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Variational Methods in Charged-Particle Collision Theory*

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A variational principle of the Kohn type is formulated for the scattering of three charged particles, with particular attention given to the breakup process. In addition, an effective-potential theory, which also allows for variational formulation, is derived for the three-body system with long-ranged Coulomb interactions properly accounted for. These results generalize previous work done for systems with short-ranged interactions; the difference lies, essentially, in the use of Coulomb-modified plane waves to describe the asymptotic states. To establish the physical justification for this modified version of scattering theory a section is included containing a time-dependent description of the collision process in which the wave packets follow classical, Coulomb-modified, trajectories in the initial and final states.

I. INTRODUCTION

It is well known that in the time-independent formulation of multiparticle-scattering theory special consideration must be given to the case where the interactions have long-ranged Coulomb components. For example, the integral-equation approach as formulated by Faddeev[1] cannot be applied directly to the Coulomb case. Indeed, the Faddeev amplitude, defined for complex values of the energy parameter, is in general singular when continued to physical energy values.[2,3] Presumably, the physical amplitude could be obtained from modified Faddeev equations in which the plane-wave basis functions are replaced by functions which properly account for the long-ranged Coulomb effects.[4] Because of the difficulty in constructing the propagator which appears in the kernel, such equations seem to be of negligible practical utility, although they may serve some purpose as a formal tool (see Appendix).

The other traditional approach to time-independent scattering theory is one based directly on the Schrödinger equation in its differential form. In particular, since variational principles of the Kohn type[5-8] have been useful in few-body problems involving short-ranged interactions, we have set out to examine the extension of such methods to include Coulomb effects. The methods developed in Secs. III and IV of this paper should be suitable for application to electron and photon ionization processes in light atoms, as well as nuclear processes such as proton-deutron scattering and breakup.

The first problem which arises in this analysis concerns the choice of boundary conditions. Asymptotic solutions of the Schrödinger equation of the (Coulomb-modified) plane-wave[9] and outgoing spherical-wave[10,11] types have been written down previously. A physical justification of this time-independent formulation of the scattering problem can be obtained by showing how it arises from a time-dependent formulation in which particles are described by wave packets following classical, Coulomb-modified trajectories in the precollision and postcollision stages. This time-dependent analysis is outlined in Sec. II below. We have followed the standard discussion,[12] altering it here by the introduction of Coulomb modifications to the plane waves from which the wave packets are constructed. As we shall show, this is equivalent to altering the form of the wave operator. Fortunately, the mathematical core of this derivation, which is the proof that this modified wave operator has a well-defined limit as the time variable is extended to infinity, is provided by a theorem of Dollard.[13] With the convergence problem solved, the remainder of the derivation, in which the scattering amplitude is represented in terms of a Green's function for the system, or, equivalently, in terms of a time-independent solution of the Schrödinger equation satisfying Coulomb-modified boundary conditions, is fairly straightforward. The discussion in Sec. II serves the purpose of combining known results and methods in a way which emphasizes an underlying coherent physical picture and which places the subsequent applications, in Secs. III and IV, on firmer theoretical footing.

In the derivation of the Kohn variational principle (Sec. III) we concentrate on the breakup (or ionization) problem in which three charged particles are free in the final state. This derivation is somewhat heuristic in its treatment of the limiting process in which the complex energy parameter approaches the real axis from the upper half-plane. An alternate derivation based on Coulomb-modified Faddeev equations is given in the Appendix to provide additional mathematical justification. Similar methods have been used

previously[7,8] in the context of scattering by short-ranged potentials. Section IV is devoted to an effective-potential formulation of the scattering problem. Calculational methods for constructing the effective-potential matrix are not discussed explicitly here. We believe, however, that the variational approach, which has been applied previously to problems involving short-ranged interactions,[14] and which can be generalized using the method of Sec. III, should prove useful in a number of atomic and nuclear scattering problems in which long-ranged Coulomb effects play a significant role.

II. TIME-DEPENDENT SCATTERING THEORY

A. Coulomb-Modified Wave Packets

We follow the standard procedure for constructing wave-packet states describing the system in its precollision and postcollision stages, but rather than use pure plane waves we take a superposition of Coulomb-modified plane-wave states. This properly accounts for Coulomb modifications in the trajectories followed by the center of each packet, as indicated below. We consider a system of N charged particles; the ith particle has charge $z_i e$ and mass m_i. To simplify the present discussion we omit explicit reference to internal degrees of freedom of the particles as well as effects of particle identity.

The modified plane waves $\chi^{(\pm)}$ are chosen such that in the region where all interparticle distances are large they take the form given by Redmond.[9] This asymptotic form is

$$\chi^{(\pm)}(\vec{q}_1, \vec{r}_1; \ldots; \vec{q}_N, \vec{r}_N) \sim (2\pi)^{-3N/2} \exp\left(i \sum_{j=1}^{N} \vec{q}_j \cdot \vec{r}_j \right) \exp\left[\pm i \sum_{\substack{\text{pairs} \\ (i,j)}} n_{ij} \ln(q_{ij} r_{ij} \mp \vec{q}_{ij} \cdot \vec{r}_{ij}) \right] . \tag{2.1}$$

Here $\hbar\vec{q}_{ij}$ and $\vec{r}_{ij}$ represent the relative momentum and position variables for the pair (ij), respectively, and n_{ij} is given by

$$n_{ij} = \frac{z_i z_j e^2}{\hbar v_{ij}} , \tag{2.2}$$

with

$$v_{ij} = \hbar \left| \frac{\vec{q}_i}{m_i} - \frac{\vec{q}_j}{m_j} \right| . \tag{2.3}$$

Equation (2.1) represents a direct generalization of the well-known two-body version.[15]

Consider now the time-dependent functions[16]

$$\Phi^{(\pm)}(\vec{p}_1, \vec{r}_1; \ldots; \vec{p}_N, \vec{r}_N; t) = \int d^3q_1 \cdots \int d^3q_N \left[\prod_{j=1}^{N} a_j(\vec{q}_j - \vec{p}_j) e^{-i\epsilon_j(q_j)t/\hbar} \right] \chi^{(\pm)}(\vec{q}_1, \vec{r}_1; \ldots; \vec{q}_N \vec{r}_N) , \tag{2.4}$$

where $\epsilon_j(q_j)$ represents the energy of the jth particle,

$$\epsilon_j(q_j) = \frac{\hbar^2 q_j^{\,2}}{2m_j} - B_j , \tag{2.5}$$

and $a_j(\vec{q}_j - \vec{p}_j)$ is a function normalized to unity which peaks at $\vec{q}_j = \vec{p}_j$. It is understood here that in the function $\Phi^{(+)}$ the time t is large and negative and the velocities $\vec{v}_j = \hbar\vec{p}_j/m_j$ are chosen to correspond to particles approaching one another in the initial state, while in $\Phi^{(-)}$, which describes the final state $t \to +\infty$, the particles are receding from one another. In the usual approximation, which amounts to the neglect of wave-packet spreading, the functions $\Phi^{(\pm)}$ can be represented as

$$\Phi^{(\pm)} \cong \chi^{(\pm)}(\vec{p}_1, \vec{r}_1; \ldots; \vec{p}_N, \vec{r}_N) \exp\left[-i \sum_{j=1}^{N} \epsilon_j(p_j) t/\hbar \right] \prod_{j=1}^{N} G_j\left(\vec{r}_j - \vec{v}_j t + \sum_{k \neq j} \frac{z_j z_k e^2}{m_j v_{jk}^{\,2}} \left(\frac{\vec{r}_{jk}}{r_{jk}} \right) \ln|t| \right) , \tag{2.6}$$

where G_j is the Fourier transform of a_j, and is therefore peaked for vanishing values of its argument. It follows that the wave packets are concentrated about the classical trajectories[9]

$$\vec{r}_j = \vec{v}_j t - \sum_{k \neq j} \frac{z_j z_k e^2}{m_j v_{kj}^{\,2}} \left(\frac{\vec{r}_{jk}}{r_{jk}} \right) \ln|t| . \tag{2.7}$$

In particular, these packets are well separated for $|t| \to \infty$. Since the functions $\chi^{(\pm)}$ are asymptotic solu-

tions of the time-independent Schrödinger equation,[9] one easily verifies that the functions $\Phi^{(\pm)}$ satisfy the time-dependent Schrödinger equation.

We note for future reference that near the classical trajectory, where $\vec{r}_{ij} \sim \vec{v}_{ij} t$, we have

$$\ln(q_{ij} r_{ij} \mp \vec{q}_{ij} \cdot \vec{r}_{ij}) \cong \ln(2 q_{ij} v_{ij} |t|) . \tag{2.8}$$

This allows us to write

$$\Phi^{(\pm)} \cong e^{-iH_{0c}(t)/\hbar} X , \tag{2.9}$$

where $H_{0c}(t)$ is the modified Hamiltonian introduced by Dollard[13] in his construction of a convergent wave operator, and X is the time-independent wave-packet state composed of *pure* plane waves,

$$X(\vec{p}_1, \vec{r}_1; \ldots; \vec{p}_N, \vec{r}_N) = \int d^3q_1 \cdots \int d^3q_N \prod_{j=1}^{N} \left[a_j(\vec{q}_j - \vec{p}_j) \frac{e^{i\vec{q}_j \cdot \vec{r}_j}}{(2\pi)^{3/2}} \right] . \tag{2.10}$$

B. The Scattering Matrix

We represent the wave function for the system at some time t_0 in the remote past as $\Phi_\alpha^{(+)}(t_0)$; to simplify notation we have suppressed the position variables and have introduced a single subscript α to denote the momenta and internal quantum numbers which define the state. The time evolution of this state is given formally, in terms of the Hamiltonian H, by

$$\Psi_\alpha^{(+)}(t; t_0) = e^{-iH(t-t_0)/\hbar} \Phi_\alpha^{(+)}(t_0) . \tag{2.11}$$

The scattering-matrix element is defined as

$$S_{\beta\alpha} = \lim_{\substack{t \to +\infty \\ t_0 \to -\infty}} (\Phi_\beta^{(-)}(t), \Psi_\alpha^{(+)}(t; t_0)) . \tag{2.12}$$

Here, and in the following, we differ from the usual treatment[12] only in the inclusion of Coulomb effects in the asymptotic solutions $\Phi_\alpha^{(+)}$ and $\Phi_\beta^{(-)}$. With the use of the asymptotic form shown in Eqs. (2.9) and (2.10), along with Eq. (2.11), we can express the scattering matrix as

$$S_{\beta\alpha} = \lim_{\substack{t \to +\infty \\ t_0 \to -\infty}} (X_\beta, e^{iH_{0c}(\beta; t)/\hbar} e^{-iHt/\hbar} \times e^{iHt_0/\hbar} e^{-iH_{0c}(\alpha; t_0)/\hbar} X_\alpha) . \tag{2.13}$$

Here $H_{0c}(\beta; t)$ is the version of Dollard's modified Hamiltonian[13] appropriate to channel β. (This channel notation is necessary since we allow in general for rearrangement and breakup collisions in addition to elastic scattering.) According to Dollard the limits in Eq. (2.13) exist; we can write

$$S_{\beta\alpha} = (X_\beta, \Omega_\beta^{(+)\dagger} \Omega_\alpha^{(-)} X_\alpha) , \tag{2.14}$$

which is unitary by virtue of the unitarity property[13] of the wave operators $\Omega_\alpha^{(\pm)}$.

The problem of computing the scattering matrix can be reduced, in the standard way,[12] to that of solving the time-independent Schrödinger equation. While no attempt is made in the derivation given in Ref. 12 to treat the time limits in a rigorous way, this is no cause for concern since, as we have just seen, convergence is assured. At this point we could take over the argument given in Ref. 12. in its entirety were it not for a technical detail: The modified plane waves $\chi^{(\pm)}$, unlike the pure plane waves which appear in the short-ranged case, will for practical reasons not be chosen to be eigenfunctions of an energy-independent Hermitian Hamiltonian if more than two charged particles are free at infinity. Consequently, we have no assurance in general that they form a complete orthonormal set. Fortunately, the derivation can be carried through without making use of this completeness property, as we shall now show.

From Eq. (2.11) we have

$$\Psi_\alpha^{(+)}(t; t_0) = e^{-iHt/\hbar} \Psi_\alpha(0; t_0) , \tag{2.15}$$

where, assuming a two-body initial state,

$$\Psi_\alpha(0; t_0) = \int d^3q_1 \int d^3q_2 a_1(\vec{q}_1 - \vec{p}_1) a_2(\vec{q}_2 - \vec{p}_2) \times e^{i(H - E_\alpha)t_0/\hbar} \chi_\alpha^{(+)} , \tag{2.16}$$

with $E_\alpha = \epsilon_1(q_1) + \epsilon_2(q_2)$. Proceeding formally, we write

$$e^{i(H-E_\alpha)t_0/\hbar} = 1 - \frac{i}{\hbar} \int_{t_0}^{0} dt' e^{i(H-E_\alpha)t'/\hbar} (H - E_\alpha) . \tag{2.17}$$

The integral can be expressed as

$$-\frac{i}{\hbar} \int_{t_0}^{0} dt' e^{i(H - E_\alpha - i\eta)t'/\hbar} (H - E_\alpha) = (E_\alpha + i\eta - H)^{-1} (H - E_\alpha) + \frac{i}{\hbar} \int_{-\infty}^{t_0} dt' e^{i(H-E_\alpha - i\eta)t'/\hbar} (H - E_\alpha) , \tag{2.18}$$

with the limit $\eta \to 0+$ understood. Now the second term on the right-hand side of Eq. (2.18), when inserted in Eq. (2.16), gives vanishing contribution in the limit $t_0 \to -\infty$ since the wave-packet construction gives weight only to those configura-

tions for which the interparticle separations grow without bound as $t_0 \to -\infty$; for such configurations $(H - E_\alpha)\chi_\alpha^{(+)}$ becomes vanishingly small. We conclude that

$$\Psi_\alpha(0; -\infty) = \int d^3q_1 \int d^3q_2 a_1(\vec{q}_1 - \vec{p}_1) \times a_2(\vec{q}_2 - \vec{p}_2)\Psi_\alpha^{(+)}, \tag{2.19}$$

where

$$\Psi_\alpha^{(+)} = \chi_\alpha^{(+)} + (E_\alpha + i\eta - H)^{-1}(H - E_\alpha)\chi_\alpha^{(+)}. \tag{2.20}$$

Since

$$(H - E_\alpha)\Psi_\alpha^{(+)} = 0, \tag{2.21}$$

we have, from Eq. (2.15),

$$\Psi_\alpha(t; -\infty) = \int d^3q_1 d^3q_2 a_1(\vec{q}_1 - \vec{p}_1)a_2(\vec{q}_2 - \vec{p}_2) \times e^{-iE_\alpha t/\hbar}\Psi_\alpha^{(+)}. \tag{2.22}$$

The S-matrix element, Eq. (2.12), is expressed as a sum

$$S_{\beta\alpha} = S_{\beta\alpha}^{(1)} + S_{\beta\alpha}^{(2)}, \tag{2.23}$$

corresponding to the representation of $\Psi_\alpha^{(+)}$, which appears in Eq. (2.22), in the form shown in Eq. (2.20). The term $\chi_\alpha^{(+)}$ gives rise to the contribution

$$S_{\beta\alpha}^{(1)} = \lim_{t \to +\infty} (\Phi_\beta^{(-)}(t), \Phi_\alpha^{(+)}(t)). \tag{2.24}$$

If the process under consideration is of the rearrangement or breakup type, in which channels α and β correspond to different groupings of particles, then $S^{(1)}$ vanishes since the wave packets have no overlap in the limit $t \to \infty$. The same conclusion holds for the elastic process. Here, even in the case of forward scattering, the integral vanishes due to the presence of a rapidly oscillating logarithmic phase factor [essentially the one shown in Eq. (2.8)] in the integrand for $t \to \infty$. The absence of disconnected contributions to the S matrix is an understandable consequence of the long-ranged nature of the Coulomb force.

The remaining contribution to the S-matrix element arises from the use of

$$\tilde{\Psi}_\alpha(E) \equiv (E - H)^{-1}(H - E_\alpha)\chi_\alpha^{(+)}, \tag{2.25}$$

with $E = E_\alpha + i\eta$, in Eq. (2.22). To simplify the formulas, we anticipate that the transition probability of interest can be expressed in terms of the S-matrix element in which initial and final states have sharply defined momenta. In this case we obtain

$$S_{\beta\alpha}^{(2)} = \lim_{\eta \to 0+} \lim_{t \to \infty} e^{i(E_\beta - E_\alpha)t/\hbar}(\chi_\beta^{(-)}, \tilde{\Psi}_\alpha(E)). \tag{2.26}$$

The limit $t \to \infty$ can be carried out with the aid of the identity

$$\lim_{t \to \infty} \frac{e^{i(E_\beta - E_\alpha)t/\hbar}}{E_\alpha + i\eta - E_\beta} = -(2\pi i)\delta(E_\alpha - E_\beta). \tag{2.27}$$

This allows us to write

$$S_{\beta\alpha}^{(2)} = -(2\pi i)\delta(E_\alpha - E_\beta)U_{\beta\alpha}^{(+)}, \tag{2.28}$$

with

$$U_{\beta\alpha}^{(+)} = \lim_{\eta \to 0+} U_{\beta\alpha}(E), \tag{2.29}$$

and

$$U_{\beta\alpha}(E) = (E - E_\beta)(\chi_\beta^{(-)}, \tilde{\Psi}_\alpha(E)). \tag{2.30}$$

We obtain an alternate form for $U_{\beta\alpha}(E)$ by writing

$$(E - E_\beta)\tilde{\Psi}_\alpha(E) = (E - H)\tilde{\Psi}_\alpha(E) + (H - E_\beta)\tilde{\Psi}_\alpha(E), \tag{2.31}$$

and making use of Eq. (2.25) in the form

$$(E - H)\tilde{\Psi}_\alpha(E) = (H - E_\alpha)\chi_\alpha^{(+)}. \tag{2.25'}$$

Equation (2.30) then becomes

$$U_{\beta\alpha}(E) = (\chi_\beta^{(-)}, (H - E_\alpha)\chi_\alpha^{(+)}) + (\chi_\beta^{(-)}, (H - E_\beta)\tilde{\Psi}_\alpha(E)). \tag{2.32}$$

The second term on the right-hand side can be transformed with the aid of Green's theorem. Since the surface terms vanish for $\eta > 0$, we have

$$U_{\beta\alpha}^{(+)} = (\chi_\beta^{(-)}, [H - E_\alpha]\chi_\alpha^{(+)}) + \lim_{\eta \to 0+}\left([H - E_\alpha]\chi_\beta^{(-)}, \frac{1}{E_\alpha + i\eta - H}[H - E_\alpha]\chi_\alpha^{(+)}\right). \tag{2.33}$$

As a check on the above analysis we can verify that for two-body elastic scattering, the S matrix takes the expected form[17] provided we replace the modified plane waves $\chi_\alpha^{(\pm)}$ in initial and final states by exact Coulomb wave functions $\psi_{\alpha c}^{(\pm)}$. This replacement leaves the wave packets $\Phi_\alpha^{(\pm)}$ unchanged for $t \to (\mp)\infty$, as can be seen by a stationary phase argument.[18] Equation (2.24) becomes[13]

$$S_{\beta\alpha}^{(1)} = (\psi_{\beta c}^{(-)}, \psi_{\alpha c}^{(+)}), \tag{2.34}$$

which can be expressed in terms of the pure Coulomb amplitude using standard techniques.[19] In the usual treatment of scattering by a modified Coulomb potential (e.g., proton-proton scattering) one can arrive at the decomposition expressed by Eqs. (2.28) and (2.34) by summing contributions from individual partial waves. The present derivation is more direct and the physical justification of the result is clearer since we have seen how it arises from a time-dependent formulation.

III. VARIATIONAL METHOD

A. Boundary Conditions in Configuration Space

We restrict our attention in the following to the three-body problem in which a pair is bound in the initial state. Only the breakup (or ionization) process is treated explicitly. Our purpose is to extend the basic result of Ref. 7, in which a Kohn-type variational principle was derived, to include Coulomb effects.

We begin by recording the asymptotic form of the wave function $\Psi_\alpha^{(+)}$ in the region where all interparticle distances are large.[10,11] The general asymptotic form, including correlation effects associated with a finite value for one of the interparticle distances, is not completely known at present, although some progress has been made.[20] The amplitude, $T_{\beta\alpha}^{(+)}$, of the outgoing scattered wave in the center-of-mass frame will be related [see Eq. (3.5), below] to the S-matrix element defined in Eqs. (2.28) and (2.33). Since we must exclude the asymptotic regions where a pair is close, this relation is established here only for scattering to three-body final states in which the relative energy of each pair is positive. We explicitly restrict the following discussion to this case.

Let $\hat{\rho}$ be the six-dimensional configuration-space vector in the center-of-mass frame; the conjugate momentum is represented as $\hbar\hat{K}$. The vectors are scaled in such a way[7] that the total energy is $E=(\hbar^2/2m)K^2$ with m a conveniently chosen reference mass, and $K^2=\hat{K}\cdot\hat{K}$. In the region where all interparticle distances are large the scattered part of the wave function

$$\tilde{\Psi}_\alpha^{(+)} = \lim_{\eta\to 0+} \tilde{\Psi}_\alpha(E_\alpha + i\eta) \tag{3.1}$$

takes the form

$$\tilde{\Psi}_\alpha^{(+)} \sim cT_{\beta\alpha}^{(+)}\rho^{-5/2}\exp\left[i\left(K\rho - \frac{m\zeta}{\hbar^2 K}\ln 2K\rho\right)\right], \tag{3.2}$$

with ζ defined by

$$\sum_{\substack{\text{pairs}\\(ij)}} \frac{z_i z_j e^2}{r_{ij}} = \frac{\zeta}{\rho}\,. \tag{3.3}$$

A factor $(2\pi)^{-3/2}\exp(i\vec{P}_\alpha\cdot\vec{R}_\alpha/\hbar)$ describing the motion of the center-of-mass has been removed. (To simplify notation we do not introduce a new symbol to distinguish center-of-mass wave functions from those defined in Sec. II.) It is easily verified that the above form, with $cT_{\beta\alpha}^{(+)}$ independent of ρ, is an asymptotic solution of the Schrödinger equation, as required by Eq. (2.25′). The choice of the outgoing, rather than incoming, wave form is consistent with the defining relation, Eq. (3.1), which implies that the scattered wave remains bounded when K takes on a positive imaginary part. The flux at infinity associated with $\tilde{\Psi}_\alpha^{(+)}$ can be computed, and the differential cross section can be expressed in terms of $|T_{\beta\alpha}^{(+)}|^2$. With the modulus of c chosen as

$$|c| = (2\pi)^{1/2}\frac{m}{\hbar^2}K^{3/2}, \tag{3.4}$$

this expression takes the conventional form,[21] thus establishing $T_{\beta\alpha}^{(+)}$ as the breakup amplitude. The phase has not yet been fixed.

We now show that by appropriate choice of phase $T_{\beta\alpha}^{(+)}$ can be related to the amplitude $U_{\beta\alpha}^{(+)}$ of Eq. (2.33) according to

$$U_{\beta\alpha}^{(+)} = \delta(\vec{P}_\beta - \vec{P}_\alpha)T_{\beta\alpha}^{(+)}, \tag{3.5}$$

where $\vec{P}_\alpha$ and $\vec{P}_\beta$ represent the total momentum before and after the collision. To establish Eq. (3.5) it is sufficient to show that $T_{\beta\alpha}^{(+)}$ can be written in the form shown in Eq. (2.33), but evaluated in the center-of-mass frame. This is equivalent to showing that, in the center-of-mass frame,

$$T_{\beta\alpha}^{(+)} = \lim_{E\to E_\beta+i0+} (E-E_\beta)(\chi_\beta^{(-)}, \tilde{\Psi}_\alpha(E)), \tag{3.6}$$

as the discussion leading from Eq. (2.29) to Eq. (2.33) implies.

Now Eq. (3.6) can be derived by adaptation of an argument applied by McCartor and Nuttall[2] to a closely related problem.[16] Sketched briefly, the argument is based on the observation that as E approaches E_β from the upper-half plane a pole in $(\chi_\beta^{(-)}, \tilde{\Psi}_\alpha(E))$ develops as a consequence of a divergence in the spatial integration. The existence of this pole can be established and the residue computed by application of the method of stationary phase to evaluate the dominant contribution to the integral in the asymptotic region. The final-state function, evaluated in the center-of-mass frame, has the asymptotic form

$$\chi_\beta^{(-)} \sim (2\pi)^{-3}\exp\left\{i\left[\hat{Q}\cdot\hat{\rho} - \sum_{\substack{\text{pairs}\\(ij)}} n_{ij}\ln(q_{ij}r_{ij} + \vec{q}_{ij}\cdot\vec{r}_{ij})\right]\right\}. \tag{3.7}$$

The phase is stationary when $K=Q$ and $\hat{\rho}$ is parallel to $\hat{Q}$. In this case the factor n_{ij} becomes

$$\frac{z_i z_j e^2}{\hbar v_{ij}} = \frac{m z_i z_j e^2}{\hbar^2 r_{ij}}\left(\frac{\rho}{Q}\right) \tag{3.8}$$

for each pair (ij). Furthermore, since the relative position and momentum vectors are parallel, we have

$$\ln(q_{ij}r_{ij}+\vec{q}_{ij}\cdot\vec{r}_{ij}) = \ln(2q_{ij}r_{ij})$$
$$= \ln 2Q\rho + \ln\left(\frac{q_{ij}}{Q}\,\frac{r_{ij}}{\rho}\right)$$
$$= \ln 2Q\rho + \ln\left[\frac{m_i m_j}{m(m_i+m_j)}\left(\frac{r_{ij}}{\rho}\right)^2\right]. \tag{3.9}$$

Collecting these results, we see that in the neighborhood of the point of stationary phase, with $\rho\to\infty$, the final state function has the form

$$\chi_\beta^{(-)} \sim (2\pi)^{-3}\exp\left[i\left(\hat{Q}\cdot\hat{\rho} - \frac{m\zeta}{\hbar^2 Q}\ln 2Q\rho - \Delta\right)\right], \tag{3.10}$$

where the angle-dependent phase factor Δ is defined as

$$\Delta = \sum_{\substack{\text{pairs}\\(ij)}}\left(\frac{\rho}{r_{ij}}\right)\frac{mz_iz_je^2}{\hbar^2 Q}\ln\left[\frac{m_im_j}{m(m_i+m_j)}\left(\frac{r_{ij}}{\rho}\right)^2\right]. \tag{3.11}$$

With the aid of Eqs. (3.2) and (3.10) the dominant contribution to the integral in Eq. (3.6) can be evaluated. The computation is straightforward and we omit the details here. We find that with the choice

$$\arg c = \tfrac{1}{4}\pi - \Delta, \tag{3.12}$$

and with $|c|$ given by Eq. (3.4), Eq. (3.6) is indeed satisfied.

Let us emphasize that the preceding discussion has been included here since the usual argument,[6] valid for short-ranged potentials, which identifies the integral expression for the scattering amplitude with the amplitude of the outgoing wave in configuration space, makes use of the simple form of free Green's function which is unavailable in the present case. Furthermore, the analysis of this subsection provides the necessary background for the following derivation of a variational principle.

B. Kohn-Type Variational Principle for Breakup Processes

We have seen that the center-of-mass breakup amplitude $T_{\beta\alpha}^{(+)}$ which appears in Eq. (3.2) can be represented as

$$T_{\beta\alpha}^{(+)} = (\chi_\beta^{(-)}, [H-E_\alpha]\chi_\alpha^{(+)}) + \lim_{\eta\to 0+}([H-E_\beta]\chi_\beta^{(-)}, G(E)[H-E_\alpha]\chi_\alpha^{(+)}), \tag{3.13}$$

with $E = E_\alpha + i\eta$, $E_\alpha = E_\beta$, and

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

A variational expression which should be useful for approximate evaluations of the scattering amplitude may be obtained by introducing the identity[7]

$$G(E) = G_t(E) + G(E)[1+(H-E)G_t(E)], \tag{3.15}$$

where $G_t(E)$ is a trial Green's function. With the definitions

$$\tilde{\Psi}_{\alpha t}(E) = G_t(E)(H-E_\alpha)\chi_\alpha^{(+)} \tag{3.16}$$

and

$$\tilde{\Psi}_\beta(E^*) = G(E^*)(H-E_\beta)\chi_\beta^{(-)}, \tag{3.17}$$

Eq. (3.13) becomes

$$T_{\beta\alpha}^{(+)} = (\chi_\beta^{(-)}, [H-E_\alpha]\chi_\alpha^{(+)}) + \lim_{\eta\to 0+}\{([H-E_\beta]\chi_\beta^{(-)}, \tilde{\Psi}_{\alpha t}(E)) + (\tilde{\Psi}_\beta(E^*), [H-E_\alpha]\chi_\alpha^{(+)}) + (\tilde{\Psi}_\beta(E^*), [H-E]\tilde{\Psi}_{\alpha t}(E))\}. \tag{3.18}$$

The second term on the right-hand side can be written as $\lim_{\eta\to 0+} I(\eta)$, with

$$I(\eta) \equiv ([H-E_\beta]\chi_\beta^{(-)}, \tilde{\Psi}_{\alpha t}(E)) = (\chi_\beta^{(-)}, [H-E_\beta]\tilde{\Psi}_{\alpha t}(E)), \tag{3.19}$$

valid for $\eta > 0$. We then have

$$I(\eta) = (E-E_\beta)(\chi_\beta^{(-)}, \tilde{\Psi}_{\alpha t}(E)) + (\chi_\beta^{(-)}, [H-E]\tilde{\Psi}_{\alpha t}(E)). \tag{3.20}$$

We can evaluate the limit $\eta\to 0+$ in the first term on the right-hand side of Eq. (3.20) with the aid of the stationary-phase method employed earlier in connection with Eq. (3.6). The result is $T_{\beta\alpha t}^{(+)}$, the trial breakup amplitude, defined in terms of the asymptotic form of $\tilde{\Psi}_{\alpha t}^{(+)}$ by an equation similar to Eq. (3.2). If we formally set $\eta = 0+$ in the integrand of the second term on the right-hand side of Eq. (3.20), as well as in the last two terms on the right-hand side of Eq. (3.18), the resulting three terms combine to give

$$(\tilde{\Psi}_\beta^{(-)}, [H-E_\alpha]\tilde{\Psi}_{\alpha t}^{(+)}) + (\chi_\beta^{(-)}, [H-E_\alpha]\tilde{\Psi}_{\alpha t}^{(+)}) + (\tilde{\Psi}_\beta^{(-)}, [H-E_\alpha]\chi_\alpha^{(+)}).$$

We shall assume here that these integrals converge rapidly enough to justify the interchange of the order of limit and integration. To support this assumption we have included an appendix in which the results of this subsection are reproduced with the aid of modified Faddeev equations

which are presumably well defined in the limit of real energies.[4] The identity, Eq. (3.18), then takes the form

$$T^{(+)}_{\beta\alpha} = T^{(+)}_{\beta\alpha t} + (\Psi^{(-)}_{\beta}, [H - E_{\alpha}]\Psi^{(+)}_{\alpha t}), \tag{3.21}$$

where

$$\Psi^{(+)}_{\alpha t} = \chi^{(+)}_{\alpha} + \tilde{\Psi}^{(+)}_{\alpha t} \tag{3.22}$$

and

$$\Psi^{(-)}_{\beta} = \chi^{(-)}_{\beta} + \tilde{\Psi}^{(-)}_{\beta} . \tag{3.23}$$

The variational expression is obtained from this identity by replacing $\Psi^{(-)}_{\beta}$ with some estimate, $\Psi^{(-)}_{\beta t}$. As discussed previously,[7] the error thus incurred is of second order if the trial functions are correct to first order.

The identity, Eq. (3.21), is of a form which is familiar in scattering theory. The usual method of derivation, for elastic and rearrangement scattering, involves the use of Green's theorem and the evaluation of a surface integral at infinity. In the present case such an approach would be difficult due to the complicated and, as yet, incompletely known asymptotic form of the wave functions, as well as the ill-behaved nature of the integrals when evaluated for real values of the energy.[7] A virtue of the derivation given here (which is based on methods developed previously for the case of short-ranged potentials[7]) lies in the fact that only the leading contribution to the asymptotic form of $\Psi^{(-)}_{\beta}$, shown in Eq. (3.7), is involved explicitly. Furthermore, the integrals encountered are all well behaved.

With regard to applications, let us represent the trial function $\Psi^{(-)}_{\beta t}$ as

$$\Psi^{(-)}_{\beta t} = \chi^{(-)}_{\beta} + \tilde{\Psi}^{(-)}_{\beta t} . \tag{3.24}$$

In the region where all interparticle distances are large, $\tilde{\Psi}^{(-)}_{\beta t}$ may be taken to be of the form[10]

$$\tilde{\Psi}^{(-)}_{\beta t} \sim A_t \rho^{-5/2} \exp\left[-i\left(Q\rho - \frac{m\zeta}{\hbar^2 Q} \ln 2Q\rho\right)\right], \tag{3.25}$$

with A_t a variational parameter. The asymptotic form of $\chi^{(-)}_{\beta}$ is shown in Eq. (3.7). We may expect that corrections to this leading term, which fall off less rapidly than $\rho^{-5/2}$, are present in the exact wave function. Since the form of such corrections is unknown, $\chi^{(-)}_{\beta}$ is to be treated as a trial function subject to Eq. (3.7). For example, we might take the product form[9]

$$\chi^{(-)}_{\beta} = (2\pi)^{-3} \exp\left[i\left(\sum_{i=1}^{3} \vec{q}_i \cdot \vec{r}_i\right)\right] \prod_{\substack{\text{pairs} \\ ij}} g^{(-)}_{ij}(\vec{r}_{ij}), \tag{3.26}$$

where $g^{(-)}_{ij}$ is defined by expressing the two-particle center-of-mass continuum wave function as

$$\psi^{(-)}_{ij}(\vec{r}_{ij}) = (2\pi)^{-3/2} \exp[i(\vec{q}_{ij} \cdot \vec{r}_{ij})] g^{(-)}_{ij}(\vec{r}_{ij}) . \tag{3.27}$$

Note, incidentally, that in the limit of vanishing charges Eq. (3.26) reproduces the exact single-scattering corrections to the leading plane-wave term.

IV. METHOD OF EFFECTIVE POTENTIALS

The utility of the effective-potential formulation of the scattering problem has been recognized for many years. Recently, minimum principles for energies below the breakup threshold and unitary variational approximations at arbitrary energies have been discussed,[14] but without explicit consideration of long-ranged Coulomb effects. We are now in a position to take such effects into account in the formalism. We would anticipate that the required modification would amount, essentially, to the replacement of pure plane waves by Coulomb-distorted waves. This is the case in a problem such as proton-proton scattering, as discussed at the end of Sec. II. Here we show that the modification is indeed of the above-mentioned character. We treat explicitly the three-body problem, including the effects of target breakup, making use of the time-independent theory described in Sec. II. To simplify the discussion we consider a problem (such as proton-deuteron scattering) in which no more than one bound state exists for each pair. The formalism is easily generalized. (In the atomic case, of course, it is not possible in practice, nor is it necessary, to build an infinite number of target states into the effective potential matrix.)

The amplitudes for elastic and rearrangement scattering will be represented in the form[22]

$$T^{(+)}_{ij} = \lim \langle \vec{k}^{(-)}_i | \mathcal{T}_{ij}(E) | \vec{k}^{(+)}_j \rangle, \tag{4.1}$$

with $E_i = E_j$. Here and in the following the notation "lim" indicates that the complex energy E approaches the physical energy from above the real axis. For $i \neq j$, $T^{(+)}_{ij}$ represents the rearrangement amplitude in which pair j is bound in the initial state and pair i is bound in the final state. For $i = j$, a pure Coulomb contribution must be added to obtain the physical elastic amplitude, as discussed earlier in connection with Eq. (2.34). The states $|\vec{k}^{(\pm)}_j\rangle$ describe the relative motion of projectile and target; they satisfy

$$\mathcal{H}_j |\vec{k}^{(\pm)}_j\rangle = \mathcal{E}_j |\vec{k}^{(\pm)}_j\rangle . \tag{4.2}$$

The effective one-body Hamiltonian $\mathcal{H}_j$ is the sum of a kinetic energy term and a potential $\mathcal{U}_j$ which accounts for the long-ranged Coulomb interaction in channel j. For $j = 1$, e.g., we define

$$\mathcal{V}_1 = e^2 z_1 (z_2 + z_3) \left| \vec{r}_1 - \frac{m_2 \vec{r}_2 + m_3 \vec{r}_3}{m_2 + m_3} \right|^{-1} . \tag{4.3}$$

The complete initial-state vector is $|\chi_j^{(+)}\rangle = |\phi_j\rangle |\vec{k}_j^{(+)}\rangle$, where $|\phi_j\rangle$, the target bound-state vector, satisfies

$$H_j |\phi_j\rangle = -B_j |\phi_j\rangle , \tag{4.4}$$

with $H_j = K_j + V_j$ representing the Hamiltonian associated with the internal state of the pair. The total energy in channel j is $E_j = \mathcal{E}_j - B_j$.

We look for integral equations to determine the operators $\mathcal{T}_{ij}(E)$ in Eq. (4.1). Toward this end we combine Eqs. (2.25) and (2.30) to obtain, in the notation of this section,

$$T_{ij}^{(+)} = \lim (E - E_i) \langle \chi_i^{(-)} | G(E)(H - E_j) | \chi_j^{(+)} \rangle , \tag{4.5}$$

with $G(E)$ given by Eq. (3.14). A more symmetric version of this equation is obtained by writing

$$G(E)(H - E_j) = G(E)(E - E_j) - 1 , \tag{4.6}$$

valid for $\mathrm{Im} E > 0$, and noting that only the first term on the right-hand side of Eq. (4.6) contributes to the residue at $E = E_i$. We therefore have the alternate form

$$T_{ij}^{(+)} = \lim (E - E_i) \langle \chi_i^{(-)} | G(E) | \chi_j^{(+)} \rangle (E - E_j) . \tag{4.7}$$

Another version of this equation will be useful in the following. Recalling the stationary phase method for evaluating the integral [see the discussion following Eq. (3.6)], we observe that it is only the part of the asymptotic form of the scattered wave $|\tilde{\Psi}_j(E)\rangle$ in which the pair i is bound that contributes. Since this part is proportional to $|\phi_i\rangle$ we can replace the state $\langle \phi_i |$ in Eq. (4.7) by $\lambda_i \langle \Gamma_i |$, restricted only by the normalization condition

$$\lambda_i \langle \Gamma_i | \phi_i \rangle = 1 . \tag{4.8}$$

Then Eq. (4.7) becomes

$$T_{ij}^{(+)} = \lim (E - E_i) \lambda_i \langle \vec{k}_i^{(-)} | \langle \Gamma_i | G(E) | \phi_j \rangle | \vec{k}_j^{(+)} \rangle (E - E_j) . \tag{4.9}$$

To obtain the desired integral equations for $\mathcal{T}_{ij}(E)$ we follow the resolvent operator approach of Grassberger and Sandhas,[23] suitably modified to include Coulomb effects. Thus, we write the three-body Hamiltonian as $H = K + V$, where K is the total kinetic energy operator and $V = \sum_{i=1}^{3} V_i$ is the sum of the pair interactions. We now decompose V in the form $V = V_A + V_B$, with

$$V_B = \sum_{i=1}^{3} \lambda_i |\Gamma_i\rangle \langle \Gamma_i | . \tag{4.10}$$

While greater generality is possible, we shall make the specific choice

$$|\Gamma_i\rangle = V_i |\phi_i\rangle , \tag{4.11}$$

$$\lambda_i^{-1} = \langle \phi_i | V_i | \phi_i \rangle . \tag{4.12}$$

We now introduce the resolvent

$$G_A = (E - H_A)^{-1} , \tag{4.13}$$

with $H_A = K + V_A$, and consider the identity

$$G(E) = G_A(E) + G_A(E) V_B G(E) . \tag{4.14}$$

Premultiplication by $\langle \Gamma_i |$ and the use of Eq. (4.10) gives

$$\langle \Gamma_i | G = \langle \Gamma_i | G_A + \sum_{k=1}^{3} \langle \Gamma_i | G_A | \Gamma_k \rangle \lambda_k \langle \Gamma_k | G . \tag{4.15}$$

To put this equation in a form with a connected kernel we define

$$G_{iA} = (E - H_{iA} - \mathcal{K}_i)^{-1} , \tag{4.16}$$

with $H_{iA} = K_i + V_{iA}$, and introduce

$$\langle \Gamma_i | G_A | \Gamma_j \rangle = \langle \Gamma_i | G_A | \Gamma_j \rangle_C + \langle \Gamma_i | G_{iA} | \Gamma_j \rangle \delta_{ij} . \tag{4.17}$$

Equation (4.15) then becomes

$$(1 - \lambda_i \langle \Gamma_i | G_{iA} | \Gamma_i \rangle) \langle \Gamma_i | G = \langle \Gamma_i | G_A + \sum_{k=1}^{3} \langle \Gamma_i | G_A | \Gamma_k \rangle_C \lambda_k \langle \Gamma_k | G . \tag{4.18}$$

To make contact with the physical scattering amplitude we analyze the structure of G_{iA}. We have the identity

$$(E - H_{iA} - \mathcal{K}_i)^{-1} = (-B_i - H_{iA})^{-1} - (-B_i - H_{iA})^{-1} \times (E - \mathcal{K}_i + B_i)(E - H_{iA} - \mathcal{K}_i)^{-1} . \tag{4.19}$$

Since

$$\langle \phi_i | V_i (-B_i - H_{iA})^{-1} = \langle \phi_i | , \tag{4.20}$$

it follows that

$$\langle \vec{k}_i^{(-)} | (1 - \lambda_i \langle \Gamma_i | G_{iA} | \Gamma_i \rangle) \underset{E \to E_i}{\sim} (E - E_i) \lambda_i \langle \vec{k}_i^{(-)} | . \tag{4.21}$$

This is just the factor which appears in Eq. (4.9) and suggests that an integral equation for the scattering operator can be obtained from Eq. (4.18), rewritten in the form

$$\Omega_{i0} = \langle \Gamma_i | G_A + \sum_{k=1}^{3} \mathcal{V}_{ik} \mathcal{G}_k \Omega_{k0} . \tag{4.22}$$

We have defined the effective potential operator

$$\mathcal{V}_{ik} = \langle \Gamma_i | G_A | \Gamma_k \rangle_C , \tag{4.23}$$

and the modified Coulomb propagator

$$\mathcal{G}_k = (\lambda_k^{-1} - \langle \Gamma_k | G_{kA} | \Gamma_k \rangle)^{-1} . \tag{4.24}$$

A formal solution of Eq. (4.22) is given by

$$\Omega_{i0} = \langle \Gamma_i | G_A + \sum_{k=1}^{3} \mathcal{T}_{ik} \mathcal{G}_k \langle \Gamma_k | G_A , \tag{4.25}$$

where the operators $\mathcal{T}_{ij}$ are defined as solutions of the coupled equations

$$\mathcal{T}_{ij} = \mathcal{V}_{ij} + \sum_{k=1}^{3} \mathcal{V}_{ik} \mathcal{G}_k \mathcal{T}_{kj} . \tag{4.26}$$

Our notation anticipates that $\mathcal{T}_{ij}$ can be identified with the scattering operator which appears in Eq. (4.1). To verify this we first observe that

$$T_{ij}^{(+)} = \lim \langle \vec{k}_i^{(-)} | \Omega_{i0} | \phi_j \rangle | \vec{k}_j^{(+)} \rangle (E - E_j) . \tag{4.27}$$

Now we replace Ω_{i0} in the above equation by the right-hand side of Eq. (4.25). The first term, arising from $\langle \Gamma_i | G_A$, has vanishing residue and therefore makes no contribution. The second term does contribute by virtue of the propagator pole

$$\mathcal{G}_j | \vec{k}_j^{(+)} \rangle \underset{E \to E_j}{\sim} (E - E_j)^{-1} | \vec{k}_j^{(+)} \rangle \tag{4.28}$$

[see Eqs. (4.21) and (4.24)] which arises in the term $k=j$, with $\langle \Gamma_j | G_A$ replaced by its disconnected part. Since $\langle \Gamma_j | G_{jA} = \langle \phi_j |$ plus terms which vanish on the energy shell [see Eq. (4.20)], we conclude that the residue is $\langle \vec{k}_i^{(-)} | \mathcal{T}_{ij} | \vec{k}_j^{(+)} \rangle$, thus completing the demonstration.

With obvious modifications of the above procedure we can derive the representation

$$\Omega_{0j} = G_A | \Gamma_j \rangle + \sum_{k=1}^{3} G_A | \Gamma_k \rangle \mathcal{G}_k \mathcal{T}_{kj} , \tag{4.29}$$

with

$$\Omega_{0j} \equiv G | \Gamma_j \rangle (1 - \lambda_j \langle \Gamma_j | G_{jA} | \Gamma_j \rangle) . \tag{4.30}$$

The breakup amplitude can then be expressed as

$$T_{0j}^{(+)} = \lim (E - E_0) \chi_0^{(-)} | \Omega_{0j} | \vec{k}_j^{(+)} \rangle , \tag{4.31}$$

where $E_0 = E_j$ and $\chi_0^{(-)}$ is the three-body modified plane wave whose asymptotic form is shown in Eq. (3.7). Once the integral equations for the amplitudes $T_{ij}^{(+)}$ have been solved, the breakup amplitude is obtained by quadratures. The term

$$V_{0j}^{(+)} \equiv \lim (E - E_0) \langle \chi_0^{(-)} | G_A | \Gamma_j \rangle | \vec{k}_j^{(+)} \rangle \tag{4.32}$$

which arises in this computation can be put into a more convenient form if we substitute

$$G_A = G_{jA} + G_A (H_A - H_{jA} - \mathcal{K}_j) G_{jA} \tag{4.33}$$

in Eq. (4.32). The disconnected part, arising from the term G_{jA}, is dropped. This can be justified by reverting to the time-dependent wave-packet description and observing that the integrand contains a logarithmic phase factor, arising from the final-state function, which is rapidly oscillating as $t \to \infty$. The argument is similar to the one given earlier in connection with the forward scattering contribution to Eq. (2.24). The second term on the right-hand side of Eq. (4.33) contains the factor

$$H_A - H_{jA} - \mathcal{K}_j = \sum_{k \neq j} V_{kA} - \mathcal{V}_j , \tag{4.34}$$

which represents the interaction between pair j and the third particle with the pure Coulomb (monopole) contribution removed. Then, defining

$$| \tilde{\chi}_j(E) \rangle = G_{jA}(E) | \Gamma_j \rangle | \vec{k}_j^{(+)} \rangle , \tag{4.35}$$

we have

$$V_{0j}^{(+)} = \lim (E - E_0) \left\langle \chi_0^{(-)} \middle| G_A(E) \left[\sum_{k \neq j} V_{kA} - \mathcal{V}_j \right] \middle| \tilde{\chi}_j(E) \right\rangle . \tag{4.36}$$

In a manner similar to that used earlier in going from Eq. (2.29) to Eq. (2.33) we can transform Eq. (4.36) to

$$V_{0j}^{(+)} = \lim \left\{ \left\langle \chi_0^{(-)} \middle| \left[\sum_{k \neq j} V_{kA} - \mathcal{V}_j \right] \middle| \tilde{\chi}_j(E_j + i\eta) \right\rangle + \left\langle (H - E_0) \chi_0^{(-)} \middle| G_A(E_j + i\eta) \left[\sum_{k \neq j} V_{kA} - \mathcal{V}_j \right] \middle| \tilde{\chi}_j(E_j + i\eta) \right\rangle \right\} . \tag{4.37}$$

Equations (4.23) and (4.37) provide definitions of the effective potential matrix elements for elastic, rearrangement, and breakup collisions which are similar in form to those given earlier[14] for the case of short-ranged forces. We recall that the motivation for this effective potential transformation lies in the simpler structure of the modified Green's function G_A compared with the original Green's function G. Thus, G_A is defined in Eq. (4.13) in terms of a Hamiltonian H_A involving two-body potentials which have been weakened by subtraction of separable components. These components [Eq. (4.10)] can be chosen such that low-lying bound states present in the original two-particle spectrum cannot be supported by the residual interaction. As a consequence the continuum threshold E_{cA} of H_A lies above the physical threshold E_c. For scattering energies which lie between E_c and E_{cA}, the variational principle for G_A, and hence for the effective potential, becomes a minimum principle, the sign of the error being rigorously determined.[14] The power of the variational approach is very much enhanced by this minimum property. Techniques introduced in the present paper allow for straightforward extension of this variational bound formulation to problems such as proton-deuteron scattering and to scattering of positrons and electrons by He^+. Numerical applications for these systems appear to be quite feasible. For energies above the breakup threshold, the variational principle still applies but the minimum property is lost. The effective-

potential approach may still be useful. For example, the residual interaction may be weak enough for perturbation methods to apply.[24] Furthermore, it allows for the variational construction of scattering amplitudes satisfying unitarity constraints.[25]

APPENDIX

The variational identity, Eq. (3.21), is rederived here using modified Faddeev equations in which the long-ranged Coulomb effects are taken into account exactly in the intermediate-state propagator as well as in the initial and final states. Correspondingly, the interactions which appear are without long-ranged Coulomb components. We expect therefore that the essential elements of Faddeev's original analysis can be applied to these modified equations[4] so that, in particular, the interchange of order of integration and limit Im$E \to 0+$ is justified.

We take as the starting point a representation of the three-body breakup amplitude of the form

$$T_{\beta\alpha} = \lim(E - E_\beta)(\chi_\beta^{(-)}, G(E)\chi_\alpha^{(+)})(E - E_\alpha), \tag{A1}$$

with $G(E)$ given by Eq. (3.14). The Hamiltonian is expressed as

$$H = K_c + \sum_{i=1}^{3} U_i, \tag{A2}$$

where all the long-ranged Coulomb interactions are contained in K_c. With $G_c(E)$ defined as

$$G_c(E) = (E - K_c)^{-1}, \tag{A3}$$

equations of the Faddeev type can be written down for the construction of $G(E)$, with G_c and U_j playing the role of "free" Green's function and potential, respectively. Unique solutions to these equations are assumed to exist for Im$E \geq 0$, and to be continuous in the limit Im$E \to 0+$. Thus, we define T_i, $i = 1, 2, 3$ by the integral equations

$$T_i = U_i + T_i G_c U_i, \tag{A4}$$

and consider Faddeev-type equations for the amplitudes $T^{(i)}$ of the form

$$T^{(i)} = T_i + \sum_{j \neq i} T^{(j)} G_c T_i. \tag{A5}$$

One easily shows that $G(E)$ can be represented as

$$G = G_c + G_c \sum_{i=1}^{3} T^{(i)} G_c. \tag{A6}$$

Let us specify that it is pair 1 which is bound in the initial state. By virtue of Eqs. (A5) we can write Eq. (A6) as

$$G = G_1 + G_c(T^{(2)} + T^{(3)})G_1, \tag{A7}$$

with

$$G_1 = G_c + G_c T_1 G_c. \tag{A8}$$

Combining Eqs. (A1) and (A7) and defining

$$\overline{\chi}_\alpha(E) = (E - E_\alpha)G_1(E)\chi_\alpha^{(+)} \tag{A9}$$

and

$$\overline{\chi}_\beta(E^*) = (E^* - E_\beta)G_c(E^*)\chi_\beta^{(-)}, \tag{A10}$$

we obtain the representation

$$\begin{aligned} T_{\beta\alpha}^{(+)} &= \lim[(E - E_\beta)(\chi_\beta^{(-)}, \overline{\chi}_\alpha(E)) \\ &\quad + (\overline{\chi}_\beta(E^*), [T^{(2)} + T^{(3)}]\overline{\chi}_\alpha(E))] \\ &\equiv \lim[T_{\beta\alpha A}(E) + T_{\beta\alpha B}(E)]. \end{aligned} \tag{A11}$$

At this stage the procedure leading to a variational expression for the breakup amplitude is very similar to that described previously in the case of short-ranged potentials.[8] We confine ourselves in the following to pointing out the modifications needed in the present case; details omitted here can be found in Ref. 8.

The term $T_{\beta\alpha B}$ in Eq. (A11) can be written with the aid of a variational identity satisfied by the solutions $T^{(i)}$ of Eq. (A5). After some algebraic manipulation, we arrive at the form [analogous to Eq. (2.36) of Ref. 8]

$$\begin{aligned} T_{\beta\alpha B}(E) &= (\Psi_\beta(E^*), [H - E]\overline{\chi}_\alpha(E)) \\ &\quad + (\hat{\Psi}_\beta(E^*), [H - E]\hat{\Psi}_{\alpha t}(E)) \\ &\quad - \sum_{j=1}^{3} (\hat{\chi}_{\beta j}(E^*), [K_c + U_j - E]\hat{\Psi}_{\alpha t}(E)). \end{aligned} \tag{A12}$$

We have defined the functions

$$\begin{aligned} \hat{\Psi}_\beta &= G_c \sum_{j=1}^{3} T^{(j)} \overline{\chi}_\beta \\ &= \Psi_\beta - \overline{\chi}_\beta, \end{aligned} \tag{A13}$$

$$\hat{\Psi}_{\alpha t} = \sum_{j \neq 1} G_c T_t^{(j)} \overline{\chi}_\alpha, \tag{A14}$$

and

$$\hat{\chi}_{\beta j} = G_c T_j \overline{\chi}_\beta. \tag{A15}$$

In Eq. (A14), $T_t^{(j)}$ represents a trial solution of Eq. (A5). Now for Im$E > 0$

$$\begin{aligned} &(\hat{\chi}_{\beta j}(E^*), [K_c + U_j - E]\hat{\Psi}_{\alpha t}(E)) \\ &\quad = ([K_c + U_j - E^*]\hat{\chi}_{\beta j}(E^*), \hat{\Psi}_{\alpha t}(E)) \\ &\quad = -(\overline{\chi}_\beta(E^*), U_j \hat{\Psi}_{\alpha t}(E)). \end{aligned} \tag{A16}$$

The last term on the right-hand side of Eq. (A12) can then be expressed as

$$\begin{aligned} \sum_{j=1}^{3} (\overline{\chi}_\beta(E^*), U_j \hat{\Psi}_{\alpha t}(E)) &= (\overline{\chi}_\beta(E^*), [H - E]\hat{\Psi}_{\alpha t}(E)) \\ &\quad - (\overline{\chi}_\beta(E^*), [K_c - E]\hat{\Psi}_{\alpha t}(E)). \end{aligned} \tag{A17}$$

Equation (A12) then becomes

$$T_{\beta\alpha B}(E) = (\Psi_\beta(E^*), [H-E]\Psi_{\alpha t}(E)) - (\bar{\chi}_\beta(E^*), [K_c - E]\hat{\Psi}_{\alpha t}(E)), \quad \text{(A18)}$$

with $\Psi_{\alpha t} = \bar{\chi}_\alpha + \hat{\Psi}_{\alpha t}$. The second term on the right-hand side of Eq. (A18) is written [see (A10)]

$$\begin{aligned} &-([K_c - E^*]\bar{\chi}_\beta(E^*), \hat{\Psi}_{\alpha t}(E)) \\ &= (E-E_\beta)(\chi_\beta^{(-)}, \hat{\Psi}_{\alpha t}(E)) \\ &= -(E-E_\beta)(\chi_\beta^{(-)}, \bar{\chi}_\alpha(E)) + (E-E_\beta)(\chi_\beta^{(-)}, \Psi_{\alpha t}(E)). \end{aligned} \quad \text{(A19)}$$

The first term in the last member of Eq. (A19) is $-T_{\beta\alpha A}(E)$ and cancels an identical term in Eq. (A11). The second term in (A19) becomes $T_{\beta\alpha t}^{(+)}$ in the limit $E \to E_\beta + i0+$, as discussed earlier in connection with Eq. (3.20). After combining these results and defining

$$\Psi_\beta^{(-)} = \lim \Psi_\beta(E^*) \quad \text{(A20)}$$

and

$$\Psi_{\alpha t}^{(+)} = \lim \Psi_{\alpha t}(E), \quad \text{(A21)}$$

we find that we have reproduced Eq. (3.21) of the text.

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[25]A detailed account of this idea, for the case of short-ranged potentials, is given by Carew and Rosenberg in the third paper listed in Ref. 14.