Scattering theory with the Coulomb potential

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Abstract. Basic features of a new surface-integral formulation of scattering theory are outlined. This formulation is valid for both short-range and Coulombic longe-range interactions. New general definitions for the potential scattering amplitude are given. For the Coulombic potentials the generalized amplitude gives the physical on-shell amplitude without recourse to a renormalization procedure. New post and prior forms for the amplitudes of breakup, direct and rearrangement scattering in a Coulomb three-body system are presented.

1. Introduction

Conventional quantum collision theory is valid only when particles interact via short-range potentials. For charged particles the theory requires modification due to the fact that the long range of the Coulomb potential distorts the incident and scattered waves right out to infinity. Formal scattering theory is generalized to include Coulomb long-range potentials using renormalization methods [1]. The renormalization theories lead to the correct cross sections for the two-body problem, however, the results from these procedures cannot be regarded as satisfactory. For instance, in screening-based renormalization methods different ways of screening lead to different asymptotic forms for the scattering wave function. These asymptotic forms differ from the exact one obtained from the solution of the Schrödinger equation. The weakest point about the renormalization methods, however, is that they give rise to a scattering amplitude that does not exist on the energy shell. This is because the amplitude obtained in these methods has complex factors which are divergent on the energy shell. Therefore, these factors must be removed (renormalized) before approaching the on-shell point. Furthermore, the renormalization factors depend on the way the limits are taken when the on-shell point is approached. In other words, depending on the way you take the limits different factors need to be removed. Thus, the *ad-hoc* renormalization procedure is based on the prior knowledge of the exact answer and has no *ab initio* theoretical justification. In quantum collision theory it is customary to define the scattering amplitude in terms of the scattering wavefunction and the potential of interaction. Despite the fact that the Coulomb wavefunction and the Coulomb potential are both known analytically, the conventional theory has not been able to provide such a standard definition for the amplitude of scattering of two charged particles, which yields the Rutherford cross section [2].

An even more complicated situation is present for a few-body system. Rigorous scattering theory for a system of three particles valid for short-range potentials was given by Faddeev [3].

For the charged particles with the long-range Coulomb interaction the theory has faced difficulties associated with the compactness of the underlying equations. A renormalization method was implemented successfully for the three-body problem when only two particles are charged [4]. There are no compact integral equations yet known for collisions of more than two charged particles that are satisfactory above the breakup threshold [1]. Furthermore, there is no theoretical proof or practical evidence that a renormalization approach can be applied to the Faddeev equations for the three-body Coulomb problem. This has serious consequences especially for three-body problems in atomic physics where all three particles are charged. See [1] for all aspects of the Coulomb problem.

As far as breakup of a bound state of two particles in a system of three charged particles is concerned, the key problem is how to extract the scattering information from the wavefunction when the latter is available. The conventional theory fails to provide a formal post-form definition of the breakup amplitude for three charged particles in terms of the total wavefunction with outgoing scattered waves describing the process. Therefore, the Coulomb interaction is screened and the formula for the short-range case is used. However, it is well known that the short-range definition of the breakup amplitude diverges when the screening radius is taken to infinity. Thus we have a situation where we cannot use the theory unless we screen the Coulomb interaction, and when we do, we end up with quantities which diverge as screening is removed. This leaves no choice but to use renormalization to fix unphysical results. As mentioned above this is not possible in all cases of interest. Therefore, a new approach to the Coulomb three-body problem that does not need renormalization is required.

Despite the aforementioned problems, a surprising, but remarkable, progress has been achieved in describing (e,2e) processes via the exterior complex-scaling (ECS) [5, 6] and the convergent close-coupling (CCC) [7] methods. The success of the ECS approach to Coulomb breakup in particular caused us to reexamine the underlying formal theory [8, 9]. In the ECS method the amplitude is calculated from Peterkop's trial integral [10] which is likely to be some kind of approximation to the exact breakup amplitude in the post form (unavailable in conventional scattering theory). In the CCC method one of the electrons is treated using a square-integrable (L^2) representation, and the breakup amplitude can be related to a particular form of Peterkop's integral. Despite the success of the computational methods in describing the measured cross sections, the traditional formal theory of scattering was unable to provide a definition for the breakup amplitude in terms of the scattered wave. This has been a long-standing problem [11].

In the present work we outline a new surface-integral approach to formulating scattering theory. This represents an extension of the general formalism of scattering theory to systems of two and three charged particles with long-range Coulombic interactions. It is made possible by the recently obtained analytic forms of the three-body asymptotic wavefunctions (see [12] and references therein). Further details of the present formalism can be found in Ref. [13].

2. Two-body scattering problem

In scattering theory we deal with functions which are not L^2. Non-L^2 functions make certain integrals emerging in the theory divergent. In case of integrals containing the interaction potential a standard procedure which ensures existence of the integrals is limiting the range of the potential which irreversibly distorts the nature of the problem. Alternatively, we first formulate the scattering problem in a finite region of coordinate space and then extend it to the full space.

Let us consider first a system of two particles interacting via long-range potential. The scattering state of this system is a solution to the Schrödinger equation (SE)

$$(\epsilon - h)\psi^{\pm}_{\vec{k}}(\vec{r}) = 0, \tag{1}$$

where $h = h_0 + V$, $h_0 = -\Delta_{\vec{r}}/2\mu$ is the free Hamiltonian operator, V is an interaction potential with the Coulomb tail, $\epsilon = k^2/2\mu$ is the energy of the relative motion, $\vec{r}$ is the relative coordinate of the particles 1 and 2 and $\vec{k}$ is their relative momentum, μ is the reduced mass.

From all possible solutions to Eq. (1) we should choose the one behaving asymptotically, in the leading order, like the Coulomb-modified plane wave and a Coulomb-modified outgoing spherical wave

$$\psi_{\vec{k}}^+(\vec{r}) \quad \overset{r \to \infty}{\sim} \quad e^{i\vec{k} \cdot \vec{r} + i\gamma \ln(kr - \vec{k} \cdot \vec{r})}[1 + O(1/r)] + f(\widehat{\vec{k} \cdot \vec{r}})\frac{e^{ikr - i\gamma \ln(2kr)}}{r}[1 + O(1/r)], \qquad (2)$$

where γ is the Sommerfeld parameter. The second suitable solution $\psi_{\vec{k}}^-(\vec{r})$ can be found from the well known relationship $\psi_{\vec{k}}^-(\vec{r}) = \left[\psi_{-\vec{k}}^+(\vec{r})\right]^*$. Note that $\vec{k} \cdot \vec{r} \neq \pm kr$, respectively for $\psi_{\vec{k}}^\pm(\vec{r})$. If $\vec{k} \cdot \vec{r} = \pm kr$, the phases of distorted plane waves do not have limits due to the logarithmic singularities. However, the strength of the present approach is that it explicitly shows how contributions from these directions exactly cancel out before they pose any problem.

As the form of Eqs. (2) suggests, the leading order term in the asymptotic region already contains all the scattering information we want. The next-order terms simply repeat this information. Therefore, all we need for extracting the scattering amplitude is the leading-order asymptotic term of the scattered wave. Let us denote the leading-order incident waves as $\phi_{\vec{k}}^{(0)\pm}(\vec{r}) = e^{i\vec{k} \cdot \vec{r} \pm i\gamma \ln(kr \mp \vec{k} \cdot \vec{r})}$, and single them out in $\psi_{\vec{k}}^\pm$ according to $\psi_{\vec{k}}^\pm(\vec{r}) = \phi_{\vec{k}}^{(0)\pm}(\vec{r}) + \psi_{\vec{k}}^{\text{sc}\pm}(\vec{r})$. This splitting represents the logical fact that the unscattered incident wave is coming from infinity and should be taken in a form valid at asymptotically large distances. Then Eq. (1) can be written in the form

$$(\epsilon - h)\psi_{\vec{k}}^{\text{sc}\pm}(\vec{r}) \quad = \quad (h - \epsilon)\phi_{\vec{k}}^{(0)\pm}(\vec{r}). \qquad (3)$$

Let us multiply Eq. (3) (for $\psi_{\vec{k}}^{\text{sc}+}$) by $\psi_{\vec{k}'}^{-*}(\vec{r})$ from the left and integrate the result over the volume of a sphere of radius r_0:

$$\langle \psi_{\vec{k}'}^- | (\epsilon - h)\psi_{\vec{k}}^{\text{sc}+} \rangle_{r_0} \quad = \quad \langle \psi_{\vec{k}'}^- | (h - \epsilon)\phi_{\vec{k}}^{(0)+} \rangle_{r_0}, \qquad (4)$$

where $\psi_{\vec{k}'}^-(\vec{r})$ is another solution of the SE at a different momentum but the same energy ϵ, i.e. $k' = k$. Subtracting $\langle (\epsilon - h)\psi_{\vec{k}'}^- | \psi_{\vec{k}}^{\text{sc}+} \rangle_{r_0} = 0$, which is valid for all r_0 due to Eq. (1), from Eq. (4) we get

$$-\langle \psi_{\vec{k}'}^- | h_0 \psi_{\vec{k}}^{\text{sc}+} \rangle_{r_0} + \langle h_0 \psi_{\vec{k}'}^- | \psi_{\vec{k}}^{\text{sc}+} \rangle_{r_0} \quad = \quad \langle \psi_{\vec{k}'}^- | (h - \epsilon)\phi_{\vec{k}}^{(0)+} \rangle_{r_0}. \qquad (5)$$

Here the two integrals containing $\epsilon - V$ canceled each other. One can argue that such integrals diverge unless V is short ranged. This is true but only for the whole space. The canceled integrals are over the limited space and are finite. This emphasizes the whole idea behind working in a limited space which is to make potentially divergent terms disappear. The left-hand side of Eq. (5) would vanish if the operator h_0 were Hermitian. Now we let $r_0 \to \infty$ on both sides of the equation

$$\lim_{r_0 \to \infty} \left[-\langle \psi_{\vec{k}'}^- | h_0 \psi_{\vec{k}}^{\text{sc}+} \rangle + \langle h_0 \psi_{\vec{k}'}^- | \psi_{\vec{k}}^{\text{sc}+} \rangle \right]_{r_0} \quad = \quad \lim_{r_0 \to \infty} \langle \psi_{\vec{k}'}^- | (h - \epsilon)\phi_{\vec{k}}^{(0)+} \rangle_{r_0}. \qquad (6)$$

In order to establish the meaning of this equation we evaluate its both sides. For the LHS of Eq. (6) we have

$$\text{LHS} \quad = \quad \lim_{r_0 \to \infty} \left[-\frac{1}{2\mu} r^2 \int d\hat{\vec{r}} \left(\psi_{\vec{k}}^{\text{sc}+} \frac{\partial \psi_{\vec{k}'}^{-*}}{\partial r} - \psi_{\vec{k}'}^{-*} \frac{\partial \psi_{\vec{k}}^{\text{sc}+}}{\partial r} \right) \right]_{r=r_0}. \qquad (7)$$

Above we used the Green's theorem to transform the volume integral into the surface one. Using the asymptotic forms for the wavefunctions and

$$e^{i\vec{k}\cdot\vec{r}\pm i\gamma\ln(kr\mp\vec{k}\cdot\vec{r})} \xrightarrow{r\to\infty} \frac{2\pi}{ikr}\left[e^{ikr-i\gamma\ln(2kr)}\delta(\hat{\vec{k}}-\hat{\vec{r}}) - e^{-ikr+i\gamma\ln(2kr)}\delta(\hat{\vec{k}}+\hat{\vec{r}})\right]. \qquad (8)$$

for the distorted plane waves $\phi_{\vec{k}}^{(0)\pm}(\vec{r})$ [2] we get from Eq. (7)

$$\text{LHS} = -\frac{2\pi}{\mu}f(\hat{\vec{k}}'\cdot\hat{\vec{k}}). \qquad (9)$$

Since the latter is simply the on-shell transition matrix $(-2\pi/\mu\ f = t)$ then we can write Eq. (6) as

$$t^{\text{prior}}(\vec{k}',\vec{k}) = \langle\psi_{\vec{k}'}^{-}|(h-\epsilon)\phi_{\vec{k}}^{(0)+}\rangle. \qquad (10)$$

Thus we have a definition for the on-shell T-matrix. We emphasize that, this definition has emerged as a result of a surface integral which has not vanished at infinity. In addition, in order to show this there was no need to use a formal solution of the SE in the integral form [2].

We now consider Eq. (3) for $\psi_{\vec{k}'}^{\text{sc}-}$ and multiply it by $\psi_{\vec{k}}^{+}$ from the right. Integrating the result over the volume of a sphere of radius r_0 we have

$$\langle(\epsilon-h)\psi_{\vec{k}'}^{\text{sc}-}|\psi_{\vec{k}}^{+}\rangle_{r_0} = \langle(h-\epsilon)\phi_{\vec{k}'}^{(0)-}|\psi_{\vec{k}}^{+}\rangle_{r_0}, \qquad (11)$$

where again $k' = k$. Subtracting $\langle\psi_{\vec{k}'}^{\text{sc}-}|(\epsilon-h)\psi_{\vec{k}}^{+}\rangle_{r_0} = 0$ from Eq. (11) we get

$$-\langle h_0\psi_{\vec{k}'}^{\text{sc}-}|\psi_{\vec{k}}^{+}\rangle_{r_0} + \langle\psi_{\vec{k}'}^{\text{sc}-}|h_0\psi_{\vec{k}}^{+}\rangle_{r_0} = \langle(h-\epsilon)\phi_{\vec{k}'}^{(0)-}|\psi_{\vec{k}}^{+}\rangle_{r_0}. \qquad (12)$$

This equation is similar to Eq. (5) in form. Taking the $r_0 \to \infty$ limit on both sides and calculating the LHS in similar way we find the second form for the T-matrix

$$t^{\text{post}}(\vec{k}',\vec{k}) = \langle(h-\epsilon)\phi_{\vec{k}'}^{(0)-}|\psi_{\vec{k}}^{+}\rangle. \qquad (13)$$

The results given above are consistent with conventional potential scattering theory for short-range interactions. The existing formulation of scattering theory relies on the condition that interaction $V(r)$ decreases faster than the Coulomb interaction when $r \to \infty$, so that $\phi_{\vec{k}}^{(0)\pm}(\vec{r}) \to e^{i\vec{k}\cdot\vec{r}}$. For the plane wave we have $(h-\epsilon)e^{i\vec{k}\cdot\vec{r}} = Ve^{i\vec{k}\cdot\vec{r}}$. Therefore, the two forms given by Eqs. (10) and (13), respectively, are in fact identical to the standard prior and post forms of the T-matrix

$$t^{\text{prior}}(\vec{k}',\vec{k}) = \langle\psi_{\vec{k}'}^{-}|V|\vec{k}\rangle \quad \text{and} \quad t^{\text{post}}(\vec{k}',\vec{k}) = \langle\vec{k}'|V|\psi_{\vec{k}}^{+}\rangle. \qquad (14)$$

On the other hand, when the interaction is pure Coulomb (no short-range component), the new forms of the scattering amplitude both give the well-known on-shell Coulomb T-matrix [2]. This confirms that the new definitions of the two-body T-matrix are indeed general for both short- and long-range interactions.

3. Three-body scattering problem

Let us consider a system of three particles of mass m_α and charge z_α, $\alpha = 1, 2, 3$. We use the Jacobi coordinates where $\vec{r}_\alpha$ is the relative coordinate, and $\vec{k}_\alpha$ is the relative momentum, between particles β and γ, $\vec{\rho}_\alpha$ is the relative coordinate of the center of mass of the pair (β, γ) and particle α, with $\vec{q}_\alpha$ being the canonically conjugate relative momentum. The corresponding reduced masses are denoted by $\mu_\alpha = m_\beta m_\gamma / (m_\beta + m_\gamma)$ and $M_\alpha = m_\alpha (m_\beta + m_\gamma) / (m_\alpha + m_\beta + m_\gamma)$. Here $\beta, \gamma = 1, 2, 3$, $\alpha \neq \beta \neq \gamma$. In addition, we introduce a hyperradius in the six-dimensional configurations space according to $R = (\mu_\alpha r_\alpha^2 + M_\alpha \rho_\alpha^2)^{1/2}$, and a five-dimensional hyperangle $\omega = (\widehat{\vec{r}}_\alpha, \widehat{\vec{\rho}}_\alpha, \varphi_\alpha)$, where $\varphi_\alpha = \arctan\left[(\mu_\alpha / M_\alpha)^{1/2} r_\alpha / \rho_\alpha \right]$, $0 \leq \varphi_\alpha \leq \pi/2$.

Consider now scattering of particle α with incident momentum $\vec{q}_{\alpha n}$ off a bound pair (β, γ) in initial state $\phi_{\alpha n}(\vec{r}_\alpha)$ of energy $E_{\alpha n}$. Here n denotes a full set of quantum numbers of the bound state (β, γ) in channel α. Assume that the energy of the projectile $q_{\alpha n}^2 / 2M_\alpha$ is enough to break up the target. Note that, in addition to direct scattering and rearrangement $(\beta + (\gamma, \alpha))$ channels, there is a breakup one. Therefore, we call this $2 \to 3$ process. In order to find the amplitudes of direct scattering, rearrangement and breakup in this collision we need the total scattering wavefunction developed from the initial channel αn and three different asymptotic wavefunctions corresponding to three final-state channels. The same amplitudes can be found in the so-called prior forms as well, which requires the knowledge of the other three types of the total scattering wavefunctions being developed to three different final-state wavefunctions. Thus, in any case, we need to specify a set of four total scattering wavefunctions together with their corresponding asymptotic forms in all relevant asymptotic domains. There are two distinct types of asymptotic domains. Let us call Ω_0 the asymptotic domain, where all interparticle distances are large, i.e, $r_\alpha \to \infty$, $\rho_\alpha \to \infty$, so that r_α / ρ_α is non-zero. In addition, we call Ω_α the asymptotic regime, where $\rho_\alpha \to \infty$, however r_α satisfies the constraint $r_\alpha / \rho_\alpha \to 0$.

The total three-body wavefunction describing the $2 \to 3$ processes satisfies the Schrödinger equation

$$(E - H)\Psi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha) = 0, \tag{15}$$

with outgoing-wave boundary conditions, where $H = H_0 + V$, $H_0 = -\Delta_{\vec{r}_\alpha}/2\mu_\alpha - \Delta_{\vec{\rho}_\alpha}/2M_\alpha$ is the free Hamiltonian, $V = V_\alpha(\vec{r}_\alpha) + V_\beta(\vec{r}_\beta) + V_\gamma(\vec{r}_\gamma)$ is the full interaction and $E = E_{\alpha n} + q_{\alpha n}^2/2M_\alpha = k_\alpha^2/2\mu_\alpha + q_\alpha^2/2M_\alpha$ is the total energy of the system. We split the wavefunction $\Psi_{\alpha n}^+$ into the initial-channel wave $\Phi_{\alpha n}^+$ and scattered wave $\Psi_{\alpha n}^{sc+}$: $\Psi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha) = \Phi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha) + \Psi_{\alpha n}^{sc+}(\vec{r}_\alpha, \vec{\rho}_\alpha)$. Then we can write Eq. (15) as

$$(E - H)\Psi_{\alpha n}^{sc+}(\vec{r}_\alpha, \vec{\rho}_\alpha) = (H - E)\Phi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha). \tag{16}$$

We now consider another scattering process which may take place within the same three-body system at the same total energy E, but the one where in the initial channel (in the time-reversed picture this will be the final state) all three particles are in the continuum which we call a $3 \to 3$ scattering. The wavefunction Ψ_0^- describing this process is also an eigenstate of the same Hamiltonian H, but with incoming scattered-wave boundary conditions. In the total wavefunction $\Psi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha)$ we separate the part describing the unscattered state of three free particles, denoted $\Phi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha)$ and which Ψ_0^- is being developed to (in the absence of the Coulomb interaction this would simply be the three-body plane wave),

$$\Psi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha) = \Phi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha) + \Psi_0^{sc-}(\vec{r}_\alpha, \vec{\rho}_\alpha). \tag{17}$$

We use $\Psi_{\alpha n}^+$ and Ψ_0^- as starting points to derive amplitudes for different scattering processes. Let us multiply Eq. (16) by $\Psi_0^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha)$ from the left and integrate the result over the volume of a hypersphere of radius R_0:

$$\langle \Psi_0^- | (E - H)\Psi_{\alpha n}^{sc+} \rangle_{R_0} = \langle \Psi_0^- | (H - E)\Phi_{\alpha n}^+ \rangle_{R_0}. \tag{18}$$

Now we subtract $\langle(E - H)\Psi_0^- | \Psi_{\alpha n}^{sc+}\rangle_{R_0} = 0$ (which is true simply due to the fact that $(E - H)\Psi_0^- = 0$ for any R_0) from Eq. (18) to get

$$\langle\Psi_0^- | (E - H)\Psi_{\alpha n}^{sc+}\rangle_{R_0} - \langle(E - H)\Psi_0^- | \Psi_{\alpha n}^{sc+}\rangle_{R_0} = \langle\Psi_0^- | (H - E)\Phi_{\alpha n}^+\rangle_{R_0}. \tag{19}$$

Despite of the fact that both Ψ_0^- and $\Psi_{\alpha n}^{sc+}$ are non-L^2 functions, terms of the form $\langle\Psi_0^- | (E - V)|\Psi_{\alpha n}^{sc+}\rangle_{R_0}$ are finite due to the limited space (regardless of the long-range nature of the potential). Therefore, canceling them we get

$$-\langle\Psi_0^- | H_0\Psi_{\alpha n}^{sc+}\rangle_{R_0} + \langle H_0\Psi_0^- | \Psi_{\alpha n}^{sc+}\rangle_{R_0} = \langle\Psi_0^- | (H - E)\Phi_{\alpha n}^+\rangle_{R_0}. \tag{20}$$

Now we will investigate the limit of this equation as $R_0 \to \infty$

$$\lim_{R_0 \to \infty} \left[-\langle\Psi_0^- | H_0\Psi_{\alpha n}^{sc+}\rangle + \langle H_0\Psi_0^- | \Psi_{\alpha n}^{sc+}\rangle \right]_{R_0} = \lim_{R_0 \to \infty} \langle\Psi_0^- | (H - E)\Phi_{\alpha n}^+\rangle_{R_0}. \tag{21}$$

As in the two-body case, the meaning of this quantity will become clear when we evaluate the limit of the LHS of the equation.

Parameter R_0 can go to infinity with the system being in Ω_0 or Ω_α, $\alpha = 1, 2, 3$. An essential feature of the term on the LHS of Eq. (21) is that it is easily transformed into an integral over the hypersurface of radius R_0 so that the result depends only on the behavior of the wavefunctions on this surface. Then for this integral the knowledge of the wavefunctions anywhere inside the surface is not required. It can be evaluated using the asymptotic forms of the wavefunctions in the corresponding asymptotic domain (see[12] and references therein). If $R_0 \to \infty$ in Ω_0 then for the LHS of Eq. (21) we have

$$\begin{aligned}
\text{LHS} &= \frac{\mu^3}{(\mu_\alpha M_\alpha)^{3/2}} \lim_{R_0 \to \infty} R_0^5 \int d\hat{\vec{r}}_\alpha d\hat{\vec{\rho}}_\alpha \int_0^{\pi/2} d\varphi_\alpha \sin^2 \varphi_\alpha \cos^2 \varphi_\alpha \\
&\times \frac{1}{2\mu} \left[\Psi_0^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_{\alpha n}^{sc+}(\vec{r}_\alpha, \vec{\rho}_\alpha) - \Psi_{\alpha n}^{sc+}(\vec{r}_\alpha, \vec{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_0^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha) \right]_{R=R_0}. \tag{22}
\end{aligned}$$

Here we first transformed H_0 into (R, ω)-variables and then made use of Green's theorem to transform the volume integral into the surface integral. Now we can use the asymptotic forms for the wave functions and perform differentiation to see that this is an extremely oscillatory integral as $R_0 \to \infty$. Therefore, only points of stationary phase in φ_α, if there are any, should contribute to the integral. Calculating the integral by means of the stationary-phase method we arrive at

$$\text{LHS} = \text{T}\left(\vec{k}_\alpha, \vec{q}_\alpha\right), \tag{23}$$

where $T(\vec{k}_\alpha, \vec{q}_\alpha)$ is the amplitude of the of the scattered wave in Ω_0. Therefore, in Ω_0 domain Eq. (21) is written as

$$T^{\text{prior}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle\Psi_0^- | (H - E)\Phi_{\alpha n}^+\rangle. \tag{24}$$

In other words, if scattering takes place into Ω_0 domain then expression $\langle\Psi_0^- | (H - E)\Phi_{\alpha n}^+\rangle_{R_0}$ represents nothing else but the breakup amplitude. If after the collision the products of scattering turn out to be back in Ω_α or in Ω_β domains then we have to differentiate whether all three particles are in continuum or just one is. If all three are in continuum then in similar way we used for Ω_0 we can show that $\langle\Psi_0^- | (H - E)\Phi_{\alpha n}^+\rangle$ again represents the breakup amplitude. Thus, Eq. (24) defines the breakup amplitude in all asymptotic domains.

Another scenario is when after the collision the products of scattering form a two-fragment channel. Then instead of Ψ_0^- we will need the total scattering wavefunction which develops into the wavefunction of this two-fragment channel. We start from Ω_α domain which corresponds to direct scattering. In this case the total scattering wavefunction we need is $\Psi_{\alpha m}^-$. Let us multiply Eq. (16) by $\Psi_{\alpha m}^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha)$ from the left and integrate the result over the volume of a hypersphere of radius R_0:

$$\langle \Psi_{\alpha m}^- | (E - H) \Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} \;\; = \;\; \langle \Psi_{\alpha m}^- | (H - E) \Phi_{\alpha n}^+ \rangle_{R_0}. \tag{25}$$

Now we subtract $\langle (E - H) \Psi_{\alpha m}^- | \Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} = 0$ from Eq. (25) to get

$$-\langle \Psi_{\alpha m}^- | H_0 \Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} + \langle H_0 \Psi_{\alpha m}^- | \Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} \;\; = \;\; \langle \Psi_{\alpha m}^- | (H - E) \Phi_{\alpha n}^+ \rangle_{R_0}. \tag{26}$$

We again consider the limit of this equation as $R_0 \to \infty$. Since this time $R_0 \to \infty$ in Ω_α then on the LHS of Eq. (26) we have

$$
\begin{aligned}
\text{LHS} \;\; = \;\; & \lim_{R_0 \to \infty} \int_{R \le R_0} d\vec{r}_\alpha d\vec{\rho}_\alpha \left[-\Psi_{\alpha m}^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha) H_0 \Psi_{\alpha n}^{\text{sc}+}(\vec{r}_\alpha, \vec{\rho}_\alpha) + \Psi_{\alpha n}^{\text{sc}+}(\vec{r}_\alpha, \vec{\rho}_\alpha) H_0 \Psi_{\alpha m}^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha) \right] \\
= \;\; & \frac{1}{2M_\alpha} \lim_{R_0 \to \infty} R_0^2 \int d\vec{r}_\alpha d\hat{\vec{\rho}}_\alpha \left[\Psi_{\alpha m}^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha) \frac{\partial}{\partial \rho_\alpha} \Psi_{\alpha n}^{\text{sc}+}(\vec{r}_\alpha, \vec{\rho}_\alpha) \right. \\
& \left. -\Psi_{\alpha n}^{\text{sc}+}(\vec{r}_\alpha, \vec{\rho}_\alpha) \frac{\partial}{\partial \rho_\alpha} \Psi_{\alpha m}^{-*}(\vec{r}_\alpha, \vec{\rho}_\alpha) \right]_{\rho_\alpha = R_0}.
\end{aligned} \tag{27}
$$

Here we transformed only one of the volume integrals into the surface integral (the other two-body space is limited). Using the asymptotic forms of the wavefunctions and the orthogonality of the the two-particle bound state wavefunctions and calculating the integral we arrive at

$$\text{LHS} \;\; = \;\; F(\vec{q}_{\alpha m}, \vec{q}_{\alpha n}), \tag{28}$$

where $F(\vec{q}_{\alpha m}, \vec{q}_{\alpha n})$ is the amplitude of the wave scattered into channel α. Thus we have established that as $R_0 \to \infty$ Eq. (26) is in fact written as

$$F^{\text{prior}}(\vec{q}_{\alpha m}, \vec{q}_{\alpha n}) \;\; = \;\; \langle \Psi_{\alpha m}^- | (H - E) \Phi_{\alpha n}^+ \rangle. \tag{29}$$

In other words we have got a definition for the direct scattering (elastic and excitation) amplitude. Finally, taking $R_0 \to \infty$ in Ω_β (i.e., the final state belongs to channel β) and calculating the limit of Eq. (26) we get a definition for the amplitude of the rearrangement scattering

$$G^{\text{prior}}(\vec{q}_{\beta m}, \vec{q}_{\alpha n}) \;\; = \;\; \langle \Psi_{\beta m}^- | (H - E) \Phi_{\alpha n}^+ \rangle. \tag{30}$$

In similar way we obtain the scattering and breakup amplitudes in the post form

$$T^{\text{post}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle (E - H) \Phi_0^- | \Psi_{\alpha n}^+ \rangle, \tag{31}$$

$$F^{\text{post}}(\vec{q}_{\alpha m}, \vec{q}_{\alpha n}) = \langle (E - H) \Phi_{\alpha m}^- | \Psi_{\alpha n}^+ \rangle, \tag{32}$$

$$G^{\text{post}}(\vec{q}_{\beta m}, \vec{q}_{\alpha n}) = \langle (E - H) \Phi_{\beta m}^- | \Psi_{\alpha n}^+ \rangle, \tag{33}$$

In particular, the definition given in Eq. (31) resolves the long-standing problem about the post form of the breakup amplitude mentioned earlier [11].

Finally, we show consistency of the new definitions for the scattering and breakup amplitudes with the conventional forms. When the interactions between all three pairs are short ranged then

$\Phi_{\alpha n}^{\pm}(\vec{r}_\alpha, \vec{\rho}_\alpha) \to e^{i\vec{q}_{\alpha n}\cdot\vec{\rho}_\alpha}\phi_{\alpha n}(\vec{r}_\alpha)$. This state satisfies the equation $(H_0 + V_\alpha - E)e^{i\vec{q}_{\alpha n}\cdot\vec{\rho}_\alpha}\phi_{\alpha n}(\vec{r}_\alpha) = 0$. At the same time if we have 3 particles in the final channel then $\Phi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha) \to e^{i\vec{k}_\alpha\cdot\vec{r}_\alpha + i\vec{q}_\alpha\cdot\vec{\rho}_\alpha}$, which is the solution to $(H_0 - E)e^{i\vec{k}_\alpha\cdot\vec{r}_\alpha + i\vec{q}_\alpha\cdot\vec{\rho}_\alpha} = 0$. Therefore, the new generalized forms of the amplitudes given by Eqs. (24) and (29)-(33) reduce to the standard definitions

$$T^{\text{prior}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle \Psi_0^- | \overline{V}_\alpha | \phi_{\alpha n}, \vec{q}_{\alpha n} \rangle, \tag{34}$$

$$F^{\text{prior}}(\vec{q}_{\alpha m}, \vec{q}_{\alpha n}) = \langle \Psi_{\alpha m}^- | \overline{V}_\alpha | \phi_{\alpha n}, \vec{q}_{\alpha n} \rangle, \tag{35}$$

$$G^{\text{prior}}(\vec{q}_{\beta m}, \vec{q}_{\alpha n}) = \langle \Psi_{\beta m}^- | \overline{V}_\alpha | \phi_{\alpha n}, \vec{q}_{\alpha n} \rangle \tag{36}$$

and

$$T^{\text{post}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle \vec{q}_\alpha, \vec{k}_\alpha | V | \Psi_{\alpha n}^+ \rangle, \tag{37}$$

$$F^{\text{post}}(\vec{q}_{\alpha m}, \vec{q}_{\alpha n}) = \langle \vec{q}_{\alpha m}, \phi_{\alpha m} | \overline{V}_\alpha | \Psi_{\alpha n}^+ \rangle, \tag{38}$$

$$G^{\text{post}}(\vec{q}_{\beta m}, \vec{q}_{\alpha n}) = \langle \vec{q}_{\beta m}, \phi_{\beta m} | \overline{V}_\beta | \Psi_{\alpha n}^+ \rangle. \tag{39}$$

where $\overline{V}_\alpha = V - V_\alpha$.

4. Conclusion

The conventional formulation of scattering theory is only valid for short-range interactions. In this paper we have given a brief account of a formalism of scattering theory [13] which is applicable to two-body and three-body systems with both short-range and Coulombic long-range potentials. The new formulation is based on a surface-integral approach and is made possible by the recently obtained analytic forms of the three-body asymptotic wavefunctions. New definitions for the potential scattering amplitude valid for arbitrary interactions are presented. For Coulombic potentials these generalized definitions of the amplitude give the physical on-shell amplitude without recourse to a renormalization procedure. New prior and post forms of the breakup amplitude for a three-body system are given that are valid for both short-range and Coulombic potentials. This resolves a long-standing problem about the conventional post form of the breakup amplitude for the long-range Coulombic interactions. An essential feature of the surface-integral formulation is that it avoids any reference to the Green's functions and formal solutions of the Schrödinger equation in integral forms are not used. Therefore, for the purpose of defining the scattering amplitudes the knowledge of a complicated analytic structure of the Green's function in the complex-energy plane is not required. This constitutes a simpler yet more general alternative to formulations adopted in textbooks on scattering theory.

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