} = \langle \Phi_E(j) | T_{jk}(+) | \Phi_E(k) \rangle .$$

Not only are on-shell matrix elements of $T_{jk}(+)$ and $U_{jk}^{(\pm)}(+)$ equal, but, by the derivation of Eq. (17), the quantities $T_{jk}(+)|\Phi_E(k)\rangle$ and $U_{jk}^{(\pm)}(+)|\Phi_E(k)\rangle$ are also identical when k is a two-body channel and the energy E in $|\Phi_E(k)\rangle$ is the same as appears in the transition operators (recall "+" $= E + i0$). As noted in the Appendix, the $T_{jk}(+)$ are similarly phase equivalent to the AGS operators[17] $U_{jk}(+)$. The reason that k is restricted to two-body channels is that the derivation of (17) makes use of Lippmann's relation,[18] which is an operator relation that can be expressed in several ways:

$$G_i(+)V_i = G_i(+)V_k + \delta_{ik}$$

or (20)

$$G_i(+)G_k^{-1}(+) = \delta_{ik},$$

and Eqs. (20) are valid *only* when acting on an initial state of energy $E\,|\Phi_E(k)\rangle$ in a two-body channel k. Hence the theory defined by Eq. (17) is in effect a half-on-shell theory, a point we take note of when we examine the discontinuity relation satisfied by the T_{jk}. This half-on-shell character will prove to be an advantage since the restriction to $z = E + i0$ in the discontinuity relation will eliminate terms which otherwise are nonzero. The restriction to initial two-body channels is not a serious limitation since the nonrelativistic collision processes of interest are generally initiated only in such channels.

Although the initial channel index k must denote a two-body channel, the final index may label a channel with an arbitrary number of fragments. In the present case this means two- or three-body channels. In either case Eqs. (20) hold and on-shell matrix elements of T_{jk} give A_{jk}. The three fragment case implies the breakup state; it can occur, for k a two-body channel, in two ways: either as a final or as an intermediate state. The former is no problem, but the latter occurs in the discontinuity relation itself, and we must therefore specify how initial breakup states enter into the channel coupling theory.

Let us define $U_{jk}^{(\pm)}(z)$ by Eqs. (3) and (4) with $G(\pm)$ replaced by $G(z) = (z - H)^{-1}$, in analogy with the definition of $G_k(z)$ given below Eq. (18). If we now retrace the derivation of Eq. (17) as given in Ref. 9 but for complex energy z, it is trivial to show[19] that

$$U_{jk}^{(+)}(z) = \sum_m T_{jm}(z)\, G_m(z)\, G_k^{-1}(z), \tag{21}$$

where $T_{jm}(z)$ obeys (17). Equation (21) holds for an arbitrary number of particles n and channels N. When k is a two-body channel, and when both sides of (21) act on $|\Phi_E(k)\rangle$, and in $\lim z \to E + i0$, then (20) immediately leads to $U_{jk}^{(+)}(+) = T_{jk}(+)$. This is a demonstration of the equivalence of $U_{jk}^{(+)}(+)$ and $T_{jk}(+)$ as well as a reminder that Eq. (17) defines a half-on-shell theory.

Our present interest is in the case of $k = 0$, the three-body or breakup channel. Instead of (20), we find[15,20]

$$G_i(+)G_0^{-1}(+) = 1 + G_i(+)V^{(i)} = 1 + G_0(+)\,t^{(i)}(+), \tag{22}$$

where $t^{(i)}(+)$, the two-body T matrix in three-body space, satisfies the relation $G_i(+)V^{(i)} = G_0(+)t^{(i)}(+)$ and obeys

$$t^{(i)}(+) = V^{(i)} + V^{(i)}G_0(+)t^{(i)}(+),$$

with $G_0(+)$ being the free three-body Green's function. Substitution of (22) into (21) (where $\lim z \to E + i0$ is now assumed) gives

$$U_{j0}^{(+)}(+) = \sum_m T_{jm}(+)\,[1 + G_m(+)V^{(m)}]. \tag{23}$$

The sum on m is over the same number of channels as is used in the derivation of (17); in the present case this means m runs from 1 to 3 or from 0 to 3. As we shall see, precisely the sum on the right-hand side of (23) enters both the discontinuity and the damping relation equations, so that transitions from a breakup channel in the W-array theory are governed by $U_{j0}^{(+)}$ (or equivalently by the AGS operator[17] U_{j0}). We note again that (23) is valid as a half-on-shell relation.

We conclude this section with several comments concerning the case $j = 0$ (transitions to breakup). From the definition (3), it is clear that

$$U_{0k}^{(+)}(\pm) = \frac{1}{2}\sum_{m=1}^{3} U_{mk}^{(+)}(+).$$

It now follows from the preceding discussion that

$$T_{0k}(\pm) = \frac{1}{2}\sum_{m=1}^{3} T_{mk}(\pm), \quad k \neq 0.$$

It is also not difficult to show[4,17] that

$$T_{0k}(\pm) = \delta_{mk}V^{(k)} + [1 + V^{(m)}G_m(\pm)]T_{mk}(\pm), \quad k \neq 0. \tag{24}$$

In fact, we prove in the Appendix, using Eq. (15) to *define* $V^{(k)}$, that (24) is valid for arbitrary numbers of particles and channels. Equation (24) enters the proof that the T_{jk} obey the correct discontinuity relation.

III. K OPERATORS AND UNITARY APPROXIMATIONS

A. Discontinuity relations

Lovelace[6] has shown that the operators $U_{jk}^{(\pm)}(\pm)$ obey the following discontinuity relation:

$$U_{jk}^{(\pm)}(+) - U_{jk}^{(\pm)}(-) = -2\pi i \sum_{l=1}^{3}\sum_{\gamma} U_{jl}^{(\pm)}(+)\Delta_{l,\gamma}(E)\,U_{lk}^{(\mp)}(-) - 2\pi i\, U_{j0}^{(\pm)}(+)\Delta_0(E)\,U_{0k}^{(\mp)}(-), \tag{25}$$

where

$$\Delta_0(E) = \delta(E - H_0) \tag{26}$$

and

$$\Delta_{l,\gamma}(E) = \delta(E - H_l) P_\gamma(l), \tag{27}$$

with $P_\gamma(l)$ being the projection operator onto the γth bound state supported by the potential $V^{(l)}$. The AGS operator U_{jk} obeys a similar relation[4,17]:

$$U_{jk}(+) - U_{jk}(-) = -2\pi i \sum_{l=1}^{3} \sum_{\gamma} U_{jl}(+) \Delta_{l,\gamma}(E) U_{lk}(-) - 2\pi i U_{j0}(+) \Delta_0(E) U_{0k}(-). \tag{28}$$

One of the advantages of the AGS formalism is that the right-hand side of the discontinuity relation involves one operator and not two, as in Eq. (25). Since, for $k \neq 0$, $T_{jk}(\pm) = U_{jk}^{(+)}(\pm) = U_{jk}^{(-)}(\pm) = U_{jk}(\pm)$, it may be expected that T_{jk} will obey a discontinuity relation similar to those of Eqs. (25) or (28), with the U's everywhere replaced by the T's, except for $l = 0$. We shall prove that this relation is ($k \neq 0$)

$$T_{jk}(+) - T_{jk}(-) = -2\pi i \sum_{l=1}^{3} \sum_{\gamma} T_{jl}(+) \Delta_{l,\gamma}(E) T_{lk}(-) - 2\pi i U_{j0}^{(+)}(+) \Delta_0(E) T_{0k}(-), \tag{29}$$

where $U_{j0}^{(+)}(+)$ is given by Eq. (23). In contrast to (25) and (28), Eq. (29) is not an operator identity but holds for physical energy values $E \pm i0$, *after application onto the corresponding channel states*. Otherwise additional terms would enter this relation. We emphasize that (29) holds for *any* choices of W, whether it is 3×3 or 4×4, and whether or not it leads to a connected, iterated kernel. We shall start with the set of integral equations (17) for the T_{jk}, thus directly establishing that the solution to these equations satisfies the discontinuity relation. The discontinuity relation can be derived either by examining the formal operator solution to (17) (see, e.g., Ref. 8) or using the inverse operators $[T(\pm)]^{-1}$. Both methods lead to the same result. We follow the latter method as it is simpler and can also be carried over to the derivation of the damping relation.

From Eq. (17) it follows that $[T(z)]^{-1}$ obeys[21]

$$[T(z)]^{-1} = [\mathcal{U}]^{-1} - \mathcal{G}(z). \tag{30}$$

Because $\mathcal{U}$ is independent of z, a little algebra shows that (30), for $z = E \pm i0$, leads to

$$[T(-)]^{-1} - [T(+)]^{-1} = \mathcal{G}(+) - \mathcal{G}(-), \tag{31}$$

or equivalently,

$$T(+) - T(-) = T(\pm)[\mathcal{G}(+) - \mathcal{G}(-)] T(\mp). \tag{32}$$

In terms of the channel space indices, j, k, and l, Eq. (32) reads

$$T_{jk}(+) - T_{jk}(-) = \sum_{l} T_{jl}(+)[G_l(+) - G_l(-)] T_{lk}(-), \tag{33}$$

where we have used Eq. (18) and chosen the upper signs on the right-hand side of (32). We also assume k to label a two-body channel. The possible occurrence of the term with $l = 0$ in (33) depends on the dimension of W in (17) (see the Appendix for details).

Differences of operators evaluated just above and just below the cuts occur on both sides of (33). We denote these differences by the symbol D, e.g.,

$$T(+) - T(-) = DT$$

or

$$T_{jk}(+) - T_{jk}(-) = DT_{jk}, \tag{34}$$

and similarly

$$DG_l = G_l(+) - G_l(-).$$

The discontinuity DG_l receives contributions from two-body bound and continuum states when channel $l \neq 0$, although only the latter ones contribute to the three-body breakup discontinuity. If $l = 0$ occurs in (33), part of the three-body discontinuity also originates from this term.

In addition to using D to represent the discontinuity, we also specify the bound state contribution D_γ and the breakup contribution D_0 to the discontinuity. That is,

$$DG_l = \sum_{\gamma} D_\gamma G_l + D_0 G_l, \tag{35}$$

with $D_\gamma G_0 = 0$. Thus (33) can be written as

$$DT_{jk} = \sum_{l} T_{jl}(+) \left[\sum_{\gamma} D_\gamma G_l + D_0 G_l \right] T_{lk}(-). \tag{36}$$

From the work of Lovelace,[6] we know that

$$D_\gamma G_l = -2\pi i \Delta_{l,\gamma}(E)$$

and

$$D_0 G_l = -2\pi i [1 + G_l(+) V^{(l)}] \Delta_0(E) [1 + V^{(l)} G_l(-)], \tag{37}$$

where the notation of Eqs. (26) and (27) has been used [we note that (37) holds for $l = 0$ since $V^{(0)} = 0$].

Substituting (37) into (36) yields

$$DT_{jk} = -2\pi i \sum_{l=1}^{3} \sum_{\gamma} T_{jl}(+) \Delta_{l,\gamma}(E) T_{lk}(-) - 2\pi i \sum_{l} T_{jl}(+) [1 + G_l(+) V^{(l)}] \Delta_0(E) \times [1 + V^{(l)} G_l(-)] T_{lk}(-). \tag{38}$$

The term on the right-hand side of (38) that contains Δ_0 can be transformed as follows. From (24) we have that

$$[1 + V^{(l)} G_l(-)] T_{lk}(-) = T_{0k}(-) - \delta_{lk} V^{(k)}, \tag{39}$$

while from the fact that we shall consider only on-shell matrix elements we find $\Delta_0(E)V^{(k)}=0$. Hence, when used in (38), Eq. (39) leads to

$$DT_{jk}=-2\pi i\sum_{l=1}^{3}\sum_{\gamma}T_{jl}(+)\Delta_{l,\gamma}(E)T_{lk}(-)$$
$$-2\pi i\left\{\sum_{l}T_{jl}(+)[1+G_l(+)V^{(l)}]\right\}$$
$$\times\Delta_0(E)T_{0k}(-). \tag{40}$$

The sum in curly brackets in (40) will include $l=0$ if W is 4×4, otherwise not, but in either case we have from (23) that this term is precisely $U_{j0}^{(+)}(+)$ $[\equiv U_{j0}(+)]$, the correct transition operator from channel 0 to channel j. This result therefore proves that the new operators T_{jk} obey the correct discontinuity relation, viz. (29). From this we conclude that our basic equation, (17), properly takes account of the singularity structure of the three-body problem. We state without proof that $DU_{j0}^{(+)}$, with $U_{j0}^{(+)}$ expressed in terms of the T_{ji} via Eq. (23), is also given by the correct expression, analogous to (40).

Equations (29) and (40), which are the correct discontinuity relations, may be contrasted with earlier but incorrect work on this topic[23] involving the transformation $\mathcal{G}\to\tilde{\mathcal{G}}$, where $\tilde{\mathcal{G}}_{ij}=\delta_{ij}G_jP(j)$ and $P(j)$ is the projection onto the bound states in channel j [in the present notation $P(j)=\sum_\gamma P_\gamma(j)$]. The reason that the $\mathcal{G}\to\tilde{\mathcal{G}}$ result is invalid is seen in Eq. (23), where the proper transition operator is $U_{j0}^{(+)}(+)$ and not T_{j0}, as was incorrectly asserted in Ref. 23. Thus the operators defined by $T=\mathcal{U}+\mathcal{U}\tilde{\mathcal{G}}T$ only describe a particular model problem, although the remarks concerning nonorthogonality in this latter work remain valid. Reexamination of the results based on $\mathcal{G}\to\tilde{\mathcal{G}}$ indicated the need for a correct treatment; the present article is a consequence of this. Subsequently, a more general analysis was given by Benoist-Gueutal,[12] who has also succeeded in establishing that the minimum number of channels N needed (i.e., the size of W) in order that the operators T will satisfy the correct discontinuity relation for the case of an arbitrary number n of distinguishable particles is N_2, the total number of two-body channels. It is obvious on this ground that the four examples of W studied in the Appendix, all of which lead to connected equations, also give rise to operators T satisfying the proper discontinuity relations.

B. Reaction operators and the damping equation

The coupled equations for the K operators in the present theory are, in matrix form,[10]

$$K=\mathcal{U}+\mathcal{U}\mathcal{G}^{(\mathcal{P})}K, \tag{41}$$

where

$$(\mathcal{G}^{(\mathcal{P})})_{ij}=\delta_{ij}G_j^{(\mathcal{P})}$$
$$=\delta_{ij}\frac{\mathcal{P}}{E-H_j} \tag{42}$$

and $\mathcal{P}$ means principal value. Since

$$G_j(\pm)=\frac{\mathcal{P}}{E-H_j}\mp\pi i\delta(E-H_j), \tag{43}$$

with $\delta(E-H_j)$ being related to DG_j by

$$DG_j(+)=-2\pi i\delta(E-H_j). \tag{44}$$

Equation (41) yields that portion of $T(\pm)$ with the singularity structure removed. Note that Eq. (35) is an alternate way of writing (44) in which the contributions of the two-body bound and continuum state portions have been separated.

Combining Eqs. (42), (43), and (44) we get

$$\mathcal{G}_{ij}(\pm)=\delta_{ij}[G_j^{(\mathcal{P})}\mp\tfrac{1}{2}DG_j(+)]. \tag{45}$$

Also, it is trivial to show from Eqs. (17) and (41) that

$$T(z)=[1-\mathcal{U}\mathcal{G}(z)]^{-1}\mathcal{U} \tag{46}$$

and

$$K=[1-\mathcal{U}\mathcal{G}^{(\mathcal{P})}]^{-1}\mathcal{U}. \tag{47}$$

These latter equations plus (17) and (41) are sufficient to establish that T and K are related by the matrix damping equation

$$T(\pm)=K\pm\tfrac{1}{2}T(\pm)D\mathcal{G}K, \tag{48}$$

where

$$D\mathcal{G}_{ij}=\delta_{ij}DG_j \tag{49}$$

and DG_j is given by Eqs. (35) and (37). The direct inclusion of the breakup channel $l=0$ depends on the size of W. Whether it contributes or not depends on the initial energy.

An alternate relation between $T(\pm)$ and K is obviously

$$T(\pm)=K\pm\tfrac{1}{2}KD\mathcal{G}T(\pm); \tag{50}$$

the arguments cited in the next subsection suffice to show that this equation also leads to unitary approximations, and so we examine only Eq. (48) in detail.

C. Unitary approximations

Equations (48) and (50) are, as noted, trivial consequences of Eqs. (17) and (41). Despite this, they are of importance because they permit unitary approximations to be introduced in a relatively simple way, as we now demonstrate. We shall

prove that *any* set of operators K_{ij} having zero discontinuity which are used in Eq. (48) result in operators T_{ij} which obey the correct discontinuity relation (29) or (40). Hence (48) provides a basis for introducing unitary approximations into the three-body problem in an extremely simple fashion, quite analogous to that used in the single channel case. If K obeys Eq. (41), the exact T is obtained from (48), but in any case, the approximate T's used will always be unitary as long as the K used in (48) has zero discontinuity.

The simplest way to prove that (48) leads to the discontinuity relation (29) is to form the analog of (48) for the inverse operators as we did for Eq. (17), leading to Eq. (30). Mutiplying from the right by K^{-1} and from the left by $[T(\pm)]^{-1}$ leads to

$$[T(\pm)]^{-1} = K^{-1} \mp \tfrac{1}{2} D\mathcal{G} . \tag{51}$$

From (51) and the assumption that K has zero discontinuity we find

$$[T(-)]^{-1} - [T(+)]^{-1} = D\mathcal{G} ,$$

which is easily seen to be equivalent to

$$T(+) - T(-) = T(+) D\mathcal{G} T(-) . \tag{52}$$

Equation (52) is clearly identical to Eq. (32), so that the arguments of the preceding section immediately show us that on-shell matrix elements of (48) satisfy (29), as required.

The preceding argument shows that (48) or (50) provides a basis for introducing unitary approximations in the three-body problem. This can be done directly from Eq. (41) defining K, without the need for intermediate equations. It is, however, worth stressing two points. First, Eqs. (48) or (50), for any K such that $DK = 0$, are only an alternate mathematical expression of the discontinuity relation (29). That is, without Eqs. (17) and (41) to express the dynamics and three-body character of the system of interest, Eqs. (48) or (50) are without physical content. It is essential first to have some kind of (connected)theory for T and K before any use can be made of the damping relation. Otherwise there is no way to ensure that an arbitrary operator K used in (48) will be an approximation applicable to the system of interest. On the other hand, whether an approximate solution of (41) will lead to an *accurate* approximation to T when used in (48) is a question to be decided in individual cases. This brings us to the second point, viz., that the purpose of the preceding analysis (or similar ones) is not to provide twice as much to do in determining T as compared to solving Eq. (17), but to present a scheme for introducing approximations of a certain kind in the hope that they will allow an accurate but approximate T to be calculated more easily than by solving (17). The above comment on accuracy is obviously pertinent. Given these remarks, we now consider other aspects of these results.

For the $N = 3$ situation ($W = 3 \times 3$), the breakup channel is not directly coupled into the sets of integral equations (17) and (41). Instead, the operators T_{0k} and K_{0k} are algebraically related to the two-body to two-body arrangement operators while the $U_{j0}^{(+)}$ obey extra integral conditions obtained by multiplying (17) from the right by $[1 + G_k(+)V^{(k)}]$, and summing over k according to (23). In an analogous way operators K_{j0} can be defined.[4] All these operators are coupled into (48) or (50). The occurrence of $U_{j0}^{(+)}$ on the right-hand side of (48) is, for instance, easily shown by inserting there the representation (37) of the discontinuity, and using (23). In the case $N = 3$, then, approximations to the two-body to two-body and three-body K operators are made first and from them a unitary approximation to $U_{j0}^{(+)}$ or T_{0k} is obtained via Eqs. (48) or (50). It is the characteristic feature of the case $N = 4$ that K_{j0} and K_{0k} both enter the analysis via (41). T operators as well as K operators for breakup are, therefore, directly determined by the sets of coupled integral equations.

For energies below the breakup threshold, Eqs. (48) and (50) are *algebraic* equations only (after an angular momentum decomposition has been made), while above breakup they are nonsingular, one-dimensional integral equations, with the integration variable ranging from 0 to a maximum value proportional to the square root of the incident energy. This statement holds for both exact and any approximate values of the matrix elements of K to be used in (48) or (50), and is one reason why approximate unitary calculations are so simple to carry out compared to solving (17). Model calculations based on this approach are in progress and will be discussed elsewhere. Our purpose here has been to demonstrate the relative ease with which a unitary approximation scheme consistent with the discontinuity relation can be introduced; in contrast, we believe, to other methods that have been proposed.[1-3] The extension of these results to the case of arbitrary n is evident and will be treated subsequently.

APPENDIX

A. Connected T operator equations

Without loss of generality, we set (the initial channel label) $k = 1$ in all four cases studied herein. Then the set (17) takes the form

$$T_{j1}(z) = V_j W_{11} + V_j \sum_m W_{1m} G_m(z) T_{m1}(z) . \tag{A1}$$

The general structure of the equations we present

here is mirrored in the structure of the K operator equations, (41): we merely need to replace $G_m(z=E+i0)$ by $G_m^{(\varphi)}$, and $T_{j1}(+)$ by K_{j1}. We consider the case $N=3$ first, for which we have found[8] two classes of W, leading to three sets of connected equations; when $N=4$, we have discovered only one choice of W, leading to six (equivalent) sets of equations.

1. $N=3$

There are two classes of W in this case, each 3×3. Only the two-body channel labels are included, so that the sum in (A1) now runs from 1 to 3. Were we to remove one of these three channels, then the resulting equations would neither satisfy unitarity[12] nor have any connected iterates of the kernel $\mathcal{U}\mathcal{G}$ occurring in (17) and (A1).

a. *Faddeev-Lovelace array.* The first set of equations is obtained by setting the free index l in W_{li} equal to the pair summation index in V_j. That is,

$$V_j=\sum_{n=1}^{3}\bar{\delta}_{nj}V^{(n)},$$

and we set $l=n$ for each n. Hence V_jW_{li} becomes

$$V_jW_{li}\to\sum_{n}\bar{\delta}_{nj}V^{(n)}W_{ni}. \tag{A2}$$

With l specified, we now select W_{ni}:

$$W_{ni}=\delta_{ni}; \tag{A3}$$

note that the choice (A3) satisfies the constraint (19).

Substituting these results into (A1) gives the set[8]

$$\begin{aligned}T_{11}&=V^{(2)}G_2T_{21}+V^{(3)}G_3T_{31},\\ T_{21}&=V^{(1)}+V^{(1)}G_1T_{11}+V^{(3)}G_3T_{31},\\ T_{31}&=V^{(1)}+V^{(1)}G_1T_{11}+V^{(2)}G_2\,T_{21},\end{aligned} \tag{A4}$$

where we have suppressed the parameter z. These equations are obviously in the standard Faddeev form.[6,15] In a more compact notation they read

$$T_{j1}=\bar{\delta}_{j1}V^{(1)}+\sum_{n=1}^{3}\bar{\delta}_{jm}V^{(m)}G_mT_{m1}, \tag{A4$'$}$$

which, from the relation $V^{(m)}G_m=t^{(m)}G_0$, can also be written as[22]

$$T_{j1}=\bar{\delta}_{j1}V^{(1)}+\sum_{m=1}^{3}\bar{\delta}_{jm}t^{(m)}G_0T_{m1}. \tag{A5}$$

The first iterate of the kernel of Eqs. (A4) or (A5) is evidently connected.

It is trivial to prove that the T_{j1} as defined by (A5) are phase equivalent to the AGS operators U_{j1} defined by[17]

$$U_{j1}=\bar{\delta}_{j1}G_0^{-1}+\sum_{m=1}^{3}\bar{\delta}_{jm}t^{(m)}G_0U_{m1}. \tag{A6}$$

The proof consists first in multiplying both sides of (A6) from the right by the operator $G_0V^{(1)}$ and noting that the resulting equation for $U_{j1}G_0V^{(1)}$ is the same as (A5). Hence we have that

$$T_{j1}(z)=U_{j1}(z)G_0(z)V^{(1)}.$$

The phase equivalence follows from the fact that $G_0(+)V^{(1)}|\Phi_E(1)\rangle=|\Phi_E(1)\rangle$. This demonstration also indicates that T_{j0} cannot be the correct operator to describe transitions from the breakup channel, since, while $U_{j0}\neq 0$, $V^{(0)}=0$, and hence $U_{j0}G_0V^{(0)}=0$.

b. *Channel permuting arrays.* These arrays have been discussed in detail elsewhere[8,9,24]; for $N=3$ there are two equivalent W's, both of which lead to the second iterate of the kernel being connected. The two arrays, which are transposes of each other, are

$$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}\text{ and }\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}.$$

Choosing the first and substituting into (A1) gives

$$\begin{aligned}T_{11}&=V_1G_2T_{21},\\ T_{21}&=V_2G_3T_{31},\\ T_{31}&=V_3+V_3G_1T_{11}.\end{aligned} \tag{A7}$$

Had we chosen the second array, a set of equations similar to (A7) but with the subscripts 2 and 3 interchanged would have resulted.

Equation (A7) is quite different in appearance from the set (A4) obtained from the Faddeev-Lovelace choice of W, Eqs. (A2) and (A3); not only is it different in structure, but the second rather than the first iterate of its kernel is connected. Nevertheless, it is a completely valid set, and it has been shown[24] that each T_{j1} in (A7) has as its exact on-shell solution just the form $U_{j1}^{(+)}(+)$ of Eq. (3). Although on-shell exact solutions of (A4) and (A7) are identical, one set may be more convenient to work with than another in specific applications; e.g., when hard core pair potentials occur, (A4) is clearly more convenient since $V^{(1)}|\Phi_E(1)\rangle$ is a well defined object.

2. $N=4$

We have found only one class of W's leading to a connected equation, and these are the six channel permuting arrays for $N=4$. The method for generating them is discussed in the first of Refs.

9, and we give only one result here, viz.,

$$\begin{aligned} T_{11} &= V_1 G_2 T_{21} , \\ T_{21} &= V_2 G_3 T_{31} , \\ T_{31} &= V_3 G_0 T_{01} , \\ T_{01} &= V + V G_1 T_{11} , \end{aligned} \tag{A8}$$

where V is the full interaction, occurring in the breakup channel $j=0$. Five other equations, equally valid, may be obtained from (A8) by (a) shifting the inhomogeneity from the $j=0$ channel to $j=2$ or $j=3$ and (b) interchanging the roles of the channels $j \neq 1$ without the inhomogeneous term. It is merely a matter of labelling.[9] The same proof[24] used in connection with (A7) suffices to show that the on-shell solutions to (A8) are given by $T_{j1}(+) = U_{j1}^{(+)}(+) = V_j + V_j G(+) V_1$.

B. Breakup channel

1. $j=0$

We assume the final channel to be the breakup channel, i.e., we take $j=0$. We shall prove Eq. (24) and then its analog for the general case of arbitrary n and N.

From Eq. (A4′), with $k \neq 0$ replacing the initial channel subscript 1, we find

$$\begin{aligned} T_{0k} &= V^{(k)} + \sum_{m=1}^{3} V^{(m)} G_m T_{mk} \\ &= V^{(k)} + V^{(m)} G_m T_{mk} + \sum_{n=1}^{3} \bar{\delta}_{mn} V^{(n)} G_n T_{nk} \\ &= \bar{\delta}_{mk} V^{(k)} + (1 + V^{(m)} G_m) T_{mk} , \end{aligned}$$

and the last line establishes Eq. (24).

A generalization is easily obtained. For arbitrary numbers of particles n, we define $V^{(l)}$ in analogy to the pair interaction of the three-body case:

$$V^{(l)} = V - V_l . \tag{A9}$$

That is, $V^{(l)}$ is the portion of the total interaction that causes binding of the clusters that form the lth channel. With this definition of $V^{(l)}$, we now examine the quantity Y given by

$$Y = [1 + V^{(l)} G_l(+)] T_{lk}(+) , \tag{A10}$$

where k is a two-body channel. We state without proof that $T_{jk}(+) \equiv U_{jk}^{(+)}(+) = V_j + V_j G(+) V_k$ when it acts on $|\Phi_E(k)\rangle$ (a proof is given in Ref. 24); hence, we may replace $T_{lk}(+)$ by

$$T_{lk}(+) = V_l + V_l G(+) V_k ,$$

which gives for (A10)

$$\begin{aligned} Y &= [1 + V^{(l)} G_l(+)][V_l + V_l G(+) V_k] \\ &= V_l + V^{(l)} G_l(+) V_l + V_l G(+) V_k \\ &\quad + V^{(l)} G_l(+) V_l G(+) V_k . \end{aligned} \tag{A11}$$

The product $G_l V_l G$, by Eq. (9), is just $G - G_l$, and using this in (A11) leads to

$$Y = V_l + V^{(l)} G_l(+)(V_l - V_k) + (V_l + V^{(l)}) G(+) V_k . \tag{A12}$$

From (A9) we see that $V_l + V^{(l)} = V$, while from (20) and our on-shell assumption, $G_l(V_l - V_k) = \bar{\delta}_{lk}$. Hence (A12) becomes

$$\begin{aligned} Y &= -\delta_{lk} V^{(l)} + (V + V G(+) V_k) \\ &= -\delta_{lk} V^{(l)} + T_{0k}(+) . \end{aligned} \tag{A13}$$

Use of (A10) in (A13) and the replacement $\delta_{lk} V^{(l)} = \delta_{lk} V^{(k)}$ then leads to

$$T_{0k}(+) = \delta_{lk} V^{(k)} + [1 + V^{(l)} G_l(+)] T_{lk}(+) , \tag{A14}$$

a generalized version of Eq. (24).

2. $k=0$

We now assume the initial channel to be the breakup channel, i.e., $k=0$. In this case j is arbitrary and $U_{j0}^{(+)}(+)$ of Eq. (23), rather than $T_{j0}(+)$, is the correct transition operator. The point we wish to comment on here is that (23) is the correct result for both the $N=3$ and $N=4$ cases. In the former case, $T_{j0}(+)$ does not enter Eq. (23), while in the latter case it does and will contribute to $U_{j0}^{(+)}(+)$. There is no paradox involved in this. For example, comparing the coupled equations for T_{j0} obtained for the $N=3$ and $N=4$ channel permuting array cases, i.e., Eqs. (A7) and (A8) with the initial channel subscript 1 replaced by 0, it might seem that the only difference they produce in Eq. (50) is T_{j0}, and since the other operators appear to be the same, this would then imply an error. In fact, the error lies in assuming the other operators to be the same. That is, the $T_{jm}(+)$ give the same results only when acting on $|\Phi_E(m)\rangle$, while the presence of $G_m(+)$ in $T_{jm}(+) G_m (+) G_0^{-1}$ ensures that $T_{jm}(+)$ will also act on states $|\Phi_{E'}(m)\rangle$, $E' \neq E$; i.e., $T_{jm}(+)$ will be evaluated off shell as well. Since off-shell values of the T_{jm} in (A7) differ from those in (A8), it should be no surprise that different structures lead to the same $U_{j0}^{(+)}(+)$.

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†SRC Senior Visiting Fellow 1974–75. Permanent address: Physics Department, Brown University, Providence, Rhode Island 02912.

[1]R. T. Cahill, Nucl. Phys. A194, 599 (1972). See also P. C. Tandy, Ph.D. thesis, The Flinders University of South Australia, 1972 (unpublished).

[2]K. L. Kowalski, Phys. Rev. D 5, 395 (1972); 6, 3705 (1972); 7, 1806 (1973).

[3]T. Sasakawa, Nucl. Phys. A203, 496 (1973); and unpublished.

[4]E. O. Alt, P. Grassberger, and W. Sandhas, (unpublished); and W. Sandhas (unpublished). Compare also W. Sandhas, in *Elementary Particle Physics*, edited by P. Urban (Springer, Wien, Germany, 1972).

[5]E.g., L. Rodberg and R. Thaler, *Introduction to the Quantum Theory of Scattering* (Academic, New York, 1967).

[6]C. Lovelace, in *Strong Interactions and High Energy Physics*, edited by R. G. Moorhouse (Oliver and Boyd, London, 1964); Phys. Rev. 135, B1225 (1964).

[7]R. D. Amado, in *Elementary Particle Physics and Scattering Theory*, edited by M. Chretien and S. S. Schweber (Gordon and Breach, New York, 1970).

[8]D. J. Kouri and F. S. Levin, Nucl. Phys. A250, 127 (1975).

[9]D. J. Kouri and F. S. Levin, Phys. Lett. 50B, 421 (1974); proceedings of the Quebec Conference, 1974, in *Few-Body Problems in Nuclear and Particle Physics*, edited by R. J. Slobodrian, B. Cujec, and K. Ramavataram (Laval University Press, Quebec, 1975), p. 47; D. J. Kouri, M. Craigie, and D. Secrest, J. Chem. Phys. 60, 1851 (1974); D. J. Kouri, F. S. Levin, M. Craigie, and D. Secrest, J. Chem. Phys. (to be published); W. Tobocman, Phys. Rev. C 9, 2466 (1974).

[10]D. J. Kouri and F. S. Levin, Bull. Am. Phys. Soc. 19, 489 (1974).

[11]D. J. Kouri and F. S. Levin, Phys. Rev. A 10, 1616 (1974); this was the first paper applying the channel coupling array method to problems involving unitarity. Not all equations based on the W array method lead to damping equations identical to Eqs. (48) or (50), e.g., those of Tobocman (Ref. 9) or those of M. Baer and D. J. Kouri, J. Math. Phys. 14, 1637 (1973). These latter authors were the first to use the W array method, although their calculations gave nonunitary approximate amplitudes. The lack of a damping equation similar to Eq. (48) in some sets of W array equations has been used to explain the occurrence of such nonunitary approximate amplitudes: D. J. Kouri, F. S. Levin, M. Craigie, and D. Secrest, J. Chem. Phys. 61, 17 (1974).

[12]P. Benoist-Gueutal, Phys. Lett. 56B, 413 (1975).

[13]The nomenclature follows that of R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[14]H. Ekstein, Phys. Rev. 101, 880 (1956); K. Hepp, Helv. Phys. Acta 42, 425 (1969).

[15]L. D. Faddeev, Zh. Eksp. Teor. Fiz. 39, 1459 (1960) [Sov. Phys. JETP 12, 1014 (1961)]; and *Mathematical Aspects of the Three-Body Problem in the Quantum Scattering Theory, Publications of the Steklov Mathematical Institute, Leningrad, 1963* (Israel Program for Scientific Translation, Jerusalem, 1965), Vol. 69.

[16]Three-body forces could be included without too much difficulty but add nothing to the physics of our approach while only complicating the formulas.

[17]E. O. Alt, P. Grassberger, and W. Sandhas, Nucl. Phys. B2, 167 (1967).

[18]B. A. Lippmann, Phys. Rev. 102, 264 (1956); see also Faddeev, Ref. 14.

[19]Such a derivation, for $z=E+i\epsilon$, is given by Tobocman, Ref. 9.

[20]Equation (22) is also discussed by Benoist-Gueutal (Ref. 12), who deals with the case of arbitrary n.

[21]It is straightforward to show that as a matrix, $[\mathcal{U}]^{-1}$ exists for the four choices of W given in the Appendix. By using the formal solution to (17) rather than the inverse, one can derive Eq. (32) for any choice of W, so we assume (32) to hold in general even if some W's may not admit an inverse $[\mathcal{U}]^{-1}$. In addition, we also assume that $[T(z)]^{-1}$ exists for all z where $T(z)$ is defined.

[22]See also Gy. Bencze, Nucl. Phys. A210, 568 (1973); E. F. Redish, Nucl. Phys. A225, 16 (1974); and the recent investigations of B. R. Karlsson and E. M. Zeiger, Phys. Rev. D 11, 939 (1975).

[23]D. J. Kouri and F. S. Levin, Phys. Lett. 53B, 27 (1974).

[24]D. J. Kouri and F. S. Levin, Nucl. Phys. A253, 395 (1975).