Unitarity in Non-Relativistic, Many-Body Scattering

I. Post-Prior Formalism

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Abstract

The unitarity (discontinuity) equations first derived by Lovelace for the three-body problem are extended to the N-channel, n-body problem using the transition operators in the usual "post-prior", rearrangement scattering form. Specific enumeration of the arrangement channels and scattering states that actually enter the problem allow for a detailed expression of results heretofore implicit in other work. Two derivations are given, one based on use of the imaginary part of the full, outgoing-wave Green function, the other based on counting the contributions from the threshold discontinuities in the various arrangement channels. The consistency of these results is used as a means of deriving modified equations for the coupled channel T and K operators discussed in the succeeding paper. An important implication of the present results is that except by coincidence, approximated calculations of scattering amplitudes based on the "post" or "prior" transition operators cannot be unitary even if all open channels are included in the calculation except by coincidence. This conclusion explains the occurrence of previously obtained non-unitary amplitudes for $e^- + H$ scattering.

1. Introduction

The unitarity condition in one-body scattering theory is of fundamental importance: it is a statement of probability conservation that leads to a relation between the imaginary part of the forward scattering amplitude and the total cross section. Although the unitarity condition in many-body scattering theory need not lead to such a simple relation, it is still of fundamental importance, not only as a statement of probability conservation, but also as a test to determine if approximate calculations are unitary.

We have recently developed a new theory of multi-channel scattering in which unitary approximations appear quite simple to introduce because of the existence, in this theory, of a K-operator matrix related to the matrix of transition operators by a damping equation.^{1,2)} As we have discussed elsewhere,¹⁾ no other formulations of many-body scattering theory seem to have such a simple damping relation built into the formalism.* Approximate calculations based on our equations have recently been made which give, to within the numerical accuracy of the computer, a unitary amplitude in low energy $e^- + H$ scattering^{5,6)}, while those based on a formalism for which a damping relation does not hold failed to give a unitary amplitude.⁵⁾ We have shown that this difference can be understood directly in terms of the existence of a damping equation in the one case, and its lack in the other.⁶⁾

Although a damping relation assures that unitary approximations can be made if a means of computing approximate K operators exists, this is not the primary form in which the expression of unitarity may be obtained. Rather

* For example, the unitary three-body theories of Kowalski³⁾ and of Cahill⁴⁾ give rise to K-operator equations that are connected to the T operators by a hierarchy of coupled integral equations, rather than directly.

it is through the relation between all the transition operators and the imaginary part of any one of them. This latter quantity is related to the discontinuity of the transition operator across the real energy axis, i.e., to the effects due to the cuts in the complex energy plane arising from the various thresholds in the problem.⁷⁾ For collisions involving many particles, the discussion of the unitarity relation is much more complicated than in the one-body case. The classic work of Lovelace⁸⁾ on unitarity in the three-body problem has been a profound influence, not only for subsequent work on the three-body problem⁹⁾, but also as a source for the treatment of unitarity in n-body scattering¹⁰⁾ [see also Levine¹¹⁾].

We have recently re-examined the unitarity relation for n-body scattering in an attempt to understand better the above-mentioned results on $e^- + H$ scattering, i.e., to try to explain further why one set of approximate calculations failed to give unitary results while another set actually produced unitary amplitudes. In so doing, we have found two results of interest. First, we have been able to derive the discontinuity relation of Lovelace for the three-body problem in a relatively simple (almost trivial) way, and have extended it to the n-body case. The key to doing this is to identify very clearly the totality of asymptotic states that can serve either as observable final states or (by time reversal invariance) as initial states which generate the scattering states of interest. Second, we have discovered an important modification in the coupled equations we have derived recently to describe multi-channel scattering.^{1,2)} The modification consists in changing each of the channel Green functions $G_1^+(E) = \lim_{\epsilon \rightarrow 0^+} (E - H_1 + i\epsilon)^{-1}$ to $\tilde{G}_1^+(E) = G_1^+(E) P(i)$, where H_1 is the Hamiltonian in channel 1 (H_1 contains no interactions between the various subsystems, or clusters of particles, forming the channel), and $P(i)$ is the projection operator onto the entire set of internal

bound states of H_1 . That is, one must remove from $G_1^+(E)$ the breakup (or continuum) states of any of the subsystems in channel 1. Only when the channel label is $i = 0$, referring to the case where all n particles are free, will breakup-like states enter, and these of course are the states in which all particles are described by plane waves.

The first of these results, a simple way to derive the N channel unitarity relation is discussed in the present paper. Our discussion involves three main items. First, a detailed and explicit enumeration of the channels and their bound states is given. Next, the detailed form of the unitarity relation is stated. Finally, these results are rederived by considering not the imaginary part of the T operators but their discontinuity, as in the work of Lovelace. The final result, twice derived, is the obvious extension to N channels of Lovelace's result for the three-body problem. It immediately allows us to draw the conclusion that, even if all open channels are included in an approximate calculation of the on-shell matrix elements of the transition operators, only by a fortuitous coincidence will the approximate amplitudes be unitary. In the second paper, the results of this present article are used as a means of first deriving the unitarity relation for our new transition operators, and then modifying the basic equations obeyed by these operators, their concomitant K operators, and the damping equation relating them.

2. Preliminaries

The scattering system is assumed to consist of n distinguishable particles labelled $1 \dots n$. Particle identity is treated by proper symmetrization of amplitudes, and will not be considered in detail in this paper. The number of arrangement channels is N ; we specify them below. Finally, the following three hypotheses are assumed to govern the dynamics:

- A. The system obeys non-relativistic quantum mechanics.
- B. Creation and annihilation of particles (including photons) may be ignored.
- C. Bound states of the interacting, n -particle system lie below all scattering state threshold energies.

The reasons for introducing these hypotheses will be made clear as we proceed.

From (A), the Hamiltonian H for the system is a sum of kinetic and potential energies; the latter may contain three-body, four-body, etc., interactions, as well as two-body interactions (long range forces are not included in the present analysis). Corresponding to each arrangement channel j , defined by stable clusters of particles or stable subsystems, H may be broken into a channel Hamiltonian H_j and a channel perturbation V_j :

$$H = H_j + V_j \quad (1)$$

Here H_j describes the internal states of the subsystems and their relative kinetic energies, while V_j is the set of interactions between the subsystems; $V_j \rightarrow 0$ as the separations between all subsystems become infinite. Since V_j is not present in H_j , H_j cannot support n -particle bound states. The channel index j sums over all possible 2-body, 3-body, etc. subsystems, including those differing only by interchange of particle labels between subsystems.

The n -particle channel is denoted 0, where H_0 is the sum of kinetic energy operators and V_0 is the total set of interactions.

Eigenstates of H_j obey

$$H_j |\Phi_\alpha(j)\rangle = E_\alpha |\Phi_\alpha(j)\rangle, \quad (2)$$

while the eigenstates of H obey

$$H |\Psi_\beta\rangle = E_\beta |\Psi_\beta\rangle. \quad (3)$$

In general, we are interested in scattering processes initiated from two-body channels at some remote time in the past. In the distant future, the system may be found in a variety of final states, all corresponding to observable stable subsystems. By time reversal invariance, any of these m -body (where $2 \leq m \leq n$) final states could serve as initial states generating scattering states of H . The observable set of channel states are the asymptotic channel states of Eckstein.¹²⁾ We shall assume that the totality of eigenstates of each H_j form a complete expansion set in the n -body Hilbert space, although as noted by Eckstein,¹²⁾ the bound states of all the H_j but H_0 are not complete. Furthermore, not all the eigenstates of H can be generated from the states of any particular H_j . This is an especially important point to keep in mind when examining the discontinuity of the full Green function across the real axis.

We consider the Green functions, or resolvent operators, next. Corresponding to the various Hamiltonians listed above are resolvent operators $G(z)$ and $G_j(z)$ defined by

$$G(z) = (z - H)^{-1} \quad (4)$$

and

$$G_j(z) = (z - H_j)^{-1}. \quad (5)$$

They are operator analytic in the complex energy Z everywhere but on the real axis, and are related by the pair of Lippmann-Schwinger (L-S) equations

$$G(Z) = G_j(Z) + G_j(Z) V_j G(Z) \quad (6)$$

and

$$G_j(Z) = G_j(Z) + G(Z) V_j G_j(Z). \quad (7)$$

Notice that all the $G_j(Z)$ are operators in the n -body Hilbert space: none of them refer to the $(n-1)$ -body problem. We call attention to the fact that $G(Z)$ and $G_j(Z)$ do not have the same analytic structure, a point we discuss in detail later. The physically interesting values of Z are $\lim_{\epsilon \rightarrow 0^+} Z = E \pm i\epsilon$, where E is a real energy. This limit is assumed to define outgoing wave Green functions $G^+(E)$ and $G_j^+(E)$, a second feature we shall discuss below.

For multi-channel scattering (rearrangement collisions), there are two transition operators^{*} whose exact, on-shell matrix elements give the amplitude for the transition¹³⁾ from a state of channel k to a state of channel j :

$$T'_{jk}(E+i\epsilon) = V_j + V_j G(E+i\epsilon) V_k \quad (8)$$

and

$$\hat{T}'_{jk}(E+i\epsilon) = V_k + V_j G(E+i\epsilon) V_k. \quad (9)$$

The amplitude of interest, $A_{jk}(E)$, is given by

$$A_{jk}(E) = \langle \Phi_E(j) | T'_{jk}(E+i0) | \Phi_E(k) \rangle \quad (10)$$

$$= \langle \Phi_E(j) | \hat{T}'_{jk}(E+i0) | \Phi_E(k) \rangle. \quad (11)$$

^{*}The operators T'_{jk} and $\hat{T}'_{jk}$ are the many-body generalizations of the 3-body operators U_{jk}^+ and U_{jk}^- introduced by Lovelace⁸⁾.

The two matrix elements are equal only if $|\Phi_E(j)\rangle$ and $|\Phi_E(k)\rangle$ are exact eigenstates of H_j and H_k respectively, and if each of their energies is equal to the energy E of the transition operators. Both $|\Phi_E(j)\rangle$ and $|\Phi_E(k)\rangle$ describe the subsystems in bound (particle-stable) states. Off-shell matrix elements of T'_{jk} and $\hat{T}'_{jk}$ are not equal.

From eq. (4), it follows that

$$G^*(Z) = G(Z^*) \quad (12)$$

and thus from (8) and (9) that

$$T'_{jk}{}^*(E \pm i\epsilon) = T'_{jk}(E \mp i\epsilon) \quad (13)$$

and

$$\hat{T}'_{jk}{}^*(E \pm i\epsilon) = \hat{T}'_{jk}(E \mp i\epsilon), \quad (14)$$

where the asterik means complex conjugate. Both $G(Z)$ and the operators $T'_{jk}(Z)$ and $\hat{T}'_{jk}(Z)$ are Hermitian analytic.⁷⁾

By time reversal invariance and the reality of the eigenvalues of H , we easily see that the following relations hold between the imaginary parts and the discontinuities of the operators of eqs. (12) - (14):

$$\Im G(E+i\epsilon) \equiv G(E+i\epsilon) - G(E-i\epsilon) = 2i \Im G(E+i\epsilon) \quad (15)$$

$$\Im T'_{jk}(E+i\epsilon) \equiv T'_{jk}(E+i\epsilon) - T'_{jk}(E-i\epsilon) = 2i \Im T'_{jk}(E+i\epsilon). \quad (16)$$

A relation similar to (16) holds for $\hat{T}'_{jk}(E+i\epsilon)$. Furthermore, from eq. (8) we have

$$\Im T'_{jk}(E+i\epsilon) = V_j \Im G(E+i\epsilon) V_k \quad (17)$$

or, equivalently,

$$\text{Im } T'_{jk}(E+i\epsilon) = V_j \text{Im } G(E+i0) V_k. \quad (18)$$

The quantity of physical interest is $T'_{jk}(E+i0)$, i.e., the limit when $\epsilon \rightarrow 0^+$. As noted by various workers,^{7,14)} both $T'_{jk}(E+i0)$ and $G(E+i0)$ are boundary values of analytic functions of Z defined in a cut plane. There are two ways of evaluating the boundary value $G(E+i0)$ and thus $T'_{jk}(E+i0)$. The first makes use of the well-known property¹³⁾

$$\text{Im } G(E+i0) = -\pi \delta(E-H), \quad (19)$$

and then relies on specification of the states of H to evaluate $\text{Im } T'_{jk}(E+i0)$. Since this is a relatively simple method which we have not heretofore seen applied to the multi-channel case, we develop it in detail first. The second method, which follows that of Lovelace for the three-body problem,⁸⁾ determines $DG(E+i0)$ by evaluating the contributions of all the cuts to the discontinuity. The two evaluations agree, as they must. The result, as we shall see, is extremely simple, once a procedure for specifying the channels is stated. Although the result we finally obtain, eq. (42), is simple, it does not seem to have been written out before, although it is implicit for example in the work of Weyers¹⁰⁾ or Levine.¹¹⁾

From (18) and (19) it follows that

$$\text{Im } T'_{jk}(E+i0) = -\pi V_j \delta(E-H) V_k, \quad (20)$$

and using the completeness relation for the states of eq. (3), viz.,

$$\int |\Psi_\alpha\rangle d\alpha \langle \Psi_\alpha| = 1, \quad (21)$$

(20) becomes

$$\text{Im } T'_{jk}(E+i0) = -\pi \int d\alpha V_j |\Psi_\alpha\rangle \delta(E-E_\alpha) \langle \Psi_\alpha | V_k. \quad (22)$$

This last equation is also a well-known result. What does not seem well-known is how to express its right hand side as a sum over products of transition operators for all the channels, even though such a result is obviously implied by the form of (22). The important step in deriving this latter result is the enumeration of those states of H which can actually contribute to the sum in (22). This will lead to an enumeration of all bound states in all channels, for, as we show below, it is only such states that can be used to generate the scattering states of H . We carry out the enumeration in the next section.

3. Specification of Asymptotic Channel States

Our goal in this section is to specify the set of states $|\Psi_\alpha\rangle$ that enter into the sum on the right hand side of eq. (22). By assumption C, none of these are bound states of H. By assumption B, the continuum states of H can only be generated from scattering experiments initiated by collisions of subsystems in an arrangement channel. That is, we do not consider states of H formed, e.g., by photon or meson absorption (or production). Furthermore, we also do not consider states of H formed as continuum states in an $(n + m)$ -body problem, e.g., formed by radioactive α -decay or heavy-ion coulomb excitation. We consider such states as a part of the set of processes in an $(n + m)$ -body system.

It follows from the above remarks that the entire set of continuum states of H can be enumerated by specifying the relevant states of the H_j used to generate them. Since we assume collisions begin in the distant past and lead to fragments (subsystems) detected in the remote future, it follows from assumption B that only particle-stable (bound) states of the H_j can generate the $|\Psi_\alpha\rangle$ of interest, i.e., by the time of detection, particle-unstable states will have decayed. By time-reversal invariance any observable final state can be used to generate a scattering state, and, as shown by Eckstein¹²⁾, scattering states of H generated by eigenstates of different H_j are orthogonal.

We thus conclude that by specifying the set of all particle-stable states of all the H_j (we include the set of free states of H_0 as well since each individual particle in isolation is assumed to be stable), we will be able to specify the set of $|\Psi_\alpha\rangle$ entering into the sum in eq. (22). Naturally,

not all such states may give a non-zero contribution, since the energy E_α may be less than E for some of them.

To specify the set of particle-stable states, we need both a notation and a means for enumerating them. The latter is required for determining the discontinuities: we need to know how many cuts contribute to DG or DT'_{jk} . States $|\Phi_\alpha(i)\rangle$ corresponding to bound subsystems (including excited states) will be denoted $|\Phi_{nq}(E_{nq}^i, i)\rangle$, obeying

$$H_i |\Phi_{nq}(E_{nq}^i, i)\rangle = E_{nq}^i |\Phi_{nq}(E_{nq}^i, i)\rangle \quad (23)$$

where

$$E_{nq}^i = E_n(i) + E_q(i), \quad (24)$$

with $E_n(i)$ denoting the sum of internal energies for the n th state of the subsystems in channel i , and $E_q(i)$ denoting the sum of the relative kinetic energies of the various subsystems in channel i .

The number of such internal bound states in each channel can be large since these bound states are products of bound states for each of the fragments. To help enumerate them, we introduce an auxiliary concept, that of reaction channel.* A reaction channel r_n corresponds to an experimentally observable grouping of n particles into m stable subsystems without regard to labelling of identical particles. An m -body arrangement channel, or simply an m -body channel, is an arrangement of n particles into m stable fragments with a specific labelling. Thus, each H_i defines a particular arrangement channel

* Our nomenclature differs from that often used in nuclear physics, where a reaction channel refers specifically to a final distribution of nucleons differing from that which initiated the collision. For example in $^{11}\text{B}(p, p')^{11}\text{B}^*$, $p + ^{11}\text{B}$ is the elastic channel, but in $^{11}\text{B}(p, d)^{10}\text{B}$, $d + ^{10}\text{B}$ is a reaction channel. For us, both of these pairs will constitute reaction channels.

in our development, since particle labelling is specified when H_i is specified. In this nomenclature, a reaction channel r_m may encompass a number of m -body arrangement channels distinguished from each other by interchange of particle labels between differing subsystems in the channel.

We illustrate these notions with the following set of nuclear reactions:

Each of (25a) - (25f) defines a reaction channel r_m , since each grouping of particles into nuclei is observable, independent of which labelled particles are in the particular nuclei. There are three r_2 channels, two r_3 channels, and one r_5 channel. (Other r_m may be energetically allowed, but the above group suffices to illustrate the basic ideas.) By assumption, each of the subsystems in any of the r_m above is in a particle-stable (bound) state. Because of this and the assumption of time reversal invariance, any of the channels to the right of the arrows can serve as an initial state for producing, among other r_m , the r_2 , $p + {}^{11}\text{B}$ channel, as an observed final channel.

We have already stated that the observable states in any channel are particle stable. Therefore, if the energy were sufficient to put one of the two ${}^6\text{Li}$ nuclei of (25c) into a continuum (breakup) state, so that e.g.,

${}^6\text{Li} \rightarrow \alpha + d$ asymptotically, then the reaction channel in this case would be (25d) rather than (25c). This result follows from the assumption that observations are made at sufficiently long times after the collision occurs, that all particle unstable states have decayed. De-excitation by electromagnetic radiation is a weak perturbation not included in our formalism by assumption B.

These examples should define clearly the method for determining which configurations belong to specific r_m channels. However, it should also be clear that each of the reaction channels can contain a number of different arrangement channels, since interchange of a pair of identical particle labels between two subsystems in an r_m does not change the reaction channel but does produce a new arrangement channel. Let $n(r_m)$ be the number of arrangement channels associated with a given r_m (recall that particle identity is dealt with at the end by proper symmetrization). For reaction (25a), $n(p + {}^{11}\text{B})$ is 6 if neutrons and protons are distinguished and is 12 if an isospin notation is used. Similarly $n(d + {}^{10}\text{B})$ of (25b) is 36 or 100 depending on whether or not neutrons and protons are distinguished. The determination of $n(r_m)$ is a counting problem: how to distribute n particles over m subsystems each containing n_m particles, some or all of which may be identical to each other.

Our aim has been to determine the total number of internal bound states making up the $\{|\Phi_{nq}(E_{nq}^i, i)\rangle\}$. This number is denoted B , and is equal to the total number of thresholds (unitarity cuts) in the n -body problem. To find B , we proceed as follows. Let $b_j(r_m)$ be the number of bound states in the j th subsystem of r_m ; $b_j(r_m)$ is evidently a number that can be determined experimentally. The total number of bound states in r_m is $b(r_m)$ given by

$$b(r_m) = \prod_{j=1}^m b_j(r_m). \quad (26)$$

This is also the total number of bound states in any one of the arrangement channels associated with this particular r_m . Since there are $n(r_m)$ such arrangement channels, the total number of bound states in the whole set of arrangement channels associated with r_m is $B(r_m)$ given by

$$B(r_m) = n(r_m) \prod_{j=1}^m b_j(r_m). \quad (27)$$

On summing (27) over all reaction channels r_m we get the total number of bound states B :

$$B = \sum_{r_m} B(r_m), \quad (28)$$

which is the desired result. The quantity B is the number of thresholds and thus the total number of cuts in the complex energy plane whose contributions must be evaluated when determining DG or DT'_{jk} .

Before making use of these results, we reconsider the argument leading from eq. (26) to eq. (27), which concerns identity of particles. In principle, there is no way to distinguish identical particles, and labelling is merely a convenient accounting device. Some account of this identity can be included by using properly symmetrized internal states for the $\{|\Phi_{n_q}(E_{n_q}^i, i)\rangle\}$. The remainder occurs by eventually forming the appropriate linear combinations of amplitudes for the process under consideration. Because masses of identical particles are identical and energy levels of identical nuclei are identical, there may be fewer bound states than B , and therefore fewer thresholds and their associated right hand cuts that contribute to DG . We ignore this in the present paper, and assume when necessary that small additional masses have been added to each identical particle mass to help distinguish one particle

from another. These additional (real) masses are set equal to zero at the end of our analysis. The forming of appropriate linear combinations of the transition operators in the case of identical particles will be seen to reduce the apparent many arrangement channel problem to a problem of fewer arrangement channels, the final number being consistent with the number of reaction channels r_m . This is discussed via an example in the following paper.

We now return to the problem of specifying the states $|\Psi_\alpha\rangle$ that enter eq. (22). Each $|\Psi_\alpha\rangle$ is to be generated from one of the $|\Phi_{nq}(E'_{nq}, i)\rangle$; choosing a labelling similar to that for the channel state we have¹³⁾

$$|\Psi_{nq}^\pm(E'_{nq}, i)\rangle = [1 + G(E'_{nq} + i\epsilon) V_i] |\Phi_{nq}(E'_{nq}, i)\rangle. \quad (29)$$

The totality of such states, $\{|\Psi_{nq}^\pm(E'_{nq}, i)\rangle\}$, is the set to be used in eq. (22). Only those states for which $E'_{nq} = E$ will contribute. With this result, we are ready to derive the discontinuity equation.

4. Derivations of the Discontinuity Equation

4.1 Development based on $\text{Im } G$

We first use eq. (22). The sum on α in that equation is to be reinterpreted as follows:

$$\sum_{\alpha} d\alpha \rightarrow \sum_{i,n} \int [d^3 q]_i, \quad (30)$$

where the double sum is over arrangement channel indices (i) and the bound states in channel i (n), while $\int [d^3 q]_i$ means an integral over all relative motion wave vectors in channel i . The number of such vector integration variables in an n -body channel is $n - 1$, since we work in the barycentric coordinate system.

Using (30) in (22) and then replacing the $\{|\Psi_{\alpha}\rangle\}$ by the $\{|\Psi_{nq}^+(E_{nq}^i, i)\rangle\}$, eq. (22) becomes

$$\begin{aligned} \text{Im } T'_{jk}(E+i0) = & -\pi \sum_{i,n} \int [d^3 q]_i V_j |\Psi_{nq}^+(E_{nq}^i, i)\rangle \delta(E - E_{nq}^i) \\ & \times \langle \Psi_{nq}^+(E_{nq}^i, i) | V_k. \end{aligned} \quad (31)$$

We may now make use of the results^{8,13)}

$$V_j |\Psi_{nq}^+(E_{nq}^i, i)\rangle = T'_{ji}(E_{nq}^i + i0) |\Phi_{nq}^i(E_{nq}^i, i)\rangle \quad (32)$$

and

$$\langle \Psi_{nq}^+(E_{nq}^i, i) | V_k = \langle \Phi_{nq}^i(E_{nq}^i, i) | \hat{T}'_{ik}(E_{nq}^i + i0) \quad (33)$$

to re-express (31) as

$$\begin{aligned} \text{Im } T'_{jk}(E+i0) = & -\pi \sum_{i,n} \int [d^3q]_i T'_{ji}(E_{nq}^i+i0) \\ & \times |\Phi_{nq}(E_{nq}^i, i)\rangle \delta(E-E_{nq}^i) \\ & \times \langle \Phi_{nq}(E_{nq}^i, i) | \hat{T}'_{ik}(E_{nq}^i-i0). \end{aligned} \quad (34)$$

The states $|\Phi_{nq}(E_{nq}^i, i)\rangle$ contain only bound internal states in channel i , in accordance with our definitions of an arrangement channel and the way in which the $|\Psi_n\rangle$ are either generated from or lead to the asymptotically observable channel states. In detail, this means that if $|\varphi_n(E_n(i), i)\rangle$ is the n th internal bound state in channel i , and $|\chi_q(E_q(i), i)\rangle$ is the relative motion state, then

$$|\Phi_{nq}(E_{nq}^i, i)\rangle = |\varphi_n(E_n(i), i)\rangle |\chi_q(E_q(i), i)\rangle. \quad (35)$$

Writing H_i as

$$H_i = h_i + K_i, \quad (36)$$

where h_i describes the internal states and K_i the relative motion, we have

$$h_i |\varphi_n(E_n(i), i)\rangle = E_n(i) |\varphi_n(E_n(i), i)\rangle \quad (37)$$

and

$$K_i |\chi_q(E_q(i), i)\rangle = E_q(i) |\chi_q(E_q(i), i)\rangle. \quad (38)$$

We now form the set of projection operators onto the bound internal states of channel i :

$$\begin{aligned} P(i) &= \sum_n P_n(i) \\ &= \sum_n |\varphi_n(E_n(i), i)\rangle \langle \varphi_n(E_n(i), i)|, \end{aligned} \quad (39)$$

so that

$$\delta(E-H_i) P(i) = \sum_n \int [d^3q]_i | \Phi_{nq}(E_{nq}^i, i) \rangle \times \delta(E-E_{nq}^i) \langle \Phi_{nq}(E_{nq}^i, i) |, \quad (40)$$

where $P(i)$ restricts the eigenstates of h_i but not those of K_1 . We note here that for channel 0, $H_0 = K_0$, the sum of all kinetic energy operators, and therefore

$$P(0) = 1. \quad (41)$$

Substituting (40) into (34) then gives the discontinuity of T'_{jk} in operator form:

$$I_m T'_{jk}(E+i0) = -\pi \sum_i T'_{ji}(E+i0) \delta(E-H_i) \times P(i) \hat{T}'_{ik}(E-i0), \quad (42)$$

where we have written $T'_{ji}(E+i0)$ and $\hat{T}'_{ik}(E-i0)$ since the energy conserving delta function $\delta(E-H_i)$ will allow us to replace E in these operators by E_{nq}^i , as in eq. (34).

The operators T'_{jk} and $\hat{T}'_{jk}$ are elements of a matrix of operators that we denote T' and $\hat{T}'$, respectively. In matrix form, eq. (42) reads

$$I_m T'(E+i0) = -\pi T'(E+i0) \tilde{\Delta}(E) \hat{T}'(E-i0), \quad (43)$$

where

$$\tilde{\Delta}_{ij}(E) = \delta_{ij} \delta(E-H_i) P(i). \quad (44)$$

Equations (42) and (43) are the desired result, and extend to the many-body case the analogous result of Lovelace⁸⁾ for the three-body problem. Thus, the quantity $\tilde{\Delta}$ is the precise analog of Lovelace's on-shell operator⁸⁾ Δ (we use $\tilde{\Delta}$ rather than Δ since in our previous work^{1,2)}, Δ was a matrix with elements $\Delta_{ij}(E) = \delta_{ij} \delta(E - H_i)$; i.e. $\tilde{\Delta}_{ij} = \Delta_{ij} P(i)$). In fact, (42) reduces to Lovelace's equation for the discontinuity of his operator U_{jk}^+ when the number of channels N is equal to 3. We remark here that N is not equal to the number of bound states B [eq. (28)] except coincidentally: the usual circumstance will be one where $B \gg N$.

In the next subsection, we shall rederive eqs. (42) and (43), by examining the discontinuity of G (and then of T). However, before doing so, we point out an extremely important implication of these equations, one that provides a further explanation of why certain of the $e^- + H$ calculations referred to above could lead to non-unitary matrix elements of the transition operator. The calculations in question used an approximation to T'_{jk} , obtained by truncating the basic set: only the $1s$, hydrogenic ground state was used in expanding the relevant channel Green function, rather than the complete set of hydrogenic states⁵⁾. But, the imaginary part of T'_{jk} will be correctly given by the product on the right hand side of (42) only when T'_{ji} and $\hat{T}'_{ik}$ are calculated exactly, for only then are on-shell matrix elements of T'_{jk} and $\hat{T}'_{jk}$ equal. Approximations to T'_{jk} and $\hat{T}'_{jk}$ are equal on-shell only by accident. In the case of $e^- + H$ scattering, where we have identical electrons, the two channels are degenerate and the problem, below the $n = 2$ threshold, is a pure one-channel problem where the S -wave amplitude (matrix element of the transition operator) should have the form $\exp(i\delta) \sin \delta$. The unitarity relation will in this case still be given by an equation like (42), but with symmetrized

operators J' and $\hat{J}'$ where $J' = T_{11}' \pm P_{21} T_{21}'$ and $\hat{J}' = \hat{T}_{11}' \pm P_{21} \hat{T}_{21}'$ with P_{21} a two-particle transposition operator. (See the following paper for details.) In order for the imaginary part of the matrix element of $J'(E + i0)$ to be $\sin^2 \delta$ (in conformity with the amplitude being $\exp(i\delta) \sin \delta$), both $J'(E + i0)$ and $\hat{J}'(E + i0)$ must be given by $\exp(i\delta) \sin \delta$. But, in an approximate calculation, J' and $\hat{J}'$ are equal only by coincidence, just as with T_{jk}' and $\hat{T}_{jk}'$, and hence matrix elements of J' and $\hat{J}'$ cannot both be given by $\exp(i\delta) \sin \delta$, except by coincidence. Only in a theory of multi-channel scattering in which one kind of operator occurs exclusively in the unitarity relation will approximate calculations yield unitary amplitudes (if all open channels are included in the calculation). This is precisely what was found in the numerical calculations⁵⁾; the above arguments clearly show why such a set of results should not be surprising.

4.2 Development based on DG

In section 2 it was shown that $DG = 2i \operatorname{Im} G$. The title of this subsection, however, refers not to this equality, but to the method of counting the contributions to DG from each of the cuts in the complex energy plane. Our purpose is not merely to verify the results of the preceding subsection, but to provide the necessary background for deriving the unitarity (discontinuity) relation obeyed by the new T operators¹⁾ T_{jk} , as discussed in the following paper.

This particular way of proceeding is the method introduced by Lovelace⁸⁾. In particular, we assume that each cut can be isolated from all others by the rotation method⁸⁾, and we refer to Lovelace's original work for details.

The resolvent $G(Z)$ is analytic everywhere in the complex energy plane except on the real axis, where there are poles at $\mathcal{E}_n$ corresponding to the n-body bound states, and cuts extending from the threshold various energies $\mathcal{E}_n(i)$ to $+\infty$ as shown in Fig. 1. By assumption C, the lowest threshold energy $\mathcal{E}^*$ is larger than the greatest bound state energy $\mathcal{E}^*$. The total number of thresholds, and thus the number of cuts on the real axis is given by B of eq. (28). These various cuts arise from the opening of the various inelastic scattering channels in each of the arrangement channels i; only one cut occurs in the free-particle channel ($i = 0$).

For calculational purposes, the domain of analyticity of $G(Z)$ can be regarded in one of two ways: either as a single Riemann sheet with B overlapping cuts on the real axis or as a multi-sheeted surface containing B sheets; in each case small circular contours are drawn about the poles, and the interior regions of these circles are excluded from the domain of analyticity. We shall use the former viewpoint, corresponding to Fig. 1. In order to evaluate DG, we must subtract $G(E - i\epsilon)$ from $G(E + i\epsilon)$, which essentially means going

from point A to point B in Fig. 2 following the dotted path. The energy E is here assumed to be larger than the maximum threshold energy, so that all of the B cuts are traversed in going from A to B. Had we considered the domain of analyticity of $G(Z)$ to be a multisheeted Riemann surface, the discontinuity would essentially be the difference of $G(E + i\epsilon)$ evaluated on the upper half plane of the uppermost sheet and $G(E - i\epsilon)$ evaluated on the lower half plane of the lowest sheet, and on passing from the uppermost to the lowest sheet, there would be a contribution from each sheet, just as there is in the preceding a contribution from each cut.

Since each cut corresponds to a threshold and the number of thresholds equals the total number of bound states B, we may write

$$D G(E + i\epsilon) = \sum_{i,n} D_{in} G(E + i\epsilon), \quad (44)$$

where $D_{in} G(E + i\epsilon)$ means the contribution to the discontinuity from the cut starting at the nth bound state in channel i.

To evaluate $D_{in} G(E + i\epsilon)$, we follow the methods introduced by Lovelace for the three-body problem.⁸⁾ From the definition (4), it follows that

$$G(Z) - G(Z') = (Z' - Z) G(Z) G(Z'), \quad (45)$$

while use of (6) and (7) in (45) lead to

$$G(Z) - G(Z') = [1 + G(Z) V_i] \{ (Z' - Z) G_i(Z) G_i(Z') \} [1 + V_i G(Z')], \quad (46)$$

where i is an arbitrary arrangement channel label. Since eq. (45) holds with G replaced by G_i , (46) may be written as

$$G(z) - G(z') = [1 + G(z)V_i] \{G(z) - G(z')\} [1 + V_i G(z')]. \quad (47)$$

Finally setting $z = E + i\epsilon$ and $z' = E - i\epsilon$, we get the contribution to the discontinuity of $G(E + i\epsilon)$ from the discontinuity of $G_1(E + i\epsilon)$:

$$\mathcal{D}_i G(E + i\epsilon) = [1 + G(E + i\epsilon)V_i] \mathcal{D}_i G_1(E + i\epsilon) [1 + V_i G(E - i\epsilon)]. \quad (48)$$

Now the discontinuity of $G_1(E + i\epsilon)$ is made up of the contributions from all the cuts in channel 1. In detail, we have

$$\begin{aligned} \mathcal{D}_i G_1(E + i\epsilon) = & \sum_n |\Phi_n(E_n(i), i)\rangle \langle \Phi_n(E_n(i), i)| \\ & \times [(E + i\epsilon - E_n(i) - K_i)^{-1} - (E - i\epsilon - E_n(i) - K_i)^{-1}] \\ & + \text{continuum state contributions.} \end{aligned} \quad (49)$$

However, we have already noted that the continuum states contribute to various other channels, each having at least one more free particle than in 1. This follows from the fact that continuum states are either generated by or lead to observable states having two or more particles. Thus, we shall not count any continuum state contributions to (49) as their effect will be included when we take all channels into account, and we must count the contribution from each cut only once. [The n free-particle states of course give one contribution when $i = 0$.] The continuous line of poles (i.e., the cut) in (49) due to each bound state is obvious in limit $\epsilon \rightarrow 0$.

It thus follows that (49) may be rewritten as

$$D G_i(E+i\epsilon) = \sum_n D_n G_i(E+i\epsilon) \quad (50)$$

where

$$D_n G_i(E+i\epsilon) = |\varphi_n(E_n(i); i)\rangle \langle \varphi_n(E_n(i); i)| \\ \times \left\{ -2i\epsilon / [(E-E_n(i)-K_i)^2 + \epsilon^2] \right\}. \quad (51)$$

Equation (51) may be rewritten with the aid of the projection operator $P_n(i)$ as

$$D_n G_i(E+i\epsilon) = -2i P_n(i) \frac{\epsilon}{(E-H_i)^2 + \epsilon^2} \quad (52)$$

Substituting (52) into (50) and then into (48) gives

$$D_i G(E+i\epsilon) = -2i \left[1 + G(E+i\epsilon) V_i \right] \frac{\sum_n P_n(i) \epsilon}{(E-H_i)^2 + \epsilon^2} \left[1 + V_i G(E-i\epsilon) \right] \\ = -2i \left[1 + G(E+i\epsilon) V_i \right] \frac{P(i) \epsilon}{(E-H_i)^2 + \epsilon^2} \left[1 + V_i G(E-i\epsilon) \right], \quad (53)$$

where the second line follows from eq. (39).

Equation (53) is the contribution from the cuts in channel i . Summing over all channels, substituting into eq. (17) and using eq. (16) gives

$$Im T'_{jk}(E+i\epsilon) = - \sum_i T'_{ji}(E+i\epsilon) \frac{P(i) \epsilon}{(E-H_i)^2 + \epsilon^2} \hat{T}'_{ik}(E-i\epsilon), \quad (54)$$

which is the general discontinuity relation. We are specifically interested in the boundary value $E + i0$. Noting that

$$\lim_{\epsilon \rightarrow 0^+} \frac{\epsilon}{(E-H_i)^2 + \epsilon^2} = \pi \delta(E-H_i), \quad (55)$$

we find for the physical value

$$\text{Im } T'_{jk}(E+i0) = -\pi \sum_i T'_{ji}(E+i0) P(i) \delta(E-H_i) \hat{T}'_{ik}(E-i0)_{42}$$

which is of course the result derived earlier by considering $\text{Im } G(E + i0)$. The purpose of the present derivation has been to demonstrate the validity of this particular approach, and in particular, the propriety of neglecting continuum (breakup) states in all channels but $i = 0$. In the succeeding article, it is only this method that we have available; the present evaluation assures us that it is valid.

5. Discussion

As pointed out at the end of section 4.1, the present development not only explains why the earlier $e^- + H$ calculations did not yield unitary amplitudes, it clearly establishes that one can expect unitary results from approximate calculations based on the T'_{jk} only as a coincidence. The need to work with a theory involving only one kind of operator rather than two, as in the present "post-prior" formalism, is obvious. The Faddeev¹⁵⁾ and Alt-Grassberger-Sandhas⁹⁾ approaches to the three-body problem do involve only one set of operators, and so approximate calculations can lead to unitary results in principle (although the technical problems^{3,4)} are complicated).

It is interesting to note that in those latter methods, only the free Green function G_0 appears; the cuts arising from the bound state thresholds enter via the two-body t matrices. A further and important point concerning the three-body problem is the evaluation of the contribution to the discontinuity arising from breakup states, or two-body scattering states with the third particle free. Lovelace⁸⁾ notes that this leads to a more complicated expression for the result obtained by considering the contribution from the three-particle cut, contained in G_0 . In fact, the breakup, or continuum, state contribution is identical to that arising from G_0 and not simply a more complicated expression. This bears out completely our procedure of neglecting the continuum contributions in eq. (49) since they will be included in the contributions from channels with more (asymptotically) free particles than are found in channel 1.

Equation (49) is also suggestive of the following: The boundary value of $\text{Im } G(Z)$, i.e. $\text{Im } G(E + i0)$, is just $-\pi \delta(E-H)$, but the boundary value of $\text{Im } G_1(Z)$ is $-\pi \delta(E-H_1) P(i)$. That is, while the boundary value of $\text{Im } G(Z)$

on the real axis is precisely what one expects, it is not true that

$\text{Im } G_i(E+i0) = -\pi \delta(E-H_i)$. The reason for this is the non-occurrence in G_i of the contributions from the threshold cuts in all channels but $i = 0$.

Thus, while eqs. (6) and (7) hold for Z defined in the domain of analyticity (the cut plane minus the bound state poles), one must approach the real axis with great care, as that is the boundary region where $G(Z)$ is singular. At this stage, these remarks are more speculative than substantive, but we shall see in the following paper that the coupled-channel formalism introduced earlier^{1,2)} is re-expressed in terms of the $\tilde{G}_1(E+i0) = G_1(E+i0)P(1)$ and not $G_1(E+i0)$ alone. This result follows from considerations of unitarity quite similar to those of the preceding sections.

Let us finally consider methods whereby the (many-body) T'_{jk} or $\hat{T}'_{jk}$ could be calculated. Single channel equations such as

$$T'_{jk}(Z) = V_j + T_{jk} G_k(Z) V_k$$

or pairs of coupled equations such as

$$T'_{jk}(Z) = V_j + V_j G_k(Z) T'_{kk}(Z)$$

and

$$T'_{kk}(Z) = V_k + V_k G_k(Z) T'_{kk}(Z)$$

are neither connected nor, because they lead to the unitarity relation (42), are they likely to lead to approximate calculations being unitary. Hence they are not satisfactory.

Connected, coupled equations (i.e., one whose iterated kernels are connected) such as those of Weyers¹⁰⁾ or of Tobocean¹⁶⁾ (based on the method discussed in the next paper, see also Refs. 1 and 2) are also unsatisfactory, because they involve the T'_{jk} , which satisfies the unitarity relation (42), and which as we have seen will in general not lead to approximate results being unitary. On the

other hand those methods for many-body scattering theory based on extensions of the methods of Faddeev¹⁵⁾ or AGS⁹⁾, such as the ones proposed by Yakubovskii¹⁷⁾, Bencze¹⁸⁾ or Redish¹⁹⁾ are not handicapped in this way and therefore are indeed satisfactory starting points for many-body calculations. If, however, one wishes to introduce unitary approximations into these latter schemes via a K matrix, then the same kinds of problems dealt with by Kowalski³⁾ and Cahill⁴⁾ will occur. Their solution will presumably be even more involved than in the three-body case^{3,4)}. On the other hand, the method we have introduced recently^{1,2)} leads to a simple unitarity expression involving only one kind of operator and also allows unitary approximations to be introduced very simply. In the next paper, we carry out an analysis for these equations similar to that of the present paper, obtaining the important modifications noted in the introduction and above.

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Figure Captions

1. The singularities of $G(Z)$ in the complex energy plane. The points labelled x are the bound state poles, whose largest value is $E^0 > E^1 > E^2$, while the heavy lines on the right depict the cuts, each originating at a threshold energy $E_n(1)$. The lowest threshold is $E^0 < E^1 < E^2$, etc. The zero of energy is arbitrarily chosen, and, since we assume distinguishable particles, no two threshold energies are assumed to be equal.
2. The points $E \pm i\epsilon$ in the complex energy plane and the path joining them. The path crosses the real axis at a point between E^0 and E^1 .

FIG. 1

FIG. 2