Reaction theory for three charged clusters

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A theory of three-body reactions is presented, applicable to atomic and nuclear interactions, in which the colliding systems may be charged and composite, subject to the condition that the total energy lies below the threshold for breakup of any of the three bound systems. A variational principle for elements of the scattering matrix is derived, and a decomposition of each trial function into open- and closed-channel parts is presented that allows for the use of a subsidiary minimum principle for the systematic improvement of the closed-channel component. A detailed analysis of the structure of the trial functions is provided through a representation of the exact wave function in terms of the solution of integral equations of the Faddeev type, generalized to allow for long-range Coulomb interactions between pairs (through the appearance of Coulomb-distorted Green's functions in the kernel of the integral equation) as well as for the internal structure of the clusters. The integral equations provide a general foundation for the theory. In particular, they lead to a formal justification of the variational identity presented here and serve to determine how the closed-channel component of the trial function is to be defined to establish the subsidiary minimum principle.

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I. INTRODUCTION

Significant advances have been made in recent years in the development of a theory of reactions involving three charged particles [1,2]. Calculational procedures have been devised [3] that avoid difficulties associated with the complicated asymptotic form of the three-body wave function, and impressive achievements have been reported [4,5]. The Merkuriev theory, on the other hand [1,2], deals directly and rigorously with these matters with the aid of an extension of the Faddeev integral equation formulation [6] to include the effects of long-range Coulomb interactions in the construction of the Green's functions that appear in the kernel of the integral equation. Applications of the theory have appeared recently [7] which, while still limited in scope, indicate the feasibility of the approach.

It seems reasonable to assume that this class of three-body charged-particle collision problems will come under computational control in the near future. In this case it is appropriate to consider, as the next logical extension, the effects of internal structure of the constituents of the three-body scattering system, for energies below the threshold for fragmentation of any of the clusters. Since the three-body asymptotics are unchanged in this extension much of the Merkuriev theory remains applicable; this will be the underlying assumption in the developments described below. A generalization of the Faddeev integral equations to apply to three composite systems, with long-range Coulomb interactions ignored, was described some time ago [8]. The modification of that theory to allow for bound systems carrying a net charge is presented here in Sec. III. This provides the basis for a channel-decomposition of the wave function, which in turn leads to integral identities for elements of the scattering matrix. Momentum-space integral equations may be replaced by an equivalent set of coupled differential equations which might provide computational advantages [9]. In particular, variational methods in configuration space can be useful, as demonstrated for the proton-deuteron system [10], and the multiparticle dynamics of the bound clusters, affecting the structure of the closed-channel part of the configuration-space wave function, may be treated effectively using familiar procedures of the Rayleigh-Ritz type [8]. The variational principle is derived in Sec. II with a method that is best described as heuristic since orders of limits and integration are exchanged with no justification provided. This is no cause for concern, however, since the well-formulated Faddeev integral equations may be invoked to provide an alternative derivation, rather more awkward and indirect, but one that avoids this defect; this was as shown earlier in a closely related problem involving neutral, structureless particles [11,12]. A separation of a scattering trial function into open- and closed-channel parts is not unique. A particular choice is proposed that allows for the use of a subsidiary minimum principle to improve the accuracy of the closed-channel component in a systematic way. The integral-equation formulation is useful in this regard, since it provides detailed information on the structure of the wave function.

II. VARIATIONAL PRINCIPLE

We seek an approximation procedure to determine the scattering amplitudes T_{ij}, where the channel index j corresponds to a projectile incident on a two-body bound state. For the moment each of the three bodies may themselves be charged bound systems; a more explicit description of the scattering model is postponed for a while. With the resolvent defined as $G(E)=(E-H)^{-1}$ the scattering amplitude may be represented as [13]

$$T_{ij}=\lim_{E\to E_i+i0+}(E-E_i)\langle\Phi_i^{(-)}|G(E)|\Phi_j^{(+)}\rangle(E-E_j), \tag{2.1}$$

where $\Phi_j^{(+)}$ is the asymptotic outgoing wave, distorted to account for the presence of a Coulomb interaction between the colliding systems in the initial state. The incoming final-state function $\Phi_i^{(-)}$ is similarly defined and the channel energies E_j and E_i are taken to be equal. To obtain a more useful form we write $(E-E_j)|\Phi_j^{(+)}\rangle=[E-H+H-E_j]|\Phi_j^{(+)}\rangle$ and set $G(E)(E-H)=1$, valid for $\mathrm{Im}\,E>0$, to obtain

$$T_{ij}=\lim(E-E_i)\langle\Phi_i^{(-)}|G(E)(H-E_j)\Phi_j^{(+)}\rangle, \tag{2.2}$$

with the limit understood as $\mathrm{Im}\,E$ approaching zero from above. Now writing $\langle\Phi_i^{(-)}|(E-E_i)=\langle\Phi_i^{(-)}|(E-H+H-E_i)$, and proceeding as above, we arrive at the form

$$T_{ij}=\langle\Phi_i^{(-)}|(H-E_j)\Phi_j^{(+)}\rangle + \lim\langle(H-E_i)\Phi_i^{(-)}|G(E)(H-E_j)\Phi_j^{(+)}\rangle. \tag{2.3}$$

A variational principle for the scattering amplitude is obtained with the introduction, in Eq. (2.3), of the resolvent identity

$$G=G_t+[1+G_t(H-E)]G, \tag{2.4}$$

where $G_t(E)$ is a trial Green's function, with $\mathrm{Im}\,E>0$ at this point. We define

$$\begin{aligned}\tilde{\Psi}_{it}(E_i-i\eta)&\equiv G_t(E_i-i\eta)(H-E_i)\Phi_i^{(-)},\\ \tilde{\Psi}_j(E_j+i\eta)&\equiv G(E_j+i\eta)(H-E_j)\Phi_j^{(+)};\end{aligned} \tag{2.5}$$

these functions approach, in the limit $\eta\to 0+$, the scattered portions of the trial final-state wave function (denoted as $\tilde{\Psi}_{it}^{(-)}$) and the exact initial-state wave function (denoted as $\tilde{\Psi}_j^{(+)}$), respectively. With these substitutions, and with the allowance for the fact that surface terms encountered in partial integrations may be ignored when η is positive, identity (2.3) may be rewritten as

$$\begin{aligned}T_{ij}=&\langle\Phi_i^{(-)}|(H-E_j)\Phi_j^{(+)}\rangle\\ &+\lim_{\eta\to 0+}\{\langle\tilde{\Psi}_{it}(E-i\eta)|(H-E_j)\Phi_j^{(+)}\rangle\\ &+\langle(H-E_i)\Phi_i^{(-)}|\tilde{\Psi}_j(E_j+i\eta)\rangle\\ &+\langle(H-E_i)\tilde{\Psi}_{it}(E-i\eta)|\tilde{\Psi}_j(E_j+i\eta)\rangle\}.\end{aligned} \tag{2.6}$$

By interchanging the order of integral and limit and combining terms, we deduce that

$$T_{ij}=\langle\Psi_{it}^{(-)}|(H-E_j)|\Phi_j^{(+)}\rangle+\langle(H-E_i)\Psi_{it}^{(-)}|\tilde{\Psi}_j^{(+)}\rangle, \tag{2.7}$$

with $\Psi_{it}^{(-)}=\Phi_i^{(-)}+\tilde{\Psi}_{it}^{(-)}$. The replacement of the scattered wave $\tilde{\Psi}_j^{(+)}$ by a trial function provides a variational estimate of the scattering amplitude, one that is correct to first order assuming that the trial functions introduce only first-order errors.

The identity (though not the variational property) is preserved with the choice $\Psi_{it}^{(-)}=\Phi_i^{(-)}$. Consider the three-body breakup channel $i=0$ and let the distorted asymptotic wave function satisfy $(H_0-E_0)|\Phi_0^{(-)}\rangle=0$ with $\overline{V}\equiv H-H_0$, a Hermitian potential energy. Then, since

$$(H-E_j)|\Phi_j^{(+)}\rangle=-(H-E_j)|\tilde{\Psi}_j^{(+)}\rangle, \tag{2.8}$$

Eq. (2.7) may be put in the form

$$T_{ij}=\langle\Phi_i^{(-)}|(E_j-H_0)\tilde{\Psi}_j^{(+)}\rangle, \tag{2.9}$$

a relation that can serve as a convenient starting point for approximate evaluation [14].

In terms of the model scattering system discussed in more detail in Sec. III, below, let us consider a Hamiltonian of the form $H=h+K+V$, where K is the total kinetic energy of the three clusters in the center-of-mass frame and $V=\Sigma_{i=1}^{3}v_i$ is the sum of interactions between pairs. Our notation is such that a pair of particles selected from the three is denoted, as a subscript, by the number of the third (missing) particle. (A more explicit notation for Jacobi coordinates, momenta, and kinetic-energy operators may be found, for example, in Ref. [11].) For simplicity, we assume that only one of the three bodies, taken as particle 3, is composite; its internal Hamiltonian is denoted as h and its ground-state wave function satisfies

$$h|\chi\rangle=\varepsilon|\chi\rangle. \tag{2.10}$$

In addition, the particles are taken to be distinguishable. The more general case can be treated by similar methods. Following Merkuriev [1] we write, for each pair,

$$v_i=\overline{v_i}+v_i^{\ell}, \tag{2.11}$$

where the long-range contribution v_i^{ℓ} represents the Coulomb interaction between particles in pair i when all three particles are well separated and vanishes when the pair is close [15]. We then make the identification $H_0=h+K+V^{\ell}$, with $V^{\ell}=\Sigma_{i=1}^{3}v_i^{\ell}$. The asymptotic state is represented as $|\Phi_0^{(-)}\rangle=|\chi\xi_0^{(-)}\rangle$. An essential feature of the Merkuriev theory is the demonstration that a well-defined procedure is available for the solution of the asymptotic wave equation $(K+V^{\ell}+\varepsilon-E_0)|\xi_0^{(-)}\rangle=0$ [16], as well as for the construction of the asymptotic resolvent $(E-K-V^{\ell}-\varepsilon)^{-1}$. An approximation procedure for determining this Green's function was described [1], starting with an eikonal first approximation that builds in the effects of the long-range Coulomb interaction and is then followed by the use of a linear integral equation to account for its shorter range component.

An application to elastic scattering of the variational principle obtained from Eq. (2.7) would provide a trial scattered wave function $\tilde{\Psi}_{jt}^{(+)}$ which could be systematically improved using a method outlined below. Use of this function in Eq. (2.9) gives an approximate breakup amplitude which, while nonvariational, does not involve the final-state scattered wave which is difficult to estimate. To illustrate in the simplest context how a subsidiary minimum principle may be used to evaluate the closed-channel component of the wave function we consider a nuclear scattering problem with repulsive Coulomb interactions (and return in the following to the case of attractive interactions). Suppose that pair 1 is bound in the initial state and that neither of the other two pairs can bind. Let ϕ_1 denote the ground-state wave function for the pair of particles 2 and 3; it satisfies

$$(h+k_1+v_1)|\phi_1\rangle=\varepsilon_1|\phi_1\rangle. \tag{2.12}$$

The total kinetic energy has been decomposed as $K=k_1+K_1$, with K_1 denoting the kinetic-energy operator associated with the relative motion of particle 1 and the pair.

We now introduce the modified Hamiltonian

$$\hat{h}=h-\varepsilon|\chi\rangle\langle\chi|. \tag{2.13}$$

whose spectrum, owing to the property $\hat{h}|\chi\rangle=0$, differs from that of h only in that the ground-state level has been displaced upward by an amount ε. It follows that while the segment of the continuous spectrum of H, representing states with three free particles at infinity, has a threshold at energy ε, the corresponding spectrum of $\hat{H}=H-\varepsilon|\chi\rangle\langle\chi|$ begins at zero energy. This provides the basis for a minimum principle for scattering energies that lie below the threshold of the continuous spectrum of the modified Hamiltonian $\hat{H}$. Thus separating off the open-channel part of the wave function explicitly, we write [with superscript $(+)$ understood when not explicitly indicated]

$$|\Psi_1^{(+)}\rangle=|\phi_1 P\rangle+|\chi Q\rangle+|M\rangle, \tag{2.14}$$

and consider the Schrödinger equation, with E now the physical energy, written as

$$\begin{aligned}(H-E)|\Psi_1^{(+)}\rangle&=(K_1+\varepsilon_1+v_2+v_3-E)|\phi_1 P\rangle+(K+\varepsilon+V\\&\quad-E)|\chi Q\rangle+(\hat{H}-E)|M\rangle+\varepsilon|\chi\rangle\langle\chi|M\rangle\\&=0.\end{aligned} \tag{2.15}$$

(While this channel decomposition is not unique, the more general analysis of the structure of the wave function given in Sec. IV leads directly to the optimum form.) We suppose that a first approximation to the wave function has been obtained and we seek an improvement in the closed-channel function M as the solution of the inhomogeneous equation

$$(\hat{H}-E)|M\rangle=-|J\rangle, \tag{2.16}$$

where the square-integrable function J is defined by

$$|J\rangle=(K_1+\varepsilon_1+v_2+v_3-E)|\phi_1 P\rangle+\overline{V}|\chi Q\rangle, \tag{2.17}$$

with $\overline{V}=\Sigma_{i=1}^3\overline{v_i}$. According to Eq. (2.15) we still have the condition

$$(K+V^\ell+\varepsilon-E)|\chi Q\rangle+\varepsilon|\chi\rangle\langle\chi|M\rangle=0, \tag{2.18}$$

which is satisfied, formally, as $|\chi Q\rangle=(E-K-V^\ell-\varepsilon)^{-1}\varepsilon|\chi\rangle\langle\chi|M\rangle$. The asymptotically decaying solution of Eq. (2.16) may be identified as the function that minimizes

$$\mathcal{M}=(M|J\rangle+\langle J|M\rangle+\langle M|(\hat{H}-E)M\rangle. \tag{2.19}$$

The minimum property follows from the fact that the energy E lies below the threshold of the continuous spectrum of the modified Hamiltonian $\hat{H}$ [17,18]. Given an improved estimate of the closed-channel function M, more accurate estimates of the open-channel functions P and Q may be obtained by application of the variational principle derived from identity (2.7). The potential advantage of this procedure lies in the fact that the multiparticle complexities of the closed-channel component of the wave function can be reduced systematically with the aid of the minimum principle. We have previously described how this procedure is to be modified to preserve the minimum principle when, as is usually the case, the bound-state function χ is imprecisely known [8,19].

Note that Eq. (2.16) has the formal solution $|M\rangle=\hat{G}(E)|J\rangle$ with

$$\hat{G}(E)=(E-\hat{H})^{-1}. \tag{2.20}$$

The minimum principle for the closed-channel function M is applicable to the approximate determination of $\hat{G}(E)$, a modified resolvent that appears prominently in the integral-equation formulation of Sec. III.

The procedure described above is readily extended to account for a finite number of bound states in each channel. For attractive Coulomb pair interactions this is of course not possible and one must proceed differently. An infinite Rydberg series of bound states may be incorporated into the wave function through the introduction of a Coulomb Green's function for each pair that consists of oppositely charged particles, as shown in Sec. IV. Anticipating that development we look for the wave function in the form

$$|\Psi_j^{(+)}\rangle=|\Phi_j^{(+)}\rangle+|R_j\rangle+|M_j\rangle, \tag{2.21}$$

where a contribution $\Phi_j^{(+)}$ associated with the incident wave in channel j, satisfying the Schrödinger equation asymptotically, has been introduced; its explicit form is provided in Sec. IV. In place of Eq. (2.15) the wave equation now takes the form

$$\begin{aligned}(H-E_j)|\Psi_j^{(+)}\rangle&=(K_j+\varepsilon_j+V-v_j-E_j)|\Phi_j^{(+)}\rangle\\&\quad+(H-E_j)|R_j\rangle+(\hat{H}-E_j)|M_j\rangle\\&\quad+\varepsilon|\chi\rangle\langle\chi|M_j\rangle.\end{aligned} \tag{2.22}$$

Setting $R_j=\Sigma_i R_j^i$, where R_j^i contains the bound states for the pair i in the region where particle i is well separated from the pair, we require that $(\hat{H}-E_j)|M_j\rangle=-|J_j\rangle$, with

$$|J_j\rangle=(K_j+\varepsilon_j+V-v_j-E_j)|\Phi_j^{(+)}\rangle+\sum_i(\overline{V}-\overline{v_i})|R_j^i\rangle. \tag{2.23}$$

We observe that $|J_j\rangle$ in this form is normalizable even when the asymptotic form of $|R_j^i\rangle$ contains terms corresponding to (an arbitrary number of) bound states in channel i. Thus the bound-state wave function provides convergence in the variable measuring the separation of the particles in the pair and convergence in the remaining region is provided by the potential $\overline{V}-\overline{v_i}$. The validity of the minimum principle for $|M_j\rangle$, based on a functional of the form (2.19), then follows. To complete the solution of Eq. (2.22) we require that, with $M_j=\Sigma_i M_j^i$,

$$(K+V^\ell+h+\overline{v_i}-E_j)|R_j^i\rangle+\varepsilon|\chi\rangle\langle\chi|M_j^i\rangle=0, \quad (2.24)$$

which is satisfied formally as $|R_j^i\rangle=G_i(E_j)\varepsilon|\chi\rangle\langle\chi|M_j^i\rangle$, with

$$G_i(E)=[E-(K+V^\ell+h+\overline{v_i})]^{-1}. \quad (2.25)$$

A decomposition of this Green's function in a form convenient for approximate evaluation is given in Sec. III.

III. EFFECTIVE THREE-BODY INTEGRAL EQUATIONS

As a preliminary to the study of the structure of the resolvent $G(E)$ we begin with an examination of the Green's function defined in Eq. (2.25). Setting $i=1$ for definiteness we define the related operator

$$\hat{G}_1(E)=[E-(K+V^\ell+\hat{h}+\overline{v_1})]^{-1}, \quad (3.1)$$

and consider the resolvent identity

$$G_1=\hat{G}_1+\hat{G}_1\varepsilon|\chi\rangle\langle\chi|G_1. \quad (3.2)$$

Since the kernel of this integral equation is separable a formal solution is available. To put this representation in useful form we introduce some notation. We define the Green's functions $G_0(E)=(E-H_0)^{-1}$ and $\hat{G}_0(E)=(E-\hat{H}_0)^{-1}$. Noting the relations

$$\hat{G}_0|\chi\rangle=|\chi\rangle(E-K-V^\ell)^{-1}, \quad (3.3a)$$

$$\langle\chi|G_0=(E-K-V^\ell-\varepsilon)^{-1}\langle\chi|, \quad (3.3b)$$

we see that the identity analogous to that shown in Eq. (3.2) may be expressed as

$$G_0(E)=\hat{G}_0(E)+|\chi\rangle\mathcal{G}(E)\langle\chi|, \quad (3.4)$$

with

$$\mathcal{G}(E)=u(E)(E-K-V^\ell-\varepsilon)^{-1}; \quad (3.5)$$

for notational convenience we have introduced the abbreviation

$$u(E)=\varepsilon(E-K-V^\ell)^{-1}. \quad (3.6)$$

To proceed we define scattering operators as solutions of the linear integral equations

$$T_1=\overline{v_1}+\overline{v_1}G_0T_1 \quad (3.7)$$

and

$$\hat{T}_1=\overline{v_1}+\overline{v_1}\hat{G}_0\hat{T}_1. \quad (3.8)$$

Comparison of these two equations, using standard operator algebra, leads to the relation

$$T_1=\hat{T}_1+\hat{T}_1|\chi\rangle\mathcal{G}\langle\chi|T_1. \quad (3.9)$$

With the expectation value of both sides taken with respect to χ, this becomes

$$\mathcal{T}_1=\mathcal{V}_1+\mathcal{V}_1\mathcal{G}\mathcal{T}_1, \quad (3.10)$$

where the effective potential for pair 1 has been defined as

$$\mathcal{V}_1=\langle\chi|\hat{T}_1|\chi\rangle. \quad (3.11)$$

The effective scattering operator for this pair consisting of particle 2 and cluster 3, in the presence of the spectator 1 and the background long-rang Coulomb potential, is given by

$$\mathcal{T}_1=\langle\chi|T_1|\chi\rangle. \quad (3.12)$$

After these preliminaries we return to Eq. (3.2) and obtain from it, after some algebra [20], the representation

$$G_1=\hat{G}_1+\varepsilon\hat{G}_1|\chi\rangle u^{-1}[\mathcal{G}+\mathcal{G}\mathcal{T}_1\mathcal{G}]u^{-1}\langle\chi|\hat{G}_1\varepsilon. \quad (3.13)$$

Another relation, useful in the expression of a bound-state pole contribution to $\mathcal{T}_1$ in terms of that in G_1, is obtained from the expectation value of the relation $G_1=G_0+G_0T_1G_0$; we readily find that

$$\langle\chi|G_1|\chi\rangle=(E-K-V^\ell-\varepsilon)^{-1}+(E-K-V^\ell-\varepsilon)^{-1}\times\mathcal{T}_1(E-K-V^\ell-\varepsilon)^{-1}. \quad (3.14)$$

The analogous relations for subsystem 2 is obtained from the above by switching indices. For pair 3, however, consisting of particles 1 and 2 treated here as structureless, we have, in place of Eqs. (3.11) and (3.12), the somewhat simpler relations

$$\mathcal{V}_3=\overline{v_3}+\overline{v_3}(E-K-V^\ell)^{-1}\mathcal{V}_3 \quad (3.15)$$

and

$$\mathcal{T}_3=\overline{v_3}+\overline{v_3}(E-K-V^\ell-\varepsilon)^{-1}\mathcal{T}_3. \quad (3.16)$$

A representation of the full Green's function $G(E)$ analogous to that derived above for the subsystem resolvent $G_i(E)$ is obtained by fairly straightforward generalization. Thus we introduce the auxiliary operator $\hat{T}$, the solution of the integral equation

$$\hat{T}=\overline{V}+\overline{V}\hat{G}_0\hat{T}. \quad (3.17)$$

The solution obtained by iteration has the form

$$\hat{T}=\sum_{i=1}^{3}\hat{T}_i+\hat{T}_c, \quad (3.18)$$

a relation which serves to define the connected part $\hat{T}_c$. The effective potential may then be expanded as

$$\mathcal{V}=\sum_{i=1}^{4}\mathcal{V}_i\,, \tag{3.19}$$

with the effective pair potentials defined, as described earlier, by

$$\mathcal{V}_i=\langle\chi|\hat{T}_i|\chi\rangle,\quad i=1,2,3. \tag{3.20a}$$

The effective three-body (connected) interaction is given by

$$\mathcal{V}_4=\langle\chi|\hat{T}_c|\chi\rangle, \tag{3.20b}$$

and the extension of Eq. (3.10) is

$$\mathcal{T}_i=\mathcal{V}_i+\mathcal{V}_i\mathcal{G}\mathcal{T}_i\,,\quad i=1,2,3,4. \tag{3.21}$$

Relation (3.10) for a subsystem scattering operator is extended to the full system as

$$\mathcal{T}=\mathcal{V}+\mathcal{V}\mathcal{G}\mathcal{T}, \tag{3.22}$$

which can be put in Faddeev form, modified by the presence of the three-body potential $\mathcal{V}_4$ [21,8]. Thus we have the representation

$$\mathcal{T}=\sum_{i=1}^{4}\sum_{j=1}^{4}\,{}^{i}\mathcal{T}^{j}, \tag{3.23}$$

with the components satisfying

$${}^{i}\mathcal{T}^{j}=\mathcal{T}_i\delta_{ij}+\sum_{l\neq j}\,{}^{i}\mathcal{T}^{l}\mathcal{G}\mathcal{T}_j\,, \tag{3.24a}$$

$${}^{i}\mathcal{T}^{j}=\mathcal{T}_i\delta_{ij}+\sum_{l\neq i}\mathcal{T}_i\mathcal{G}\,{}^{l}\mathcal{T}^{j}. \tag{3.24b}$$

The derivation of the three-body extension of Eq. (3.13) begins with the resolvent identity

$$G=\hat{G}+\hat{G}\varepsilon|\chi\rangle\langle\chi|G, \tag{3.25}$$

which, in parallel with the derivation of Eq. (3.13), may be converted to the form

$$G=\hat{G}+\varepsilon\hat{G}|\chi\rangle u^{-1}[\mathcal{G}+\mathcal{G}\mathcal{T}\mathcal{G}]u^{-1}\langle\chi|\hat{G}\varepsilon. \tag{3.26}$$

This relation serves as the starting point for an analysis of the structure of the wave function in a manner that allows for the presence of subsystem bound states and propagators to be exhibited explicitly.

IV. WAVE FUNCTION AND SCATTERING AMPLITUDES

The structure of the resolvent operator displayed in Eq. (3.26) provides the basis for the derivation of a channel decomposition of the wave function of the type anticipated in Eqs. (2.14) and (2.21). The starting point is provided by the representation

$$|\Psi_j^{(+)}\rangle=\lim_{E\to E_j+i0+}G(E)|\Phi_j^{(+)}\rangle(E-E_j). \tag{4.1}$$

The incident Coulomb-distorted wave introduced earlier is now defined more explicitly as

$$|\Phi_j^{(+)}\rangle=|\phi_j\mathbf{q}_j^{(+)}\rangle, \tag{4.2}$$

where ϕ_j is the ground-state wave function of the pair j, satisfying an equation of the form shown in Eq. (2.12) for $j=1$. The relative motion of this pair and the projectile, particle j, is described by a modified plane wave satisfying the wave equation

$$K_{jc}|\mathbf{q}_j^{(+)}\rangle=(E_j-\varepsilon_j)|\mathbf{q}_j^{(+)}\rangle, \tag{4.3}$$

with outgoing-wave boundary conditions. Here we have defined $K_{jc}=K_j+w_j$, where w_j is an auxiliary potential introduced to account for the monopole component of the Coulomb interaction acting, in the asymptotic region, between the center of mass of the pair and the projectile. The limit in Eq. (4.1) is evaluated by identifying the residue at the bound-state pole in the scattering operator $\mathcal{T}_j$ appearing in Eq. (3.24a). We set $j=1$ temporarily, and refer to Eq. (3.14) for this evaluation. To isolate the pole contribution we introduce the expansion

$$G_1(E)=g_1(E)+G_1(E)U_1g_1(E), \tag{4.4}$$

where

$$U_1=v_2^{\ell}+v_3^{\ell}-w_1 \tag{4.5}$$

represents the multipole component of the asymptotic Coulomb interaction and

$$g_1(E)=[E-(h+k_1+v_1+K_{1c})]^{-1} \tag{4.6}$$

is the resolvent for the pair from which the pole contribution

$$g_{1P}(E)=|\phi_1\rangle(E-\varepsilon_1-K_{1c})^{-1}\langle\phi_1| \tag{4.7}$$

is extracted. The replacement of g_1 with g_{1P} in Eq. (4.4) defines G_{1P}, and provides us with the relation

$$\langle\chi|G_{1P}|\chi\rangle=\langle\chi|g_{1P}|\chi\rangle+\langle\chi|G_1U_1g_{1P}|\chi\rangle. \tag{4.8}$$

With the use of Eq. (3.14) we have the separation $\mathcal{T}_1=\mathcal{T}_{1P}+\mathcal{T}_{1Q}$, with $\mathcal{T}_{1Q}$ free of the pole singularity.

Now from Eq. (3.26) combined with Eq. (4.1) we see that the factor $\hat{G}|\Phi_1^{(+)}\rangle$ stands to the right in the expression for the wave function, but only the part of $\hat{G}$ that contributes to the pole need be retained. We identify that part by writing the eigenvalue equation (2.12) as

$$|\phi_1\rangle=\hat{g}_1(\varepsilon_1)\varepsilon|\chi\rangle\langle\chi|\phi_1\rangle, \tag{4.9}$$

with

$$\hat{g}_1(\varepsilon_1)=[\varepsilon_1-(\hat{h}+k_1+v_1)]^{-1}. \tag{4.10}$$

This suggests that we introduce the resolvent identity

$$\hat{G}(E)=\hat{g}_1(\varepsilon_1)+\hat{G}(E)(V^1+K_{1c}+\varepsilon_1-E)\hat{g}_1(\varepsilon_1), \tag{4.11}$$

with

$$V^1 = v_2 + v_3 - w_1. \tag{4.12}$$

We keep only the first term on the right in Eq. (4.11), apply the adjoint of Eq. (4.9), the representation (4.7), and the wave equation (4.3) to verify the relation

$$\lim_{E\to E_1+i0+} u(E)\langle\chi|G_{1P}|\chi\rangle\varepsilon\langle\chi|\hat{g}_1(\varepsilon_1)|\Phi_1^{(+)}\rangle(E-E_1)$$
$$=|f_1\mathbf{q}_1^{(+)}\rangle. \tag{4.13}$$

Here we defined (for $j=1$, 2, or 3 to allow for the extension specified below)

$$|f_j\rangle = u\langle\chi|(1+G_jU_j)|\phi_j\rangle. \tag{4.14}$$

The form of Eq. (3.24a) leads to the wave-function decomposition

$$|\Psi_j^{(+)}\rangle = \sum_{i=1}^{4} |\Psi_j^{i(+)}\rangle, \tag{4.15}$$

and, with the aid of the limiting relation (4.13), the representation

$$|\Psi_j^{i(+)}\rangle = \varepsilon\hat{G}|\chi\rangle u^{-1}\left[\delta_{ij} + \mathcal{G}\sum_{l\neq j} {}^{i}\mathcal{T}^{\,l}\right]|f_j\mathbf{q}_j^{(+)}\rangle. \tag{4.16}$$

The extension made here to include the initial channel $j=2$ is immediate; the verification of this form for $j=3$ requires separate treatment, given in the Appendix.

Results just obtained allow us to develop a channel decomposition of the wave function. As a first step we consider a nuclear scattering problem (deuteron scattering by a tightly bound nucleus would provide an example) involving only repulsive Coulomb interactions. We assume that each pair can support a single bound state. The incident channel is taken as $j=1$. Then, with the first term on the right in Eq. (4.16) written as $|\Psi_{1,\mathrm{inc}}\rangle\delta_{ij}$, and referring back to Eq. (4.14), we have

$$|\Psi_{1,\mathrm{inc}}\rangle = \varepsilon\hat{G}|\chi\rangle\langle\chi|(1+G_1U_1)|\Phi_1^{(+)}\rangle. \tag{4.17}$$

This form may be decomposed as

$$|\Psi_{1,\mathrm{inc}}\rangle = |\phi_1 P_{1,\mathrm{inc}}\rangle + |\chi Q_{1,\mathrm{inc}}\rangle + |M_{1,\mathrm{inc}}\rangle, \tag{4.18}$$

with expressions for these channel functions obtained as follows. We make use of Eqs. (4.11) and (4.9) to find

$$\hat{G}|\chi\rangle\varepsilon\langle\chi|\phi_1\mathbf{q}_1^{(+)}\rangle$$
$$=|\phi_1\mathbf{q}_1^{(+)}\rangle + \hat{G}[V^1+K_{1c}+\varepsilon_1-E]|\phi_1\mathbf{q}_1^{(+)}\rangle. \tag{4.19}$$

The resolvent identity (4.4), along with the decomposition $g_1=g_{1P}+g_{1Q}$, is now used to expand the second term in brackets in Eq. (4.17). With g_{1P} given by the bound-state pole term shown in Eq. (4.7) we arrive at the form

$$|P_{1,\mathrm{inc}}\rangle = |\mathbf{q}_1^{(+)}\rangle + (E-\varepsilon_1-K_{1c})^{-1}\langle\phi_1|W_1|\Phi_1^{(+)}\rangle, \tag{4.20}$$

with the limit $\mathrm{Im}\,E\to 0+$ understood, and with [22]

$$W_1 = U_1 + U_1G_1U_1. \tag{4.21}$$

There remains a contribution to the closed-channel component $|M_{1,\mathrm{inc}}\rangle$, the full expression of which is recorded below.

The first term in the expansion $g_1=g_{1P}+g_{1Q}$ having been accounted for we consider the second, nonsingular term. With the aid of Eqs. (3.3a) and (3.6) we find that

$$\varepsilon\hat{G}|\chi\rangle = (1+\hat{G}\overline{V})|\chi\rangle u, \tag{4.22}$$

from which we obtain

$$|Q_{1,\mathrm{inc}}\rangle = u\langle\chi|g_{1Q}W_1|\Phi_1^{(+)}\rangle. \tag{4.23}$$

The complete form for $|M_{1,\mathrm{inc}}\rangle$ is now determined as

$$|M_{1,\mathrm{inc}}\rangle = \hat{G}\{[V^1+K_{1c}+\varepsilon_1-E]|\phi_1P_{1,\mathrm{inc}}\rangle + \overline{V}|\chi Q_{1,\mathrm{inc}}\rangle\}. \tag{4.24}$$

This analysis can be extended to include the scattered-wave part of the expression shown in Eq. (4.16). We make use of Eq. (3.24b) to write

$${}^{i}\mathcal{T}^{\,l} = \mathcal{T}_i\delta_{il} + \sum_{m\neq i}\mathcal{T}_i\mathcal{G}^m\mathcal{T}^{\,l}, \tag{3.24b$'$}$$

with $\mathcal{T}_i$ expanded as $\mathcal{T}_{iP}+\mathcal{T}_{iQ}$. In parallel with the derivation of Eq. (4.20) we find, for channels $j=1$ or 2 and $i=1$ or 2,

$$|P_j^i\rangle = |P_{j,\mathrm{inc}}\rangle\delta_{ij} + (E-\varepsilon_i-K_{ic})^{-1}\langle f_i|\left\{\sum_{l\neq j}\sum_{m\neq i}{}^{m}\mathcal{T}^{\,l}\right.$$
$$\left. + \mathcal{G}^{-1}(1-\delta_{ij})\right\}|f_j\mathbf{q}_j^{(+)}\rangle. \tag{4.25}$$

Turning now to the contribution arising from the final-state interaction $\mathcal{T}_{iQ}$ we make use of Eq. (4.22) to obtain

$$|Q_j^i\rangle = |Q_{j,\mathrm{inc}}\rangle\delta_{ij} + \mathcal{G}\left\{\mathcal{T}_{iQ}(1-\delta_{ij})\right.$$
$$\left. + \sum_{l\neq j}\sum_{m\neq i}\mathcal{T}_{iQ}\mathcal{G}^m\mathcal{T}^{\,l}\right\}|f_j\mathbf{q}_j^{(+)}\rangle, \tag{4.26}$$

and for $i=4$ we have

$$|Q_j^4\rangle = \mathcal{G}\sum_{l\neq j}{}^{4}\mathcal{T}^{\,l}|f_j\mathbf{q}_j^{(+)}\rangle. \tag{4.27}$$

The complete closed-channel contribution is

$$|M_j^i\rangle = \hat{G}\{[V^i+K_{ic}+\varepsilon_i-E]|\phi_iP_j^i\rangle + \overline{V}|\chi Q_j^i\rangle\}. \tag{4.28}$$

Results for channel 3 (particles 1 and 2 interacting in initial or final states) require a slightly different treatment, given in the Appendix. These results combine to give the desired channel decomposition

$$|\Psi_j^{i(+)}\rangle=|\phi_1 P_j^i\rangle+|\chi Q_j^i\rangle+|M_j^i\rangle. \tag{4.29}$$

It should be emphasized that with all subsystem bound states separated off, as done above, the function Q_j^i appearing in the second term on the right in Eq. (4.28) behaves asymptotically as a three-body outgoing wave (see, for example, Ref. [11] for a review of the kinematics for this process). Then, with the additional "protection" coming from the potential $\overline{V}$, the function that is operated upon by the modified resolvent $\hat{G}$ is normalizable. The conclusion that M_j^i is asymptotically decaying is then valid, as required for the applicability of the minimum principle discussed in Sec. II. If a finite number of subsystem bound states exist they must all be separated off using a straightforward extension of the procedure described above. Clearly, a different approach is required to treat problems such as electron-atom impact ionization where attractive Coulomb interactions appear. We return to this matter below.

Scattering amplitudes may be determined by application of the rule given in Eqs. (2.1) and (4.1) and results given in Eqs. (4.25)–(4.29). We then have, for i, $j=1,2,3$,

$$T_{ij}=\lim_{E\to E_i+i0+}(E-E_i)\langle \mathbf{q}_i'^{(-)}|P_j^i\rangle, \tag{4.30}$$

where $|\mathbf{q}_j'^{(-)}\rangle$ satisfies an equation of the form of Eq. (4.3) with incoming-wave boundary conditions. We then find that

$$T_{ij}=T_{j,\mathrm{inc}}\delta_{ij}+\langle f_i\mathbf{q}_i'^{(-)}|\sum_{l\neq j}\sum_{m\neq i}[{}^m\mathcal{T}^{\,l}+\mathcal{G}^{-1}(1-\delta_{ij})]\times|f_j\mathbf{q}_j^{(+)}\rangle. \tag{4.31}$$

where

$$T_{j,\mathrm{inc}}=\langle\Phi_j^{(-)}|W_j|\Phi_j^{(+)}\rangle \tag{4.32}$$

arises from the first term on the right in Eq. (4.25) for P_j^i [23].

We now consider the matrix element T_{0j}, $j=1$, 2, and 3, representing the amplitude for breakup of the bound state of pair j upon impact with particle j. Following the notation of Sec. II, the final-state wave function is represented as $|\Phi_0^{(-)}\rangle=|\chi\xi_0^{(-)}\rangle$ with $(K+V^\ell+\varepsilon-E_0)|\xi_0^{(-)}\rangle=0$. We then have

$$T_{0j}=\lim_{E\to E_0+i0+}(E-E_0)\langle\xi_0^{(-)}|Q_j\rangle, \tag{4.33}$$

after taking into account the fact that the functions P_j and M_j lack the appropriate singularity and therefore vanish in the limit. For the same reason the final-state interactions $\mathcal{T}_{iQ}$ appearing in expression (4.26) for Q_j^i may be replaced by $\mathcal{T}_i$ since the bound-state pole term makes no contribution in the limit. Then, with the notation $\mathcal{T}^{\,l}=\Sigma_{i=1}^4\,{}^i\mathcal{T}^{\,l}$, we have

$$T_{0j}=T_{0j,\mathrm{inc}}+\langle\xi_0^{(-)}|\sum_{l\neq j}\mathcal{T}^{\,l}|f_j\mathbf{q}_j^{(+)}\rangle. \tag{4.34}$$

The term $T_{0j,\mathrm{inc}}$ arises from the first term on the right in Eq. (4.26) for Q_j^i. Replacing g_{jQ} with g_j (as justified above), we are led to the expression

$$|Q_{j,\mathrm{inc}}\rangle=u\langle\chi|g_jW_j|\Phi_j^{(+)}\rangle. \tag{4.35}$$

A more convenient form is obtained using the relation $g_jW_j=G_jU_j$. We may then apply the identity $G_j=G_0+G_0\overline{v_j}G_j$ and make use of Eqs. (3.3b) and (3.5) to obtain

$$T_{0j,\mathrm{inc}}=\lim_{E\to E_0+i0+}(E-E_0)\langle\Phi_0^{(-)}|\mathcal{G}(U_j+\overline{v_j}G_jU_j)|\Phi_j^{(+)}\rangle. \tag{4.36}$$

Writing Eq. (3.5) as $\mathcal{G}=(E-K-V^\ell-\varepsilon)^{-1}-(E-K-V^\ell)^{-1}$, and recognizing that the second term on the right does not contribute in the limit, we have

$$T_{0j,\mathrm{inc}}=\langle\Phi_0^{(-)}|(U_j+\overline{v_j}G_jU_j)|\Phi_j^{(+)}\rangle. \tag{4.37}$$

In atomic physics applications we deal with attractive Coulomb interactions. For such problems a different channel decomposition of the wave function is required, not only to justify the expressions derived above for the scattering matrix but also to preserve the subsidiary minimum principle for the closed-channel component. We therefore retrace our steps, starting once again with Eq. (4.1) for the wave function, combined with Eqs. (3.26) and (3.24a) for the Green's function $G(E)$ and scattering operator ${}^i\mathcal{T}^{\,j}$. With the entrance channel taken temporarily to be $j=1$, we note that the first term on the right in Eq. (4.17) reduces, unchanged, to the expression shown in Eq. (4.19). With regard to the second term in Eq. (4.17), of the form $\hat{G}|\chi\rangle\varepsilon\langle\chi|G_1U_1|\Phi_1^{(+)}\rangle$, we may wish to separate off a finite number of bound-state pole contributions to the Green's function G_1, but if an infinite number of bound states exist for the pair the difficulty regarding the minimum principle would remain. Here, to be specific, we leave the Green's function as it stands but "expose" it as a final-state propagator by first introducing the resolvent identity

$$\hat{G}=\hat{G}_1+\hat{G}(\overline{v_2}+\overline{v_3})\hat{G}_1, \tag{4.38}$$

and then making the replacement [similar to that made in Eq. (3.25)]

$$\hat{G}_1|\chi\rangle\varepsilon\langle\chi|G_1=G_1-\hat{G}_1. \tag{4.39}$$

At this stage we have a contribution to the complete wave function Ψ_1 of the form

$$\Psi_{1,\mathrm{inc}}=|\phi_1\mathbf{q}_1^{(+)}\rangle+|R_{1,\mathrm{inc}}\rangle+|M_{1,\mathrm{inc}}\rangle, \tag{4.40}$$

with

$$|R_{1,\mathrm{inc}}\rangle=(G_1-\hat{G}_1)U_1|\Phi_1^{(+)}\rangle \tag{4.41}$$

and

$$|M_{1,\text{inc}}\rangle=\hat{G}[V^1|\phi_1\mathbf{q}_1^{(+)}\rangle+(\overline{V}-\overline{v_1})|R_{1,\text{inc}}\rangle]. \quad (4.42)$$

The analysis of the scattered-wave part of the expression shown in Eq. (4.16) proceeds as was done previously, with the introduction of expansion (3.24b′) for the scattering operator. For the final-state interaction we use Eq. (3.14) in the form

$$u^{-1}\mathcal{G}\mathcal{T}_i\mathcal{G}=\langle\chi|G_i-G_0)|\chi\rangle u, \quad (3.14')$$

which is reduced further by writing $G_i-G_0=G_1\overline{v_i}G_0$ and using the adjoint of Eq. (3.3b). In this way we arrive at the representation, for $j=1$, 2, or 3,

$$|\Psi_j^{i(+)}\rangle=|\phi_j\mathbf{q}_j^{(+)}\rangle\delta_{ij}+|R_j^i\rangle+|M_j^i\rangle, \quad (4.43)$$

with

$$|R_j^i\rangle=|R_{j,\text{inc}}\rangle\delta_{ij}+(G_i-\hat{G}_i)\overline{v_i}|\chi\rangle\mathcal{G}\Bigg[\sum_{l\neq j}\sum_{m\neq i}{}^m\mathcal{T}^{\,l}+\mathcal{G}^{-1}(1-\delta_{ij})\Bigg]|f_j\mathbf{q}_j^{(+)}\rangle \quad (4.44)$$

and

$$|M_j^i\rangle=\hat{G}[V^j|\dot{\phi}_j\mathbf{q}_j^{(+)}\rangle\delta_{ij}+(\overline{V}-\overline{v_i})|R_j^i\rangle]. \quad (4.45)$$

As remarked earlier in the discussion following Eq. (2.23), the function operated on by the modified resolvent $\hat{G}$ in Eq. (4.45) is normalizable owing to the presence of the potential $\overline{V}-\overline{v_i}$ even when the function R_j^i contains terms corresponding to an infinite number of bound states in channel i. The function M_j is then normalizable in this form, as required for its proper identification as the closed-channel component in the determination of the scattering matrix from the full wave function. The fact that it decays asymptotically is also required, as mentioned, for the applicability of the minimum principle.

V. SUMMARY

With the recognition of significant progress currently being made in the computation of three-body scattering amplitudes, accounting for effects of long-range Coulomb interactions, inquiries into the possibility of multiparticle extensions become relevant. One may be interested, for example, in the study of deuteron-nucleus scattering, or electron-impact ionization of helium with frozen-core approximations lifted. With one or more of the three particles composite, and for scattering energies lying below the threshold for fragmentation of any of the clusters, existing formal treatments of three-body collision theory involving charged particles [1,2] can be extended, as shown here, with the introduction of effective potentials that account for virtual excitations of the clusters. In terms of these potentials a set of generalized Faddeev integral equations was established (in Sec. III) which, by virtue of the use of Coulomb-modified Green's functions in the kernel, are mathematically well defined. This allows for a rigorously valid decomposition of the scattering wave function into open- and closed-channel components from which the elements of the scattering matrix are identified, as shown in Sec. IV. A solution of the integral equations presents a formidable task and while approximation methods are available (separable representations of the effective potentials have proved useful in the past) we have focused attention here on the application of well-studied variational methods. Two principal advantages are gained in the use of the channel-decomposition of the wave function as a model for the choice of trial functions. First, convergence difficulties that can arise, in standard variational treatments, when imprecisely known subsystem bound states and propagators are introduced, are avoided when such functions are contained in the structure of the wave function, as in Eqs. (4.29) and (4.43), rather than appearing only in the asymptotic forms. [One simply treats these functions, formally, as exact until acted upon by the Hamiltonian in a variational expression such as that shown in Eq. (2.7) and only then are the approximations introduced.] In addition, the closed-channel component of the wave function has been so defined, in terms of a modified Hamiltonian from whose spectrum the three-body continuum segment has effectively been projected out, as to allow the use of a Rayleigh-Ritz type of minimum principle as an aid in its construction, as described in Sec. II. More generally, we have attempted here to provide a consistent framework for multiparticle extensions of techniques developed, with some success, in recent studies of three-body collision processes.

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APPENDIX

Here we complete the derivation of the channel decomposition of the wave function [Eq. (4.15)] involving channel 3, in which the structureless particles 1 and 2 are bound along with the composite particle 3. The bound state in this channel is of the product form $|\phi_3\rangle=|\chi\xi_3\rangle$, with $(k_3+v_3)|\xi_3\rangle=(\varepsilon_3-\varepsilon)|\xi_3\rangle$. As in the text, the analysis begins with Eqs. (4.1)–(4.3) with the resolvent represented by Eqs. (3.26) and (3.24). The statement in the text that Eq. (4.16) holds for $j=3$ is verified as follows. The expansion

$$\hat{G}=\hat{g}_3+\hat{G}V^3\hat{g}_3, \quad (A1)$$

with $V^3=v_1+v_2-w_3$, is used in place of Eq. (4.11). The asymptotic form of w_3 represents the monopole Coulomb interaction between the two bound clusters. We find that

$$\langle\chi|\varepsilon\hat{g}_3|\mathbf{\Phi}_3^{(+)}\rangle=\frac{\varepsilon}{E-(k_3+v_3+K_{3c})}|\xi_3\mathbf{q}_3^{(+)}\rangle=|\xi_3\mathbf{q}_3^{(+)}\rangle, \quad (A2)$$

and observe that only the first term on the right in Eq. (A1) contributes to the limit $E\to E_3$ in Eq. (4.1). To evaluate the limit, the relation between the scattering operator $\mathcal{T}_3$ and resolvent G_3, given by Eq. (3.14′) with $i=3$, is used, along with the identity

$$G_3=g_3+G_3U_3g_3. \tag{A3}$$

This extends Eq. (4.4), with $U_3=v_1^\ell+v_2^\ell-w_3$. The limit is now evaluated by replacing g_3 in Eq. (A3) by its bound-state pole term and this leads to Eq. (4.16).

We may represent the wave function components in the form shown in Eq. (4.29), now extended to include the entrance channel $j=3$ and exit channel $i=3$. In obtaining these results we make use of Eqs. (A1) and (A3) along with the identity $\hat{G}=\hat{G}_0+\hat{G}\overline{V}\hat{G}_0$. Thus we define

$$|P_{3,\mathrm{inc}}\rangle=|\mathbf{q}_3^{(+)}\rangle+\frac{\varepsilon}{E-(\varepsilon_3-\varepsilon)-K_{3c}}\frac{1}{E-\varepsilon_3-K_{3c}}\times\langle\phi_3|W_3|\Phi_3^{(+)}\rangle, \tag{A4}$$

with $W_3=U_3+U_3G_3U_3$. The extension of Eq. (4.23) is

$$|Q_{3,\mathrm{inc}}\rangle=u\langle\chi|g_{3Q}W_3|\Phi_3^{(+)}\rangle. \tag{A5}$$

Expressions given in the text for the wave-function components are now completed with the specification, for $j=1$, 2, or 3:

$$|P_j^3\rangle=|P_{3,\mathrm{inc}}\rangle\delta_{3j}+\frac{\varepsilon}{E-(\varepsilon_3-\varepsilon)-K_{3c}}\frac{1}{E-\varepsilon_3-K_{3c}}\times\langle f_3|\sum_{l\neq j}\sum_{m\neq 3}{}^m\mathcal{T}^{\,l}+\mathcal{G}(1-\delta_{3j})|f_j\mathbf{q}_j^{(+)}\rangle, \tag{A6}$$

$$|Q_j^3\rangle=|Q_{3,\mathrm{inc}}\rangle\delta_{3j}+\mathcal{G}\left\{\mathcal{T}_{3Q}(1-\delta_{3j})+\sum_{l\neq j}\sum_{m\neq 3}\mathcal{T}_{3Q}\mathcal{G}^m\mathcal{T}^{\,l}\right\}|f_j\mathbf{q}_j^{(+)}\rangle \tag{A7}$$

[as in Eq. (4.26) with $i=3$] and

$$|M_j^3\rangle=\hat{G}\{V^3|\phi_3P_j^3\rangle+\overline{V}|\chi Q_j^3\rangle\}. \tag{A8}$$

[1] S. P. Merkuriev, Ann. Phys. (N.Y.) **130**, 395 (1980).
[2] L. D. Faddeev and S. P. Merkuriev, *Quantum Scattering Theory for Several-Particle Systems* (Kluwer, Dordrecht, 1993).
[3] A review of some of the recent work was given by S. P. Lucey, J. Rasch, and C. T. Whelan, Proc. R. Soc. London, Ser. A **455**, 349 (1999).
[4] M. Baertschy, T. N. Rescigno, and C. W. McCurdy, Phys. Rev. A **64**, 022709 (2001).
[5] I. Bray, J. Phys. B **33**, 581 (2000).
[6] L. D. Faddeev, Zh. Eksp. Teor. Fiz. **39**, 1459 (1960) [Sov. Phys. JETP **12**, 1041 (1961)].
[7] Z. Papp, C.-Y. Hu, Z. T. Hlousek, B. Kónya, and S. L. Yakovlev, Phys. Rev. A **63**, 062721 (2001).
[8] L. Rosenberg, Phys. Rev. C **13**, 1406 (1976).
[9] C. R. Chen, J. L. Friar, and G. L. Payne, Few-Body Syst. **31**, 13 (2001).
[10] A. Kievsky, M. Viviani, and S. Rosati, Phys. Rev. C **64**, 024002 (2001).
[11] M. Lieber, L. Rosenberg, and L. Spruch, Phys. Rev. D **5**, 1330 (1972).
[12] M. Lieber, L. Rosenberg, and L. Spruch, Phys. Rev. D **5**, 1347 (1972).
[13] See, for example, L. Rosenberg, Phys. Rev. D **8**, 1833 (1973).
[14] Expressions similar to those in Eqs. (2.7) and (2.9) appeared previously in Ref. [12]. As discussed there, it is necessary in certain cases to remove oscillations in such integrals by means of an averaging procedure. Identity (2.7) of Ref. [4] is of a similar type. Numerical convergence was achieved there through the use of an "exterior complex scaling" procedure that avoids difficulties associated with the complicated asymptotic behavior of the three-body wave function.
[15] The precise definition is found in Eq. (5.105) of Ref. [2]. The virtue of this definition lies in the fact that enough of the long-range nature of the Coulomb interaction is contained in $\Sigma_{i=1}^3 v_i^\ell$ so that the effect of the residual interaction can be accounted for using well-defined integral equations. Furthermore, the long-range components vanish in a sufficiently large region of configuration space that they cannot support subsystem bound states.
[16] See also, E. O. Alt and A. M. Mukhamedzhanov, Phys. Rev. A **47**, 2004 (1993); A. M. Mukhamedzhanov and M. Lieber, *ibid.* **54**, 3078 (1996).
[17] If discrete states of $\hat{H}$ exist with energies below E they must be "subtracted out" in order to preserve the minimum property. Multichannel generalizations can be developed to account for additional subsystem bound states or resonances that increase the number of open channels. See Ref. [18] for further discussion in the context of a closely related problem.
[18] L. Rosenberg, Phys. Rev. D **9**, 1789 (1974).
[19] One might be concerned that the use of imprecisely known bound-state functions ϕ_1 and χ in the construction of trial scattering functions would introduce convergence problems (as it would in some variational approaches) since the trial function is not an asymptotic solution. This difficulty is avoided by the choice of trial function shown in Eq. (2.14); bound-state functions appear explicitly there, not just in the asymptotic form. We may treat these functions, temporarily, as exact, as done in arriving at Eq. (2.15). Then, in the actual calculation, approximate forms may be substituted. At this stage, first-order errors in the bound-state functions will lead to first-order errors in the calculated scattering amplitude. Of course, one may evaluate the bound-state functions variationally [18], thus removing all first-order errors.
[20] The derivation is similar to that leading to Eq. (3.19) of Ref. [18].

[21] R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966).

[22] The operator $W_j = U_j + U_j G_j U_j$ represents the scattering due to the long-range inverse-power potentials generated by the multipole components of the Coulomb field, an effect that plays an important role in low-energy atomic collisions.

[23] Since here the distorted waves account for the full effect of the monopole Coulomb potential, the pure Coulomb transition amplitude must be included to obtain the physical elastic transition amplitude; see Ref. [21], p. 194 or Ref. [13].