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Three-cluster states in reaction theory*

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In recent work it was shown how a rigorous subsidiary minimum principle of the Rayleigh-Ritz type could be used as an aid in the construction of the closed-channel part of the scattering wave function, thereby making available a potentially powerful new tool in the variational approach to multiparticle scattering problems. The earlier discussion, which was restricted to scattering below the threshold for target breakup, is generalized here to the case where both two-body and three-body channels are open. The scattering problem is formally reduced to an equivalent three-body problem. Effective two-body and three-body potentials are defined explicitly (without the use of projection operators) and integral equations of the Faddeev type are derived. This analysis, which suggests a variety of cluster approximations, is used here as the basis for a decomposition of the wave function into an open-channel part, which contains the two-body and three-body outgoing scattered waves, and a decaying closed-channel part. The closed-channel part is shown to satisfy a minimum principle whose rigor can be maintained even when the target bound-state wave functions are imprecisely known. A calculational procedure which combines this minimum principle with the Kohn variational construction of the scattering amplitude is described.

[NUCLEAR REACTIONS Scattering theory. Effective three-body formulation. Derivation of extremum principle for the wave function.]

I. INTRODUCTION

A considerable effort has been devoted in recent years toward the development of reliable approximation techniques for three-body scattering problems,[1] and a good deal of progess has been made. There are a few "pure" three-body systems in atomic and nuclear physics (such as the electron-hydrogen and nucleon-deuteron systems) which have served as testing grounds for calculational methods. Much of the motivation for these studies lies in the recognition that for a wide class of multiparticle systems the model of three interacting clusters gives a useful first approximation. The deuteron-α particle and electron-lithium systems provide examples in which the picture of two particles and a tightly bound core is quite a reasonable one, particularly for scattering energies below the threshold for breakup of the core.[2] Models of nuclear reactions based on core excitation mechanisms have come under study recently.[3] In a more general sense, apart from any particular model of the scattering process, it is clear that the effects of three-cluster states must be properly accounted for in a complete theory of reactions. For example, unless such states are built into the approximation scheme explicitly there seems little chance that the requirements of flux conservation will be satisfied in the energy range where three-cluster states can propagate asymptotically. If the explicit introduction of three-cluster states is to be carried out as part of a systematic approach to the scattering problem a precise, unambiguous definition of the effective interactions among the clusters must be provided. This allows for a well-defined procedure for determining corrections to the tight-binding (or equivalent three-body) approximation.

A systematic analysis of three-cluster interactions can be carried out in a variety of ways.[4] The approach adopted here arises as a natural extension of an earlier analysis of effective two-body scattering problems.[5,6] The usefulness of the effective two-body (or optical) potential method in the study of low-energy reactions has long been recognized.[7] It provides for a unified description of resonance reactions and, by means of the Hermiticity condition on the effective potential, allows for the requirements of unitarity. There is some freedom in the manner in which the effective potential is defined. It was shown[5,6] that a particular choice could be made which had the merit of allowing for the use of rather powerful Rayleigh-Ritz bound-state techniques as a computational aid. This is important since the construction of the effective potential is in general a complicated multiparticle dynamical problem. The method has two significant features, both of which are maintained in the generalization developed in the present work. Firstly, the subsidiary Rayleigh-Ritz-

type minimum principle, whose applicability depends on a separation of the wave function into open- and closed-channel parts, can be maintained rigorously even when (as is usually the case) the target wave function is imprecisely known. Secondly, the above-mentioned channel separation can be carried out effectively without the introduction of Feshbach projection operators.[7] This is significant since the projection operators are difficult to construct in practice when rearrangement processes can occur. A brief outline of this earlier work is given in Sec. II below. That discussion serves as a point of departure for the generalizations taken up subsequently.

When rearrangement processes (such as deuteron stripping) are considered, or when the effects of three-body open channels are significant, it is more appropriate to analyze the system in terms of effective three-body (rather than two-body) equations; this is worked out in Sec. III. It will be clear from the derivation that systematic generalizations are possible, in which effective n-body equations are introduced; they would be appropriate at still higher scattering energies. However, we shall for simplicity restrict our present considerations to the energy domain below the threshold for breakup into four or more bound clusters. The effective three-body equations are of the form given by Newton[8]; they represent the modification of the original three-body Faddeev equations[9] which is appropriate when both two-body and three-body forces are present. The two-body effective potentials which appear here have been introduced earlier.[5] The three-body effective potential is of course a new feature. These effective interactions are here defined explicitly in terms of the original multiparticle Hamiltonian.

The Faddeev-Newton equations are of interest in their own right. They may serve, for example, as the basis for unitary approximation schemes in analogy with the use of the usual three-body Faddeev equations for that purpose.[1] For our present purposes they serve as a formal tool in the analysis of the structure of the wave function. This analysis leads to the specific decomposition into open- and closed-channel components developed in Sec. IV. The decomposition provides the basis for a variational formulation of the problem in configuration space. We have previously described[6] how a subsidiary minimum principle for the closed-channel component can be used in conjunction with the Kohn variational principle for the scattering amplitude to give a tractable calculational procedure. The generalization of that procedure applicable to reactions above the three-body breakup threshold is described in Sec. V. A summary of our results appears in Sec. VI.

II. PRELIMINARIES: TWO-CLUSTER STATES

In this section we shall consider the scattering of a structureless particle by a composite system in its ground state. The target ground-state wave function χ satisfies

$$h|\chi\rangle = \epsilon|\chi\rangle . \tag{2.1}$$

The Schrödinger equation for the scattering process is written as

$$(h+k+v)|\psi\rangle = e|\psi\rangle . \tag{2.2}$$

Here k is the kinetic energy operator for the relative motion of the projectile and the center of mass of the target, while v represents the interaction potential. To simplify the present discussion the scattering energy e is assumed to lie below the threshold for the onset of rearrangement processes and for target excitation. We now introduce the modified target Hamiltonian

$$\hat{h} \equiv h - \epsilon|\chi\rangle\langle\chi| , \tag{2.3}$$

whose spectrum differs from the spectrum of h only in that the ground-state level has been displaced upward by an amount ϵ.[10] Equation (2.2) can evidently be rewritten as

$$(\hat{h}+k+v-e)|\psi\rangle = -\epsilon|\chi\rangle\langle\chi|\psi\rangle . \tag{2.4}$$

The solution can be represented formally in terms of the resolvent

$$\hat{g}(e) = (e-\hat{h}-k-v)^{-1} \tag{2.5}$$

as

$$|\psi\rangle = \hat{g}(e)\epsilon|\chi\rangle\langle\chi|\psi\rangle . \tag{2.6}$$

A decomposition of the wave function into open- and closed-channel components can be obtained directly from Eq. (2.6). We introduce the resolvent equation

$$\hat{g} = \hat{g}_0 + \hat{g}v\hat{g}_0 , \tag{2.7}$$

where

$$\hat{g}_0(e) = (e-\hat{h}-k)^{-1} . \tag{2.8}$$

It follows directly from the eigenfunction expansion of $\hat{g}_0(e)$ that

$$\hat{g}_0(e)|\chi\rangle = |\chi\rangle(e-k)^{-1} . \tag{2.9}$$

Hence, by combining Eqs. (2.6) and (2.7) and defining the effective single-particle wave function f according to

$$|f\rangle = \frac{\epsilon}{e-k}\langle\chi|\psi\rangle , \tag{2.10}$$

we find that

$$|\psi\rangle = (1+\hat{g}v)|\chi\rangle|f\rangle . \tag{2.11}$$

This representation is of the form

$$|\psi\rangle = |\chi f\rangle + |m\rangle , \tag{2.12}$$

where we have written $|\chi\rangle|f\rangle = |\chi f\rangle$ and have defined

$$|m\rangle = \hat{g} v |\chi f\rangle . \tag{2.13}$$

Now $\hat{g}(e)$ is a bounded operator since, by assumption, e lies below the level of the first excited state of h and hence below the lowest energy level of $\hat{h}$. Then, since $v|\chi f\rangle$ is a vector of finite length the same is true for $|m\rangle$; that is, the configuration-space representation of $|m\rangle$ is a function which decays asymptotically. We may therefore identify $|m\rangle$ in Eq. (2.12) as the closed-channel component of the scattering wave function, and $|\chi f\rangle$ as the open-channel component. This decomposition is of course not unique. However, as discussed in detail in Ref. 6 (see also Sec. V below), it has the merit of allowing for the use of a subsidiary minimum principle in determining accurate approximations to $|m\rangle$. Significantly, the rigor of the minimum principle can be maintained even when the target function χ is imprecisely known.[5,6] A variational procedure for finding approximations to the single-particle wave function f, which may be used in conjunction with the minimum principle for the function m, was outlined in Ref. 6. A knowledge of the exact form of the defining equation for f is useful in this connection. To determine this equation we make use of Eq. (2.11) and the adjoint of (2.7) to write

$$\langle\chi|\psi\rangle = |f\rangle + \langle\chi|[\hat{g}_0 + \hat{g}_0 v \hat{g}] v |\chi f\rangle . \tag{2.14}$$

This may be rewritten, with the aid of Eqs. (2.9) and (2.10), as

$$\left[\frac{e-k}{\epsilon} - 1\right] |f\rangle = \frac{1}{e-k}\langle\chi|v + v\hat{g}v|\chi f\rangle . \tag{2.15}$$

If we rearrange Eq. (2.15) slightly and define the effective potential

$$\nu(e) = \langle\chi|v + v\hat{g}v|\chi\rangle , \tag{2.16}$$

we may put Eq. (2.15) in the form

$$(e - k - \epsilon)|f\rangle = \frac{\epsilon}{e-k}\nu(e)|f\rangle . \tag{2.17}$$

Equivalently, we have the integral equation[11]

$$|f\rangle = |\vec{p}\rangle + \frac{1}{e-k-\epsilon}\frac{\epsilon}{e-k}\nu(e)|f\rangle , \tag{2.18}$$

where $|\vec{p}\rangle$ is the momentum eigenstate representing the relative motion in the initial state. The eigenvalue problem for bound states can be formulated in terms of the homogeneous version of Eq. (2.18), a result which will be of use to us later on.

Much of the above analysis can be reformulated in the language of Feshbach projection operators. When rearrangement processes are possible (Pauli exchange is of course always possible when identical particles are present) the required projection operators are difficult to construct. The approach outlined above, on the other hand, is easily generalized to account for rearrangement and target excitation processes. [The generalization of Eq. (2.3), providing the modified Hamiltonian appropriate in such cases, appears in Ref. 5]. However, for scattering energies high enough so that three-cluster channels are open, a substantial modification is required in order to retain the subsidiary minimum principle for the closed-channel component of the wave function. The necessary generalizations will be worked out in the following three sections.

III. EQUIVALENT THREE-BODY FORMULATION

A. Statement of the problem

We wish to generalize the discussion of Sec. II to the case where the scattering process can lead to three-body final states. For definiteness we assume that one of the bodies is a bound cluster C while the other two are neutral structureless particles, labeled 1 and 2, which are distinguishable from each other and the constituents of C. The more general case, where all three bodies are composite, and where Pauli exchange processes are accounted for, can be treated by similar methods. To account properly for long-ranged Coulomb effects in three-body channels is a far more difficult task.[12]

The Hamiltonian for the system is written as

$$H = h + K + V . \tag{3.1}$$

Here K is the three-body kinetic energy operator associated with the relative motion of particles 1, 2, and the center of mass of C; V is of the form

$$V = v_1 + v_2 + v_3 . \tag{3.2}$$

We have represented the interaction between particles 1 and 2 as v_3, while v_i, $i = 1, 2$, represents the total interaction potential between particle i and the constituents of C. To complete the definition of H, we identify h in Eq. (3.1) as the Hamiltonian of the cluster C in its own center-of-mass frame. The ground state of C is defined by the eigenvalue equation (2.1). We assume that bound states exist for the subsystems (1 2), (1 C), and (2 C); the ground states are defined by the equations (appropriate in each case to the center of mass of the subsystem)

$$(k_3 + v_3)|\phi_3\rangle = \epsilon_3|\phi_3\rangle , \quad \text{subsystem (1 2)} ; \tag{3.3a}$$

$$(h+k_i+v_i)|\phi_i\rangle=\epsilon_i|\phi_i\rangle\,, \quad \text{subsystem } (iC)\,, \quad i=1,2\,. \tag{3.3b}$$

For simplicity we ignore the possibility of additional subsystem bound states, thus limiting the number of open channels which need be considered. Multichannel generalizations can easily be worked out (indeed, as mentioned earlier, such generalizations are required if Pauli exchange processes are to be properly accounted for) but their inclusion at this point would add an inessential complication. As it is, we deal with four open channels, or equivalently, with four different initial (or final) states which must be considered. Thus, the initial state for channel 1 is given by

$$|\Phi_1\rangle=|\phi_1\vec{p}_1\rangle\,, \tag{3.4}$$

where $|\vec{p}_1\rangle$ is a momentum eigenstate for the relative motion of the center of mass of subsystem $(1C)$ and particle 2. It satisfies

$$K_1|\vec{p}_1\rangle=(E-\epsilon_1)|\vec{p}_1\rangle\,, \tag{3.5}$$

where K_1 is the kinetic-energy operator associated with the relative motion and E is the total energy. The initial state Φ_2 for channel 2 is analogously defined. In channel 3 subsystems $(1\,2)$ and C are both bound. The initial state is

$$|\Phi_3\rangle=|\chi\phi_3\vec{p}_3\rangle\,, \tag{3.6}$$

where $|\vec{p}_3\rangle$, the momentum eigenstate for the relative motion of the two bound subsystems, satisfies

$$K_3|\vec{p}_3\rangle=(E-\epsilon-\epsilon_3)|\vec{p}_3\rangle\,. \tag{3.7}$$

The initial state associated with the three-cluster channel 0 is given by

$$|\Phi_0\rangle=|\chi\vec{p}_0\rangle\,, \tag{3.8}$$

with

$$K|\vec{p}_0\rangle=(E-\epsilon)|\vec{p}_0\rangle\,. \tag{3.9}$$

The Schrödinger equation for the scattering problem is

$$(H-E)|\Psi_j\rangle=0\,, \quad j=0,\ 1,\ 2,\ \text{or } 3\,. \tag{3.10}$$

The index j specifies the channel which contains the incident wave. The energy E is taken to be low enough so that channels other than the four enumerated above are closed.

B. Effective three-body Faddeev-Newton equations

In analogy with the two-cluster treatment discussed in Sec. II we write the Schrödinger equation (3.10) in the form

$$(\hat{H}-E)|\Psi_j\rangle=-\epsilon|\chi\rangle\langle\chi|\Psi_j\rangle\,, \tag{3.11}$$

with

$$\hat{H}=\hat{h}+K+V\,. \tag{3.12}$$

The solution can be expressed formally as

$$|\Psi_j\rangle=\hat{G}(E)\epsilon|\chi\rangle\langle\chi|\Psi_j\rangle\,, \tag{3.13}$$

where

$$\hat{G}(E)=(E-\hat{H})^{-1}\,. \tag{3.14}$$

We have the resolvent identity

$$\hat{G}=\hat{G}_0+\hat{G}V\hat{G}_0\,, \tag{3.15}$$

with

$$\hat{G}_0(E)=(E-\hat{h}-K)^{-1}\,. \tag{3.16}$$

In analogy with Eq. (2.9) we have

$$\hat{G}_0(E)|\chi\rangle=|\chi\rangle(E-K)^{-1}\,. \tag{3.17}$$

These results may be used to write Eq. (3.13) in the form

$$|\Psi_j\rangle=|\chi\overline{F}_j\rangle+|\overline{M}_j\rangle\,,$$

with

$$|\overline{F}_j\rangle=\frac{\epsilon}{E-K}\langle\chi|\Psi_j\rangle$$

and

$$|\overline{M}_j\rangle=\hat{G}V|\chi\overline{F}_j\rangle\,.$$

While the formal analogy with Eq. (2.12) is clear the argument given below Eq. (2.13) cannot be generalized to show that $\overline{M}_j$ is a square-integrable function. The reason lies in the fact that V is a sum of two-body potentials and is therefore *not* everywhere decaying in configuration space. Hence $V|\chi\overline{F}_j\rangle$ is not represented by a square-integrable function. The argument based on the boundedness of $\hat{G}$ then breaks down. In fact, it is not difficult to verify directly that $\overline{F}_j$ does not contain the complete outgoing-wave part of the wave function; the remainder must be contained in $\overline{M}_j$. The above decomposition fails to provide the desired separation of the wave function into open- and closed-channel parts. To achieve our objective a more careful treatment of the disconnected parts of the interaction is required. In the remainder of this subsection we prepare the way for such a treatment by studying the structure of the effective three-body wave function $\langle\chi|\Psi_j\rangle$. The channel decomposition of Ψ_j is taken up in Sec. IV.

We proceed by projecting both members of Eq. (3.13) onto the state $\langle\chi|$. To evaluate $\langle\chi|\hat{G}$ we use the resolvent identity in the form

$$\hat{G}=\hat{G}_0+\hat{G}_0V\hat{G}\,, \tag{3.18}$$

along with the analog of Eq. (3.17). We then find

$$\langle\chi|\Psi_j\rangle=\frac{\epsilon}{E-K}\langle\chi|\Psi_j\rangle+\frac{1}{E-K}\mathcal{U}(E)\frac{\epsilon}{E-K}\langle\chi|\Psi_j\rangle\,, \tag{3.19}$$

where we have defined the effective potential

$$\mathcal{U}(E) = \langle\chi|\hat{T}(E)|\chi\rangle , \tag{3.20}$$

with

$$\hat{T}(E) = V + V\hat{G}(E)V . \tag{3.21}$$

Equation (3.19) may be rewritten as

$$(E - K - \epsilon)\langle\chi|\Psi_j\rangle = \mathcal{U}\frac{\epsilon}{E-K}\langle\chi|\Psi_j\rangle . \tag{3.22}$$

The effective potential may be expressed as a sum of disconnected and connected parts. This is accomplished by expressing $\hat{T}$ as the solution of

$$\hat{T} = V + V\hat{G}_0\hat{T} . \tag{3.23}$$

These equations can be put in the usual Faddeev form, as shown in Appendix B. For our present purposes it is sufficient to note the representation

$$\hat{T} = \sum_{i=1}^{3}\hat{T}_i + \hat{T}_c , \tag{3.24}$$

where the disconnected parts $\hat{T}_i$ satisfy the integral equations

$$\hat{T}_i = v_i + v_i\hat{G}_0\hat{T}_i , \quad i = 1,2,3 . \tag{3.25}$$

Equation (3.24) serves to define the connected part $\hat{T}_c$. Accordingly, we may expand the effective potential in the form

$$\mathcal{U} = \sum_{i=0}^{3}\mathcal{U}_i , \tag{3.26}$$

with

$$\mathcal{U}_i = \langle\chi|\hat{T}_i|\chi\rangle , \quad i = 1,2,3 , \tag{3.27}$$

and

$$\mathcal{U}_0 = \langle\chi|\hat{T}_c|\chi\rangle . \tag{3.28}$$

The operators $\mathcal{U}_i$, $i = 1,2,3$, are effective pair potentials, while $\mathcal{U}_0$ is a three-body (connected) interaction.

The solutions to Eq. (3.22) may now be put in a form which clearly exhibits their structure. Considering first the case $j = 0$ (three bodies free in the initial state) we write in place of Eq. (3.22) the Lippmann-Schwinger-type integral equation

$$\langle\chi|\Psi_0\rangle = |\vec{p}_0\rangle + \frac{1}{E-\epsilon-K}\mathcal{U}\frac{\epsilon}{E-K}\langle\chi|\Psi_0\rangle . \tag{3.29}$$

The solution is of the form

$$\langle\chi|\Psi_0\rangle = |\vec{p}_0\rangle + \frac{1}{E-\epsilon-K}\mathcal{T}|\vec{p}_0\rangle . \tag{3.30}$$

Here $\mathcal{T}$, the effective three-body scattering operator, is defined by the integral equation

$$\mathcal{T} = \mathcal{U} + \mathcal{U}\mathcal{G}\mathcal{T} , \tag{3.31}$$

with the modified three-body propagator given by[11,13]

$$\mathcal{G} = (E - \epsilon - K)^{-1} - (E - K)^{-1} . \tag{3.32}$$

With the use of standard methods,[8] Eq. (3.31) can be put in Faddeev form, modified by the presence of the three-body potential $\mathcal{U}_0$. Thus, we first define the operators $\mathcal{T}_i$ as the solutions of the integral equations

$$\mathcal{T}_i = \mathcal{U}_i + \mathcal{U}_i\mathcal{G}\mathcal{T}_i , \quad i = 0,1,2,3 . \tag{3.33}$$

Then $\mathcal{T}$ may be represented as

$$\mathcal{T} = \sum_{i=0}^{3}\sum_{j=0}^{3}{}^{i}\mathcal{T}^{j} , \tag{3.34}$$

with the components ${}^{i}\mathcal{T}^{j}$ satisfying

$${}^{i}\mathcal{T}^{j} = \mathcal{T}_i\delta_{ij} + \sum_{l\neq j}{}^{i}\mathcal{T}^{l}\mathcal{G}\mathcal{T}_j , \tag{3.35a}$$

$${}^{i}\mathcal{T}^{j} = \mathcal{T}_i\delta_{ij} + \sum_{l\neq i}\mathcal{T}_i\mathcal{G}{}^{l}\mathcal{T}^{j} . \tag{3.35b}$$

The definitions

$$\mathcal{T}^{j} = \sum_{i=0}^{3}{}^{i}\mathcal{T}^{j} , \tag{3.36a}$$

$${}^{i}\mathcal{T} = \sum_{j=0}^{3}{}^{i}\mathcal{T}^{j} \tag{3.36b}$$

will prove to be convenient later on.

One of the appealing features of the usual Faddeev equations lies in the physical interpretation, in terms of subsystem scattering processes, that can be given to the input amplitudes. We shall now provide an analogous physical interpretation of the operators $\mathcal{T}_i$, $i = 1,2,3$, defined above. Thus, the operator $\mathcal{T}_1$ plays the role of the effective scattering operator for particle 1 and the cluster C in the presence of the spectator 2. This follows from the representation

$$\mathcal{T}_1 = \langle\chi|T_1|\chi\rangle ; \tag{3.37}$$

here the operator T_1 satisfies

$$T_1 = v_1 + v_1G_0T_1 , \tag{3.38}$$

with

$$G_0 = (E - h - K)^{-1} . \tag{3.39}$$

Equivalently, we have the familiar representation of the physical scattering operator,

$$T_1 = v_1 + v_1G_1v_1 , \tag{3.40}$$

with

$$G_1 = (E - h - K - v_1)^{-1} . \tag{3.41}$$

To verify Eq. (3.37), we compare the solution of

Eq. (3.25) for $i=1$ with Eq. (3.38) to find[14]

$$T_1 = \hat{T}_1 + \hat{T}_1(G_0 - \hat{G}_0)T_1 . \tag{3.42}$$

Furthermore, from the eigenfunction expansions of G_0 and $\hat{G}_0$ we have

$$G_0 - \hat{G}_0 = |\chi\rangle g\langle\chi| . \tag{3.43}$$

When we take the expectation value of each member of Eq. (3.42) with respect to χ and make use of Eq. (3.43), along with Eq. (3.27) defining $\mathcal{U}_1$, we find that $\langle\chi|T_1|\chi\rangle$ satisfies the integral equation (3.33) defining $\mathcal{T}_1$. The identification (3.37) then follows. When $\mathcal{T}_1$ is evaluated in momentum space and a momentum conserving δ function associated with the spectator particle is factored out the result is a particular off-shell extension of the physical amplitude for elastic scattering of particle 1 from the bound cluster C. An identical discussion, with the roles of particles 1 and 2 interchanged, holds for $\mathcal{T}_2$. Turning now to the operator $\mathcal{T}_3$ we first observe that the expectation value in Eq. (3.27) for $i=3$ can be evaluated directly to give

$$\mathcal{U}_3 = v_3 + v_3\frac{1}{E-K}\mathcal{U}_3 . \tag{3.44}$$

Comparison of this integral equation with Eq. (3.33) for $i=3$ gives[14]

$$\mathcal{T}_3 = v_3 + v_3\frac{1}{E-\epsilon-K}\mathcal{T}_3 . \tag{3.45}$$

Thus $\mathcal{T}_3$ satisfies the Lippmann-Schwinger equation in its usual form and may therefore be identified with the conventional scattering operator for the pair (12) with C the spectator.

It should be clear that $\mathcal{T}_1$ and $\mathcal{T}_2$ are multiparticle operators, i.e., they each account for the scattering of a particle by a multiparticle system. The description of this scattering problem is essentially that given in Sec. II; in the absence of the spectator particle the effective potential takes the form (2.16). This is to be contrasted with the appearance of a *two*-particle potential in the integral equation (3.45) for $\mathcal{T}_3$.

We now turn to the analysis of Eq. (3.22) for the case of two-body initial states ($j=1,2,3$). In this case we have the *homogeneous*[9] integral equation

$$\langle\chi|\Psi_j\rangle = (E-\epsilon-K)^{-1}\mathcal{U}\frac{\epsilon}{E-K}\langle\chi|\Psi_j\rangle . \tag{3.46}$$

To identify the scattered wave we introduce the representation

$$\langle\chi|\Psi_j\rangle = \langle\chi|\Phi_j\rangle + \langle\chi|\tilde{\Psi}_j\rangle \tag{3.47}$$

on the right-hand side of Eq. (3.46). The incident wave Φ_j is defined in Eqs. (3.3)–(3.9). To proceed we note the relations

$$(E-\epsilon-K)^{-1}\mathcal{U}_j\frac{\epsilon}{E-K}\langle\chi|\Phi_j\rangle = \langle\chi|\Phi_j\rangle , \tag{3.48}$$

which are essentially eigenvalue equations for the two-body bound-state functions ϕ_j in the presence of the third spectator particle. For $j=1,2$, the eigenvalue equation referred to is of the form (2.17) with $e=\epsilon_j$ and $f=f_j$ defined by

$$|f_j\rangle = \frac{\epsilon}{\epsilon_j - k_j}\langle\chi|\phi_j\rangle . \tag{3.49}$$

To verify Eq. (3.48) for $j=3$ we first write

$$\mathcal{U}_3(E-K)^{-1} = v_3(E-K-v_3)^{-1} , \tag{3.50}$$

a relation easily derived from Eq. (3.44). We next observe that by virtue of the eigenfunction expansion of the resolvent $(E-\epsilon-v_3)^{-1}$ we have

$$\epsilon(E-K-v_3)^{-1}|\phi_3\vec{p}_3\rangle = |\phi_3\vec{p}_3\rangle . \tag{3.51}$$

These relations allow us to reduce Eq. (3.48), $j=3$, to the eigenvalue equation in its standard form

$$(E-\epsilon-K)^{-1}v_3|\phi_3\vec{p}_3\rangle = |\phi_3\vec{p}_3\rangle . \tag{3.52}$$

Having established Eq. (3.48) we use it along with Eqs. (3.46) and (3.47) to derive an inhomogeneous integral equation for the scattered wave of the form

$$\langle\chi|\tilde{\Psi}_j\rangle = (E-\epsilon-K)^{-1}\sum_{l\neq j}\mathcal{U}_l\frac{\epsilon}{E-K}\langle\chi|\Phi_j\rangle + (E-\epsilon-K)^{-1}\mathcal{U}\frac{\epsilon}{E-K}\langle\chi|\tilde{\Psi}_j\rangle . \tag{3.53}$$

The solution can be represented as

$$\langle\chi|\tilde{\Psi}_j\rangle = (E-\epsilon-K)^{-1}\sum_{l\neq j}\mathcal{T}^l\frac{\epsilon}{E-K}\langle\chi|\Phi_j\rangle \tag{3.54}$$

by virtue of the relation

$$\mathcal{T}^l = \mathcal{U}_l + \mathcal{U}g\mathcal{T}^l . \tag{3.55}$$

We therefore have, for $j=1,2,3$, the representation

$$\langle\chi|\Psi_j\rangle = \langle\chi|\Phi_j\rangle + (E-\epsilon-K)^{-1}\sum_{l\neq j}\mathcal{T}^l\frac{\epsilon}{E-K}\langle\chi|\Phi_j\rangle . \tag{3.56}$$

In analogy with Faddeev's treatment of the pure three-body wave function[9] we may introduce the decomposition

$$\langle\chi|\Psi_j\rangle = \sum_{i=0}^{3}\langle\chi|\Psi_j^i\rangle . \tag{3.57}$$

For $j=0$ we have, from Eq. (3.30),

$$\langle\chi|\Psi_0^i\rangle = |\vec{p}_0\rangle\delta_{i0} + \frac{1}{E-\epsilon-K}{}^i\mathcal{T}|\vec{p}_0\rangle , \tag{3.58}$$

while from Eq. (3.56) we have

$$\langle\chi|\Psi_j^i\rangle=\langle\chi|\Phi_j\rangle\delta_{ij}+\frac{1}{E-\epsilon-K}\sum_{l\neq j}{}^iT^l\frac{\epsilon}{E-K}\langle\chi|\Phi_j\rangle \tag{3.59}$$

for $j=1,2,3$. The coupled equations for ${}^iT^j$ imply a set of coupled equations for the components $\langle\chi|\Psi_j^i\rangle$. As may be readily verified, these equations take the form

$$(E-\epsilon-K)\langle\chi|\Psi_j^i\rangle=v_i\frac{\epsilon}{E-K}\sum_{l=0}^{3}\langle\chi|\Psi_j^l\rangle\,. \tag{3.60}$$

Most of the analysis given above has its counterpart in the scattering theory of three structureless particles. In fact, it is easy to see that in the extreme tight-binding (or "frozen-core") limit, in which virtual excitations of the cluster C no longer play a role, the above formalism reduces identically to the usual Faddeev version. This formalism therefore provides a convenient starting point for a systematic investigation of corrections to the frozen-core model. In particular, Eqs. (3.60) reduce, in the tight-binding limit, to the coupled equations satisfied by the Faddeev components of the three-body wave function. As they stand, however, Eqs. (3.60) incorporate the multiparticle effects exactly. Note that one can anticipate on general grounds that multiparticle effects will not only alter the pair potentials but will also induce a three-body potential term in the coupled equations.[8] Here we have succeeded in expressing these potentials explicitly in terms of the original Hamiltonian.

IV. CHANNEL DECOMPOSITION OF THE WAVE FUNCTION

The wave function Ψ_j can be expanded as

$$|\Psi_j\rangle=\sum_{i=0}^{3}|\Psi_j^i\rangle\,, \tag{4.1}$$

where, recalling the representation (3.13),

$$|\Psi_j^i\rangle=\hat{G}\epsilon\,|\chi\rangle\langle\chi|\Psi_j^i\rangle\,; \tag{4.2}$$

$\langle\chi|\Psi_j^i\rangle$ is given by Eq. (3.58) for $j=0$ and by Eq. (3.59) for $j=1,2,3$. These relations provide the basis for a decomposition of the wave function into open- and closed-channel parts. In this section we consider those cases where Ψ_j evolves from a two-body initial state, i.e., we consider entrance channels $j=1,2,3,$. The case $j=0$ (three-body initial state) is somewhat more complicated and is taken up in Appendix B. To begin with, we set $i=0$ in Eq. (4.2) and introduce the resolvent identity, Eq. (3.18), in the equivalent form

$$\hat{G}=\hat{G}_0+\hat{G}V\hat{G}_0\,. \tag{4.3}$$

Use of Eq. (3.17) then allows us to write

$$|\Psi_j^0\rangle=|\chi F_j^0\rangle+|M_j^0\rangle\,, \tag{4.4}$$

with

$$|M_j^0\rangle=\hat{G}V|\chi F_j^0\rangle \tag{4.5a}$$

and

$$|F_j^0\rangle=\frac{\epsilon}{E-K}\langle\chi|\Psi_j^0\rangle\,. \tag{4.5b}$$

We note that in configuration space the function F_j^0 is defined by coordinates appropriate to a "pure" three-body system, and satisfies outgoing wave boundary conditions in the region where all three interparticle separations are large. Two-body bound states do not appear in the asymptotic form of F_j^0, as may be seen by examination of Eq. (3.59) with $i=0$. The function $V\chi F_j^0$ falls off rapidly enough to be square integrable. We conclude that M_j^0 is square integrable. Equation (4.4) then represents a decomposition of the wave function into open- and closed-channel components. This particular decomposition serves as the basis for the introduction of a subsidiary minimum principle for the construction of the closed-channel component. We shall return in Sec. V for a detailed discussion of this approach. Here we complete the analysis of the structure of the wave function by considering the remaining three components $\langle\chi|\Psi_j^i\rangle$, $i=1,2,3$.

We first observe that use of Eq. (4.3) fails to provide the desired decomposition in these cases because of the appearance of two-body bound states; such states must be completely accounted for in the construction of the open-channel component of the wave function. Thus, for $i=3$ we use, in place of Eq. (4.3), the identity

$$\hat{G}=\hat{G}_3+\hat{G}V^3\hat{G}_3\,, \tag{4.6}$$

where $V^3\equiv V-v_3$ and

$$\hat{G}_3=(E-\hat{h}-K-v_3)^{-1}\,. \tag{4.7}$$

The eigenfunction expansion of $\hat{G}_3$ may be used to verify the relation

$$\hat{G}_3|\chi\rangle=|\chi\rangle(E-K-v_3)^{-1}\,. \tag{4.8}$$

Use of these results in Eq. (4.2) leads to the decomposition

$$|\Psi_j^3\rangle=|\chi F_j^3\rangle+|M_j^3\rangle\,, \tag{4.9}$$

with

$$|M_j^3\rangle=\hat{G}V^3|\chi F_j^3\rangle \tag{4.10}$$

and

$$|F_j^3\rangle=\frac{\epsilon}{E-K-v_3}\langle\chi|\Psi_j^3\rangle\,. \tag{4.11}$$

From Eq. (3.59) with $i=3$ and Eq. (3.51) we find

$$|F_j^3\rangle = |\phi_3 \vec{p}_3\rangle \delta_{j3} + \frac{1}{E-K-v_3}\frac{\epsilon}{E-K-\epsilon} \times \sum_{l\neq j} {}^3\mathcal{T}^l \frac{\epsilon}{E-K}\langle\chi|\Phi_j\rangle . \quad (4.12)$$

The function F_j^3 is a three-body wave function. In the asymptotic domain it contains, in addition to a three-body outgoing-wave contribution, a component which describes the relative motion of the bound pair (12) and the cluster C. If desired, an explicit separation of these two-body and three-body components could be obtained, though for simplicity we shall not do so here. (This separation is not necessary in the variational approach described in Sec. V provided the two-particle bound-state function ϕ_3 is assumed known.) Since $V^3\chi F_j^3$ is square integrable the same holds for the function M_j^3.

The open-channel part of Ψ_j^1 contains both two-body and three-body components. We wish to separate off these open-channel components explicitly, obtaining a representation of Ψ_j^1 in the form

$$|\Psi_j^1\rangle = |\phi_1 F_{jP}^1\rangle + |\chi F_{jR}^1\rangle + |M_j^1\rangle . \quad (4.13)$$

Here F_{jP}^1 and F_{jR}^1 are effective two-body and three-body scattering functions, respectively. The function M_j^1 is the closed-channel component. To derive Eq. (4.13), and thereby obtain a prescription for the construction of the closed-channel component, we first observe that the two-body component $\phi_1 F_{jP}^1$ arises from the part of ${}^1\mathcal{T}^l$ in Eq. (3.59) which contains the bound-state pole associated with subsystem 1. We therefore write

$$\mathcal{T}_1 = \mathcal{T}_{1P} + \mathcal{T}_{1R} , \quad (4.14)$$

where $\mathcal{T}_{1P}$ contains the bound-state pole. The separation is of course not unique; a particularly convenient form for our purposes is derived in Appendix A. When the decomposition (4.14) is inserted in the right-hand side of Eq. (3.35b) we find

$${}^1\mathcal{T}^l = {}^1\mathcal{T}_P^l + {}^1\mathcal{T}_R^l , \quad (4.15)$$

with

$${}^1\mathcal{T}_P^l \equiv \mathcal{T}_{1P}\delta_{1l} + \sum_{m\neq 1} \mathcal{T}_{1P}\mathcal{G}^m\mathcal{T}^l . \quad (4.16)$$

Referring to Eqs. (3.59) and (4.2) we see that the decomposition (4.15) leads to a corresponding decomposition of the wave function

$$|\Psi_j^1\rangle = |\Psi_{jP}^1\rangle + |\Psi_{jR}^1\rangle . \quad (4.17)$$

Explicitly, we have

$$|\Psi_{jP}^1\rangle = \hat{G}\epsilon\,|\chi\rangle\langle\chi|\Psi_{jP}^1\rangle , \quad (4.18)$$

with

$$\langle\chi|\Psi_{jP}^1\rangle = \langle\chi|\Phi_j\rangle\delta_{1j} + (E-\epsilon-K)^{-1}\sum_{l\neq j} {}^1\mathcal{T}_P^l \frac{\epsilon}{E-K}\langle\chi|\Phi_j\rangle . \quad (4.19)$$

By construction, the function Ψ_{jP}^1 contains the complete outgoing scattered wave in exit channel 1 (1 and C bound in the final state). To decompose Ψ_{jP}^1 into open- and closed-channel parts we introduce the resolvent identity

$$\hat{G}(E) = \hat{g}_1(\epsilon_1) + \hat{G}(E)(K_1 + V^1 - E + \epsilon_1)\hat{g}_1(\epsilon_1) , \quad (4.20)$$

where $V^1 = V - v_1$ and

$$\hat{g}_1(\epsilon_1) = (\epsilon_1 - \hat{h} - k_1 - v_1)^{-1} . \quad (4.21)$$

According to Eq. (2.6) we may express the eigenvalue equation in the form

$$|\phi_1\rangle = \hat{g}_1(\epsilon_1)\epsilon\,|\chi\rangle\langle\chi|\phi_1\rangle . \quad (4.22)$$

Thus, when Eqs. (4.18)–(4.20) are combined, with $\mathcal{T}_{1P}$ given by Eq. (A7), we obtain the representation

$$|\Psi_{jP}^1\rangle = [1 + \hat{G}(K_1 + V^1 - E + \epsilon_1)]\,|\phi_1 F_{jP}^1\rangle , \quad (4.23)$$

with F_{jP}^1 defined in Eq. (A8). In a similar way we obtain for the residual component Ψ_{jR}^1 the representation

$$|\Psi_{jR}^1\rangle = \hat{G}\epsilon\,|\chi\rangle\langle\chi|\Psi_{jR}^1\rangle . \quad (4.24)$$

Use of the resolvent identity in the form (4.3) allows us to write

$$|\Psi_{jR}^1\rangle = (1 + \hat{G}V)\,|\chi F_{jR}^1\rangle . \quad (4.25)$$

Combining these results, we arrive at the form (4.13) with the asymptotically decaying closed-channel component given by

$$|M_j^1\rangle = \hat{G}[(K_1 + V^1 - E + \epsilon_1)\,|\phi_1 F_{jP}^1\rangle + V\,|\chi F_{jR}^1\rangle] . \quad (4.26)$$

In verifying that M_j^1 is normalizable note that F_{jP}^1 has the oscillatory asymptotic behavior of a two-body scattering function of energy $E - \epsilon_1$; then $(K_1 - E + \epsilon_1)F_{jP}^1$ vanishes asymptotically. This can be seen explicitly from Eq. (A8). Since $\hat{G}$, a bounded operator, acts on a sum of normalizable functions the stated property of M_j^1 is confirmed. We see again that a proper treatment of the components of the wave function involving subsystem bound states is crucial in this analysis. The difficulties mentioned in the discussion following Eq. (3.17) have been overcome. The decomposition of Ψ_j^2 into two-body, three-body, and closed-channel components is achieved in a manner identical to that just described for Ψ_j^1.

To summarize, we have obtained the channel decomposition

$$|\Psi_j\rangle = |\phi_1 F^1_{jP}\rangle + |\phi_2 F^2_{jP}\rangle + |\chi F_{jR}\rangle + |M_j\rangle . \quad (4.27)$$

Here F^1_{jP} and F^2_{jP} are effective two-body wave functions. The three-body open-channel component is represented by

$$|F_{jR}\rangle \equiv |F^1_{jR}\rangle + |F^2_{jR}\rangle + |F^3_j\rangle + |F^0_j\rangle . \quad (4.28)$$

The function $M_j \equiv \sum_{i=0}^{3} M^i_j$ represents the complete closed-channel component.

We turn now to the identification of the matrix element T_{ij} for transition from initial "plane-wave" state Φ_j to final state Φ'_i in which the clusters separate from one another with relative momentum $\vec{p}'_i$. The transition-matrix elements can be determined by identifying the amplitude of the scattered wave in each channel. Since the asymptotic form of the wave function is determined by the singularities in its momentum-space representation (see, e.g., J. Nuttall, Ref. 16) one arrives at the equivalent prescription[11]

$$T_{ij}(\vec{p}'_i, \vec{p}_j) = \lim_{\eta \to 0} i\eta \langle \Phi'_i | \Psi_j \rangle . \quad (4.29)$$

From Eqs. (3.30) and (3.56) we find that

$$T_{00}(\vec{p}'_0, \vec{p}_0) = \langle \vec{p}'_0 | \mathcal{T} | \vec{p}_0 \rangle \quad (4.30)$$

and

$$T_{0j}(\vec{p}'_0, \vec{p}_j) = \sum_{l \neq j} \langle \vec{p}'_0 | \mathcal{T}^l | f_j \vec{p}_j \rangle , \quad j = 1,2,3 . \quad (4.31)$$

Here, to simplify notation, we use

$$| f_j \vec{p}_j \rangle \equiv \frac{\epsilon}{E - K} \langle \chi | \Phi_j \rangle . \quad (4.32)$$

The time-reversed amplitude may be determined as

$$T_{i0}(\vec{p}'_0, \vec{p}_0) = \sum_{l \neq i} \langle f_i \vec{p}'_i | {}^l\mathcal{T} | \vec{p}_0 \rangle , \quad i = 1,2,3 . \quad (4.33)$$

From Eqs. (4.12) and (A8) we find that, for $i,j = 1,2,3$,

$$T_{ij}(\vec{p}'_i, \vec{p}_j) = B_{ij}(\vec{p}'_i, \vec{p}_j)(1 - \delta_{ij}) + \sum_{l \neq i} \sum_{m \neq j} \langle f_i \vec{p}'_i | {}^l\mathcal{T}^m | f_j \vec{p}_j \rangle , \quad (4.34)$$

where

$$B_{ij}(\vec{p}'_i, \vec{p}_j) = \langle f_i \vec{p}'_i | \left(\frac{E - K}{\epsilon} \right) (E - \epsilon - K) | f_j \vec{p}_j \rangle . \quad (4.35)$$

As remarked earlier [in connection with Eq. (3.49)] the functions f_1 and f_2 are effective single-particle bound-state functions determined by homogeneous integral equations involving the effective subsystem interaction potential.

V. APPROXIMATION METHODS

The scattering equations given above suggest a number of approximation techniques. For example, a cluster approximation is a very natural one to attempt in the present context. That is, one assumes that at each stage of the scattering process the system can be analyzed in terms of three interacting clusters. This amounts to the neglect of the three-body potential $\mathcal{U}_0$ in Eqs. (3.60) or, equivalently, the amplitude $\mathcal{T}_0$ in Eqs. (3.35). Note that this approximation does not violate unitarity. The equations in this cluster approximation are of the usual three-body Faddeev form and will generate unitary amplitudes (for energies below the four-body threshold) provided that the Hermiticity property of the effective pair potentials is maintained. A variational method for determining Hermitian approximations to these pair interactions has been described previously.[5] The approximations may be represented in separable form to facilitate the numerical solution of the Faddeev equations.[15] While this approach should be useful in a variety of scattering problems it suffers from the intrinsic limitation of the neglect of $\mathcal{U}_0$.

One can attempt to refine the calculational procedure by introducing approximations to $\mathcal{U}_0$. We shall not take this course here, however. We consider instead what appears to be a simpler approach based on the Kohn variational principle. With the aid of subsidiary minimum principles for the construction of trial functions this method allows for systematic improvement. Such a method was described previously for the case where only two-body channels are open.[6] Here we merely outline the modifications required to account for the appearance of propagating three-body states.

We are interested in determining the scattering amplitude T_{ij} in which two bodies are incident in the entrance channel and either two or three bodies emerge in the exit channel. The Kohn-type variational approximation for T_{ij} is of the form[16]

$$T_{ijv} = T_{ijt} + \langle \Psi^{(-)}_{it} | H - E | \Psi^{(+)}_{jt} \rangle . \quad (5.1)$$

Here T_{ijt} is a trial scattering amplitude, determined as the amplitude of the outgoing wave in channel i associated with the trial wave function $\Psi^{(+)}_{jt}$. The superscript on the symbol $\Psi^{(-)}_{it}$ indicates incoming-wave boundary conditions. Alternatively, standing-wave boundary conditions may be adopted. This would be appropriate for the variational construction of the K matrix, with the T matrix subsequently determined from a set of multichannel Heitler equations.[17] In this way unitarity can be preserved in the approximation procedure. To make use of the variational principle (for either the K matrix or the T matrix) we require a pre-

scription which enables us to generate trial functions in such a way that the many-body complexities of the problem can be accounted for systematically. The cluster representation of the exact wave function developed in Sec. IV is useful in this connection; it provides us with an explicit separation of open- and closed-channel components of the wave function. It is in the construction of the closed-channel components that the many-body nature of the problem is encountered. Thus, we express Ψ_{jt} [the superscript $(\pm)$ is dropped since the choice of boundary conditions plays no role in the following discussion] in the form

$$|\Psi_{jt}\rangle = \sum_{l=0}^{3} |\Psi_{jt}^{l}\rangle , \tag{5.2}$$

as suggested by Eq. (4.1). To simplify the present discussion we consider only two-body initial states $j=1$, 2, or 3. The components Ψ_{jt}^{l} are to be chosen in accordance with the exact representations, Eqs. (4.4), (4.9), and (4.13). For example, we would choose Ψ_{jt}^{1} in the form

$$|\Psi_{jt}^{1}\rangle = |\phi_1 F_{jPt}^{1}\rangle + |\chi F_{jRt}^{1}\rangle + |M_{jt}^{1}\rangle . \tag{5.3}$$

We are assuming temporarily that the bound-state functions ϕ_1 and χ are known precisely. The procedure for introducing trial bound-state functions is described below. Recall that the function F_{jPt}^{1} is a two-body wave function, depending on a single interparticle distance; F_{jRt}^{1} is a three-body function. Each of these trial functions can be expressed as an expansion in some convenient set of basis functions which incorporate the proper asymptotic boundary conditions. This is the same procedure as that used in the pure three-body problem. We shall assume that these trial functions can be constructed with sufficient flexibility to provide satisfactory approximations to the true open-channel components F_{jP}^{1} and F_{jR}^{1}. The choice of the basis functions in the expansion of the asymptotically decaying closed-channel component M_{jt}^{1} is more difficult since these are functions of all of the particle coordinates. Experience in multiparticle bound-state calculations indicates that these basis functions should be kept flexible by inclusion of nonlinear variational parameters; otherwise the number of basis functions required to obtain convergent results may increase to the point where the calculation becomes unmanageable. Of course, in bound-state calculations the Rayleigh-Ritz minimum principle can be used in the search for the optimum set of nonlinear parameters. As we shall now show, an analogous minimum principle is available for the construction of the trial function M_{jt}^{1}. We first note that Eq. (4.26) which defines the exact function M_{j}^{1} can be rewritten as the inhomogeneous differential equation

$$(\hat{H} - E)\,|M_{j}^{1}\rangle = -\,|J_{j}^{1}\rangle , \tag{5.4}$$

with the square-integrable function J_{j}^{1} defined by

$$|J_{j}^{1}\rangle = (K_1 + V^1 - E + \epsilon_1)\,|\phi_1 F_{jP}^{1}\rangle + V\,|\chi F_{jR}^{1}\rangle . \tag{5.5}$$

Alternatively, we can characterize the solution of Eq. (5.4) as the function which minimizes the functional

$$\mathfrak{M}_{j}^{1} = \langle M_{j}^{1}|J_{j}^{1}\rangle + \langle J_{j}^{1}|M_{j}^{1}\rangle + \langle M_{j}^{1}|\hat{H} - E\,|M_{j}^{1}\rangle . \tag{5.6}$$

The minimum property follows from the fact that the energy E lies below the threshold of the continuous spectrum of the modified Hamiltonian $\hat{H}$. (If there are discrete eigenstates of $\hat{H}$ with energies below E they must be "subtracted out" in order to preserve the minimum property.[5,6] To simplify the discussion we shall assume that such states are not actually present.) The above discussion suggests that the nonlinear variational parameters in the trial function M_{jt}^{1} may be determined by minimizing the functional

$$\mathfrak{M}_{jt}^{1} = \langle M_{jt}^{1}|J_{jt}^{1}\rangle + \langle J_{jt}^{1}|M_{jt}^{1}\rangle + \langle M_{jt}^{1}|\hat{H} - E\,|M_{jt}^{1}\rangle , \tag{5.7}$$

where

$$|J_{jt}^{1}\rangle = (K_1 + V^1 - E + \epsilon_1)\,|\phi_1 F_{jPt}^{1}\rangle + V\,|\chi F_{jRt}^{1}\rangle . \tag{5.8}$$

The above procedure is essentially equivalent to that in which the trial function M_{jt}^{1} is chosen in the form

$$|M_{jt}^{1}\rangle = \hat{G}_t\,|J_{jt}^{1}\rangle , \tag{5.9}$$

with the trial Green's function $\hat{G}_t$ determined with the aid of the minimum principle satisfied by $\hat{G}$.[5] More generally, we could write, for each closed-channel component,

$$|M_{jt}^{l}\rangle = \hat{G}_t\,|J_{jt}^{l}\rangle , \quad l = 0,1,2,3 , \tag{5.10}$$

with

$$|J_{jt}^{0}\rangle = V\,|\chi F_{jt}^{0}\rangle , \tag{5.11}$$

$$|J_{jt}^{3}\rangle = V^3\,|\chi F_{jt}^{3}\rangle , \tag{5.12}$$

and J_{jt}^{2} given by an equation similar to (5.8) with $1 \to 2$.

Having fixed the form of the trial function Ψ_{jt} we must make use of the variational principle, Eq. (5.1), to determine the open-channel components of the wave function. One would make an initial guess at the open-channel components in terms of which the functions J_{jt}^{l} are defined, and then construct the closed-channel components as in Eq. (5.10). With the functions M_{jt}^{l} fixed, Eq. (5.1) would be used to generate variational approxima-

tions to the scattering matrix and, at the same time, improved approximations to the open-channel components. If it were desired this process could be iterated. A more detailed discussion of this and alternative procedures is given in Ref. 6.

We discuss, in conclusion, the manner in which the above procedure must be modified to account for the fact that the bound-state functions χ, ϕ_1, and ϕ_2 are in general imprecisely known. Firstly, we note that subsidiary minimum principles for the trial functions M^l_{jt} can be maintained, in the form shown in Eq. (5.7) for $l=1$, by making the replacement $\hat{H} \to \hat{H}_t$, with

$$\hat{H}_t = h - \frac{h|\chi_t\rangle\langle\chi_t|h}{\langle\chi_t|h|\chi_t\rangle} + K + V . \tag{5.13}$$

This reduces to $\hat{H}$ if χ_t is exact. We have previously shown[10] that for χ_t sufficiently accurate the operator $\hat{H}_t - E$ will be positive, thus ensuring the validity of the minimum principle.

The effect of the imprecisely known bound-state functions must also be accounted for in matching the boundary conditions at infinity. Clearly some care must be exercised here since the trial function Ψ_{jt} fails to satisfy the Schrödinger equation asymptotically if inexact bound-state functions appear in the asymptotic form. The integral on the right-hand side of Eq. (5.1) diverges under these circumstances. To avoid divergent integrals we may proceed formally[18] by evaluating $(H-E)|\Psi^l_{jt}\rangle$ with the assumption that the exact bound-state functions are used in the representation of Ψ^l_{jt}. Here we take advantage of the fact that the bound-state functions appear explicitly in factored form, as shown in Eq. (5.3) for the $l=1$ component. The variational functional (5.1), when constructed in this way, will involve the bound-state functions explicitly. If at *this* stage approximations are introduced for these bound-state functions the integrals remain finite.[18] To preserve the variational principle (5.1), the approximate bound-state functions must be correct to first order. Such functions can be obtained with the aid of the variational principle for bound-state wave functions proposed in Ref. 5. Here too one has subsidiary minimum principles to aid in the determination of the trial functions which appear in the variational principle for the bound-state wave functions.

VI. SUMMARY AND CONCLUSION

As an example of the type of problem for which the formalism developed here would be appropriate, consider the low-energy collision of a deuteron with a tightly bound nucleus. In addition to elastic scattering we are interested in the amplitudes for rearrangement (one of the nucleons in the deuteron is captured by the nucleus) and breakup of the deuteron. The scattering energy is assumed to lie below the threshold for breakup of the target nucleus. In first approximation we may think of this as a problem in three-body scattering theory, with corrections required to account for the internal structure of the nucleus. With regard to the three-body dynamics we have available some fairly well-developed approximation techniques, based, for example, on the use of separable kernels in the Faddeev equations or on variational methods. Our concern is then shifted to the problem of accounting consistently for the fact that the nucleus is a compound system. For example, in forming the final-state wave function for the rearrangement process we must consider the binding of a nucleon with the nucleus. In our picture the effective nucleon-nucleus potential is given by Eq. (2.16); the equivalent two-body wave function is determined by the homogeneous version of Eq. (2.18). This is the wave function which appears in the formally exact expression (4.34) for the matrix element. The operators ${}^l\mathcal{T}^m$ in that expression are determined by the generalized[8] three-body Faddeev equations (3.35). The input to these equations are the multiparticle operators $\mathcal{T}_i$ which satisfy the Lippmann-Schwinger equations (3.33). The original Faddeev equations[9] involve three subsystem scattering operators; here there are four, since in addition to the effective pair interactions we have an induced three-body potential. The "free" three-body propagator is given by Eq. (3.32). The appearance of the second term on the right-hand side may seem somewhat unusual; it would be absent in a Feshbach projection-operator formulation. We have avoided using that formalism since we are unable to construct the required projection operators. As an alternative to Eqs. (3.35) we have the coupled equations (3.60) for the Faddeev components of the wave function associated with the equivalent three-body system. Since these latter equations involve the effective potentials directly rather than the subsystem scattering operators they may be simpler to work with in practice.

The analysis of the wave function given in Sec. IV serves two purposes. Firstly, it allows us, with the aid of Eqs. (4.29), to identify the physical scattering matrix elements. Secondly, it provides us with a specific decomposition of the wave function into open-channel components, which behave like standing waves or outgoing waves at infinity, and asymptotically decaying closed-channel components. This decomposition is carried out with the help of two separate techniques. One of them is based on the introduction of the modified target

Hamiltonian defined in Eq. (2.3). As discussed in greater detail previously,[5,6] this procedure plays a role analogous to the use of Feshbach projection operators, in that a certain class of continuum states is "subtracted out", and is more easily generalized to cases where rearrangement and Pauli exchange effects are present. The second technique is to partially solve the basic equations to the extent that subsystem scattering and binding effects are explicitly included in the formalism.[9] As indicated in the discussion following Eq. (4.26), both techniques are required to properly identify the closed-channel part of the wave function. Corresponding to this formal decomposition of the wave function we can devise a computational procedure in which variational methods of the Rayleigh-Ritz type are used in the construction of the decaying components. It is at this stage that one comes to grips with the multiparticle complexities of the target nucleus. Having "subtracted out" the effects of the continuum we achieve a very much needed simplification of this stage of the calculation. There still remains the problem of determing the open-channel components of the wave function. This is essentially a three-body (not a many-body) problem on which a considerable amount of computational experience can be brought to bear. In Sec. V we have outlined a variational approach as one of a number of possible computational methods. Our goal, more generally, has been to provide a consistent theoretical framework for the development of three-body models of multiparticle scattering processes.

APPENDIX A

Here we derive Eq. (4.14), which expresses the subsystem scattering operator $\mathcal{T}_1$ as the sum of a pole term plus a nonsingular remainder. We first note that the operators $\mathcal{T}_1$, G_0, and G_1, defined by Eqs. (3.38), (3.39), and (3.41), respectively, satisfy the well-known relation

$$G_1 = G_0 + G_0 T_1 G_0 . \tag{A1}$$

When we take the expectation value with respect to χ of both sides of Eq. (A1) and make use of the relations

$$G_0(E)\,|\chi\rangle = |\chi\rangle(E - \epsilon - K)^{-1} , \tag{A2}$$

$$\langle\chi|\,G_0(E) = (E - \epsilon - K)^{-1}\langle\chi| , \tag{A3}$$

along with Eq. (3.37), we find

$$\langle\chi|\,G_1\,|\chi\rangle = (E - \epsilon - K)^{-1} + (E - \epsilon - K)^{-1}\mathcal{T}_1(E - \epsilon - K)^{-1} . \tag{A4}$$

We now write

$$G_1 = G_{1P} + G_{1R} , \tag{A5}$$

with G_{1P} defined as the bound-state contribution to the eigenfunction expansion of G_1, namely,

$$G_{1P} = |\phi_1\rangle(E - \epsilon_1 - K_1)^{-1}\langle\phi_1| . \tag{A6}$$

The decomposition of G_1 when combined with Eq. (A4) leads to the desired representation Eq. (4.14), with $\mathcal{T}_{1P}$ determined by

$$\langle\chi|\,\phi_1\rangle(E - \epsilon_1 - K_1)^{-1}\langle\phi_1\,|\chi\rangle = (E - \epsilon - K)^{-1}\mathcal{T}_{1P}(E - \epsilon - K)^{-1} . \tag{A7}$$

We may now replace ${}^1\mathcal{T}^l_P$ in Eq. (4.19) by the right-hand side of Eq. (4.16) with the above form for $\mathcal{T}_{1P}$. This leads to Eq. (4.23) with

$$|F^1_{jP}\rangle = |\vec{p}_1\rangle\delta_{1j} + (E - \epsilon_1 - K_1)^{-1}\langle\phi_1\,|\chi\rangle\left[(E - \epsilon - K)(1 - \delta_{1j}) + \sum_{l\neq j}\sum_{m\neq 1}\frac{\epsilon}{E - K}{}^m\mathcal{T}^l\right]\frac{\epsilon}{E - K}\langle\chi\,|\Phi_j\rangle . \tag{A8}$$

APPENDIX B

The discussion of Sec. IV leading to a channel decomposition of the wave function was restricted to the case of two-body initial states. If one wishes to extend that discussion to include three-body initial states (as would be required, for example, in the application of the variational approach of Sec. V to breakup scattering) one encounters a new feature, related to the appearance of a new class of terms in the asymptotic form of the wave function.[19] Thus, according to Eq. (3.13), the wave function which evolves from a three-body initial state is represented by

$$|\Psi_0\rangle = \hat{G}\epsilon\,|\chi\rangle\langle\chi\,|\Psi_0\rangle , \tag{B1}$$

with $\langle\chi\,|\Psi_0\rangle$ given by Eq. (3.30). In the analysis of the asymptotic form of this effective three-body wave function separate consideration must be given to the first few terms in the multiple scattering expansion.[19] We therefore write

$$\langle\chi\,|\Psi_0\rangle = |\vec{p}_0\rangle + (E - \epsilon - K)^{-1}\left[\sum_{l=1}^{3}\mathcal{T}_l + \sum_{l=1}^{3}\sum_{m=1}^{3}\mathcal{T}_l\mathcal{G}\mathcal{T}_m(1 - \delta_{lm})\right]|\vec{p}_0\rangle + \langle\chi\,|\tilde{\Psi}_0\rangle . \tag{B2}$$

The asymptotic form of $\langle\chi|\tilde{\Psi}_0\rangle$ is the same as that of $\langle\chi|\tilde{\Psi}_j\rangle$, $j=1,2,3$, defined in Eq. (3.47) and the decomposition of the function

$$|\tilde{\Psi}_0\rangle \equiv \hat{G}\epsilon|\chi\rangle\langle\chi|\tilde{\Psi}_0\rangle \tag{B3}$$

into open-and closed-channel parts proceeds exactly as described in Sec. IV. A different procedure is necessary for the remaining terms, which decay less rapidly at infinity. Thus, consider the contribution of the plane wave $|\vec{p}_0\rangle$ in Eq. (B2); when inserted in the right-hand side of Eq. (B1) we obtain the function

$$|I_0\rangle \equiv \hat{G}\epsilon|\chi\rangle|\vec{p}_0\rangle . \tag{B3'}$$

This function consists of disconnected and connected parts which must be treated separately. The separation is achieved by expressing $\hat{G}$ as a sum of disconnected and connected parts. For this purpose we write

$$\hat{G} = \hat{G}_0 + \hat{G}_0\hat{T}\hat{G}_0 \tag{B4}$$

and introduce a Faddeev-type analysis of the operator $\hat{T}$. We have the decomposition

$$\hat{T} = \sum_{l=1}^{3} \hat{T}^l , \tag{B5}$$

with the components $\hat{T}^l$ defined as the solutions of the Faddeev equations

$$\hat{T}^l = \hat{T}_l + \sum_{m\neq l} \hat{T}^m\hat{G}_0\hat{T}_l . \tag{B6}$$

This leads, when combined with Eq. (B4), to the decomposition

$$\hat{G} = \hat{G}_0 + \sum_{l=1}^{3} \hat{G}_0\hat{T}_l\hat{G}_0 + \sum_{l=1}^{3}\sum_{m\neq l} \hat{G}_0\hat{T}^m\hat{G}_0\hat{T}_l\hat{G}_0 . \tag{B7}$$

The scattering operators may be eliminated in favor of the potentials (which are often simpler to deal with in practice) with the aid of the relations

$$\hat{G}_0\hat{T}_l = \hat{G}_l v_l , \tag{B8}$$

$$\hat{G}_0\hat{T}^m = \hat{G}v_m . \tag{B9}$$

These results, along with the relation

$$\hat{G}_0\epsilon|\chi\vec{p}_0\rangle = |\chi\vec{p}_0\rangle \tag{B10}$$

[which can be deduced from Eqs. (3.17) and (3.9)] lead to the expansion

$$|I_0\rangle = |\chi\vec{p}_0\rangle + \sum_{l=1}^{3}|I_{0l}\rangle + \sum_{l=1}^{3}\sum_{m\neq l}\hat{G}v_m|I_{0l}\rangle , \tag{B11}$$

with

$$|I_{0l}\rangle = \hat{G}_l v_l|\chi\vec{p}_0\rangle . \tag{B12}$$

In the first term in Eq. (B11) we recover the three-body incident plane wave, a function we take to be known in the present discussion. The function I_{0l} represents a contribution to the closed-channel part of the wave function for the pair l, with the third particle playing the role of a spectator. As mentioned in Sec. II (and discussed in detail in Ref. 6) a subsidiary minimum principle is available for determining approximations to this two-body closed-channel wave function. Let us suppose we have constructed an approximation to I_{0l} in this manner. Turning then to the third group of terms in Eq. (B11) we note that $v_m I_{0l}$, for $m\neq l$, is square integrable. The function $\hat{G}v_m I_{0l}$ is therefore square integrable; it represents a contribution to the closed-channel part of the wave function Ψ_0. In this way we arrive at a decomposition of the function I_0, Eq. (B11), into open- and closed-channel parts of the desired form. To complete the analysis we would consider the single- and double-scattering terms in Eq. (B2) as contributions to $\langle\chi|\Psi_0\rangle$ on the right-hand side of Eq. (B1). The channel decomposition of this part of Ψ_0 would then proceed in a manner very similar to that just described for the function I_0 and we omit further details of this analysis here.

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[11]It should be understood that the total physical energy has added to it, in the usual way, an imaginary part $i\eta$ with the limit $\eta\to 0$ performed at a suitable stage of the

calculation.

[12]Recall that the usual three-body Faddeev equations do not apply to charged-particle scattering and a practical alternative remains to be found.

[13]The second term on the right-hand side of Eq. (3.32) is nonsingular if, as we have assumed, E lies below the threshold for breakup of the cluster C.

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