

Generalisation of scattering theory to charged particles

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Abstract. Generalisation of scattering theory to charged particles is presented. It is based on a surface-integral approach. New general definitions for the breakup amplitude in a three-body system valid for both short-range and long-range Coulombic interactions are given.

1. Introduction

In scattering of charged particles the incident and scattered waves are distorted right out to infinity due to the long-range nature of the Coulomb interaction. Therefore the Coulomb potential often receives a special treatment known in scattering theory as screening and renormalization [1]. The *ad-hoc* renormalization procedure leads to the correct cross sections for the two-body problem, however, it is based on prior knowledge of the exact answer and has no *ab initio* theoretical justification. A renormalization method was implemented successfully for the three-body problem when only two particles are charged [2]. However, no practical renormalization method exists that is valid for a system of three charged particles above the breakup threshold.

Another issue is how to extract the breakup amplitude 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. 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 invoke renormalization to fix unphysical results. As mentioned above this is not possible in all cases of interest. Therefore, a new approach to Coulomb few-body problems that does not need renormalization is required. Below we present a different approach to the same problem based on surface integrals. We use the recently derived analytic forms of the total scattering wavefunctions in asymptotic domains [3, 4] in order to develop well-defined prior and post forms of the breakup amplitude valid for short-range and Coulombic potentials.

2. Surface-integral approach to scattering theory

We shall now briefly explain the derivation of the new definitions for the breakup amplitude in order to outline the surface-integral approach. Consider scattering of particle α with incident momentum $\vec{q}_{\alpha n}$ off a bound pair (β, γ) in initial state $\phi_{\alpha n}$ of energy $E_{\alpha n}$ above the breakup threshold. The total wavefunction describing this process satisfies the Schrödinger equation

$$(E - H)\Psi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha) = 0, \quad (1)$$

with outgoing-spherical wave boundary conditions. Here $H = H_0 + V$, $H_0 = -\Delta_{\vec{r}_\alpha}/2\mu_\alpha - \Delta_{\vec{\rho}_\alpha}/2M_\alpha$ is the free Hamiltonian, $V = v + V_\alpha + V_\beta + V_\gamma$ is the full interaction, v is a three-body interaction and V_α is a Coulombic interaction between particles β and γ , $E = E_{\alpha n} + q_{\alpha n}^2/2M_\alpha = k_\alpha^2/2\mu_\alpha + q_\alpha^2/2M_\alpha$ is the total energy of the system. We use the Jacobi coordinates where \vec{r}_α and \vec{k}_α are respectively the relative coordinate and momentum between particles β and γ . The coordinate of particle α relative to the center of mass of the pair (β, γ) is $\vec{\rho}_\alpha$, with \vec{q}_α being the canonically conjugate relative momentum. The corresponding reduced masses are denoted by μ_α and M_α . Another process which may take place within the same system at the same energy E is called $3 \rightarrow 3$ scattering. The wavefunction Ψ_0^- describing this process is also an eigenstate of the same Hamiltonian H , however we impose on it incoming-wave boundary conditions. It develops to the final state where all three particles are in the continuum.

In scattering theory we deal with functions which are not square-integrable (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. To this end we introduce a partial inner product of two arbitrary functions Ψ_i and Ψ_f in the space of functions describing various states and arrangements in a three-body system according to $\langle \Psi_f | \Psi_i \rangle_{R_0} = \int_{R \leq R_0} d\vec{r}_\alpha d\vec{\rho}_\alpha \Psi_f^* \Psi_i$. Here R is a hyperradius in the 6-dimensional configurations space $R = (\mu_\alpha r_\alpha^2 + M_\alpha \rho_\alpha^2)^{1/2}$. The integration is limited to the volume of a 6-dimensional hypersphere of radius R_0 .

We want to use $\Psi_{\alpha n}^+$ and Ψ_0^- as starting points to derive prior and post forms of the breakup amplitude. If we split $\Psi_{\alpha n}^+$ into the initial-channel wave $\Phi_{\alpha n}^+$ and scattered wave $\Psi_{\alpha n}^{\text{sc}+}$ then Eq. (1) transforms to

$$(E - H)\Psi_{\alpha n}^{\text{sc}+}(\vec{r}_\alpha, \vec{\rho}_\alpha) = (H - E)\Phi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha). \quad (2)$$

We multiply Eq. (2) by Ψ_0^{-*} from the left and integrate the result over a volume of a hypersphere of radius R_0 :

$$\langle \Psi_0^- | (E - H)\Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} = \langle \Psi_0^- | (H - E)\Phi_{\alpha n}^+ \rangle_{R_0}. \quad (3)$$

For simplicity we assume V to be real. Then we have $\langle (E - H)\Psi_0^- | \Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} = 0$, which is true for any R_0 simply due to $(E - H)\Psi_0^- = 0$. Now we subtract this from Eq. (3). Despite the fact that both Ψ_0^- and $\Psi_{\alpha n}^{\text{sc}+}$ are non- L^2 functions, terms of the form $\langle \Psi_0^- | (E - V)\Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0}$ are finite due to the limited space (regardless of the nature of the potential). Therefore, canceling them we get

$$-\langle \Psi_0^- | H_0 \Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} + \langle H_0 \Psi_0^- | \Psi_{\alpha n}^{\text{sc}+} \rangle_{R_0} = \langle \Psi_0^- | (H - E)\Phi_{\alpha n}^+ \rangle_{R_0}. \quad (4)$$

Now we calculate the limit of this equation as $R_0 \rightarrow \infty$. An essential feature of the term on the left-hand side (LHS) of Eq. (4) 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. Therefore, the knowledge of the wavefunctions anywhere inside the surface is not required. Then it can be evaluated using the asymptotic forms of the wavefunctions. If $R_0 \rightarrow \infty$ with all interparticle distances being large then for the limit of the LHS of Eq. (4) we have

$$\frac{1}{2(\mu_\alpha M_\alpha)^{3/2}} \lim_{R_0 \rightarrow \infty} R_0^5 \int d\hat{r}_\alpha d\hat{\rho}_\alpha \int_0^{\pi/2} d\varphi_\alpha \sin^2 \varphi_\alpha \cos^2 \varphi_\alpha \left[\Psi_0^{-*} \frac{\partial \Psi_{\alpha n}^{\text{sc}+}}{\partial R} - \Psi_{\alpha n}^{\text{sc}+} \frac{\partial \Psi_0^{-*}}{\partial R} \right]_{R=R_0}. \quad (5)$$

Here we first transformed H_0 into (R, ω) -variables, where ω is a 5-dimensional hyperangle $(\hat{r}_\alpha, \hat{\rho}_\alpha, \varphi_\alpha)$ with $\varphi_\alpha = \arctan [(\mu_\alpha/M_\alpha)^{1/2} r_\alpha/\rho_\alpha]$. Then we made use of Green's theorem to transform the volume integral into the surface integral. The asymptotic forms of Ψ_0^- and $\Psi_{\alpha n}^{\text{sc}+}$ were given in Ref. [3] and [4], respectively. The asymptotic form of scattered wave $\Psi_{\alpha n}^{\text{sc}+}$ contains the breakup amplitude as a function of the coordinates. The above integral is infinitely oscillatory as $R_0 \rightarrow \infty$. Calculating it by means of the stationary-phase method we find that it reduces to $T(\vec{k}_\alpha, \vec{q}_\alpha)$ which is the breakup amplitude. Therefore, the limit of Eq. (4) is written as

$$T(\vec{k}_\alpha, \vec{q}_\alpha) = \lim_{R_0 \rightarrow \infty} \langle \Psi_0^- | (H - E) \Phi_{\alpha n}^+ \rangle_{R_0}. \quad (6)$$

We can also use Ψ_0^- as a starting point. If we separate Ψ_0^- into Coulomb-distorted three-body plane wave Φ_0^- and scattered wave $\Psi_0^{\text{sc}-}$ then the Schrödinger equation for Ψ_0^- can be written as

$$(E - H) \Psi_0^{\text{sc}-}(\vec{r}_\alpha, \vec{\rho}_\alpha) = (H - E) \Phi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha). \quad (7)$$

Take complex conjugate of Eq. (7) and multiply it by $\Psi_{\alpha n}^+$ from the right. Then integrating the result over the volume of a hypersphere of radius R_0 we get

$$\langle (E - H) \Psi_0^{\text{sc}-} | \Psi_{\alpha n}^+ \rangle_{R_0} = \langle (H - E) \Phi_0^- | \Psi_{\alpha n}^+ \rangle_{R_0}. \quad (8)$$

From Eq. (1) we have $\langle \Psi_0^{\text{sc}-} | (E - H) \Psi_{\alpha n}^+ \rangle_{R_0} = 0$. Subtracting this from (8) we get

$$-\langle H_0 \Psi_0^{\text{sc}-} | \Psi_{\alpha n}^+ \rangle_{R_0} + \langle \Psi_0^{\text{sc}-} | H_0 \Psi_{\alpha n}^+ \rangle_{R_0} = \langle (H - E) \Phi_0^- | \Psi_{\alpha n}^+ \rangle_{R_0}. \quad (9)$$

We again investigate the limit of this equation as $R_0 \rightarrow \infty$. However, this time we have the situation of three free particles in the initial state. In the final state we may have three free particles or two of the particles may form a bound state. In the latter case the limit of LHS of Eq. (9) is written as

$$\frac{1}{2M_\alpha} \lim_{R_0 \rightarrow \infty} R_0^2 \int d\hat{r}_\alpha d\hat{\rho}_\alpha \left[\Psi_{\alpha n}^+ \frac{\partial}{\partial \rho_\alpha} \Psi_0^{\text{sc}-*} - \Psi_0^{\text{sc}-*} \frac{\partial}{\partial \rho_\alpha} \Psi_{\alpha n}^+ \right]_{\rho_\alpha=R_0}. \quad (10)$$

An essential difference from Eq. (5) here is that only one of the three-dimensional volume integrals is transformed into the surface integral. The remaining volume integral is limited due to presence of a bound state in channel α . Calculating the limit of this equation as $R_0 \rightarrow \infty$ we obtain

$$T(\vec{k}_\alpha, \vec{q}_\alpha) = \lim_{R_0 \rightarrow \infty} \langle (H - E) \Phi_0^- | \Psi_{\alpha n}^+ \rangle_{R_0}. \quad (11)$$

The same analysis can be performed on the right-hand side of Eqs. (6) and (11) to yield $T(\vec{k}_\alpha, \vec{q}_\alpha)$. So the general prior and post forms of the breakup amplitude, valid for both short-range and Coulombic potentials, are written as

$$T^{\text{prior}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle \Psi_0^- | (H - E) \Phi_{\alpha n}^+ \rangle, \quad (12)$$

$$T^{\text{post}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle (H - E) \Phi_0^- | \Psi_{\alpha n}^+ \rangle. \quad (13)$$

3. Consistency of the results

The new definitions are consistent with the well-known ones for short-range interactions. To see this we note that when the interactions are short-ranged we have $\Phi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha) \rightarrow e^{i\vec{q}_{\alpha n}\vec{\rho}_\alpha}\phi_{\alpha n}(\vec{r}_\alpha)$. This leads to $(H - E)\Phi_{\alpha n}^+(\vec{r}_\alpha, \vec{\rho}_\alpha) = (V - V_\alpha)e^{i\vec{q}_{\alpha n}\vec{\rho}_\alpha}\phi_{\alpha n}(\vec{r}_\alpha)$. At the same time if we have three particles in the final channel then $\Phi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha) \rightarrow e^{i\vec{k}_\alpha\vec{r}_\alpha+i\vec{q}_\alpha\vec{\rho}_\alpha}$. Then we have $(H - E)\Phi_0^-(\vec{r}_\alpha, \vec{\rho}_\alpha) = Ve^{i\vec{k}_\alpha\vec{r}_\alpha+i\vec{q}_\alpha\vec{\rho}_\alpha}$. Therefore, the general forms of the amplitudes (12) and (13) reduce to the standard definitions for short-range interactions

$$T^{\text{prior}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle \Psi_0^- | V - V_\alpha | \phi_{\alpha n}, \vec{q}_{\alpha n} \rangle, \quad (14)$$

$$T^{\text{post}}(\vec{k}_\alpha, \vec{q}_\alpha) = \langle \vec{q}_\alpha, \vec{k}_\alpha | V | \Psi_{\alpha n}^+ \rangle. \quad (15)$$

4. Summary

Summarizing, we have given a brief account of a formalism of scattering theory which is applicable to three-body systems with both short-range and Coulombic potentials. The new formulation is based on a surface-integral approach. It was made possible by the recently obtained analytical forms of the three-body asymptotic wavefunctions. New representations for the breakup amplitude in a three-body system have been given. Further details of the present formalism can be found in Ref. [5].

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