Annals of Physics 324 (2009) 1516–1546

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Surface-integral formulation of scattering theory

A.S. Kadyrov [a,*], I. Bray [a], A.M. Mukhamedzhanov [b], A.T. Stelbovics [a]

[a] ARC Centre for Antimatter-Matter Studies, Curtin University of Technology, P.O. Box U1987, Perth, WA 6845, Australia
[b] Cyclotron Institute, Texas A&M University, College Station, TX 77843, USA

ARTICLE INFO

Article history:
Received 8 January 2009
Accepted 5 February 2009
Available online 10 March 2009

PACS:
03.65.Nk
21.45.−v
24.10.−i
34.10.+x

Keywords:
Scattering theory
Few-body systems
Coulomb breakup
Renormalization

ABSTRACT

We formulate scattering theory in the framework of a surface-integral approach utilizing analytically known asymptotic forms of the two-body and three-body scattering wavefunctions. This formulation is valid for both short-range and long-range Coulombic interactions. New general definitions for the potential scattering amplitude are presented. 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 Coulomb three-body breakup amplitude are derived. This resolves the problem of the inability of the conventional scattering theory to define the post form of the breakup amplitude for charged particles. The new definitions can be written as surface-integrals convenient for practical calculations. The surface-integral representations are extended to amplitudes of direct and rearrangement scattering processes taking place in an arbitrary three-body system. General definitions for the wave operators are given that unify the currently used channel-dependent definitions.

1. Introduction

Scattering in a few-body system is one of the central subjects of quantum mechanics, and yet our knowledge of the field is still incomplete. It is well known that conventional quantum collision theory is formally valid only when the particles interact via short-range potentials, see, e.g. [1]. 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. In the time-depen-

* Corresponding author.
E-mail address: A.Kadyrov@curtin.edu.au (A.S. Kadyrov).

0003-4916/$ - see front matter © 2009 Elsevier Inc. All rights reserved.
doi:10.1016/j.aop.2009.02.003

dent formulation, formal scattering theory is generalized to include Coulomb long-range potentials by choosing appropriately modified time evolution operators [2,3]. This is equivalent to choosing various forms of renormalization methods [4–9] in the time-independent formulation. The renormalization theories lead to the correct cross-sections for the two-body problem, however, the results from these procedures cannot be regarded as completely satisfactory. For instance, in screening-based renormalization methods [5,8] different ways of shielding lead to different asymptotic forms for the scattering wave function. Generally, these asymptotic forms differ from the exact one obtained from the solution of the Schrödinger equation (SE), see, e.g. [10]. The weakest point about these methods, however, is that they give rise to a scattering amplitude that does not exist on the energy shell. In other words, the resulting amplitude cannot be used for calculating cross-sections. This is because the amplitude obtained in these methods has complex factors which are divergent on the energy shell [8,11–16]. These factors, often containing branch point singularities, 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. The following question summarizes a part of formal problems. In the simple case of two charged particles, the Coulomb scattering amplitude, which yields the Rutherford cross-section, is known. However, what is the standard definition for this amplitude in terms of the Coulomb wavefunction and the potential of the interaction which are both known analytically? These issues have been the focii of our recent research [17]. We have been able to demonstrate that there was a practical approach to the two-body collision problem with a Coulomb-like potential that did not lead to the formal difficulties described above. Our approach is based on a representation of the scattering amplitude in a surface-integral form.

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 [18,19] and Merkuriev and Faddeev [20,21]. For the charged particles with the long-range Coulomb interaction, the theory has faced difficulties associated with the compactness of the underlying equations. For the repulsive Coulomb interactions, the compactness of the Faddeev integral equations for so-called $2 \to 2$ reactions (two fragments in the initial channel and two fragments in the final channel) has been proven in [22,23]. However, each iteration term of the Faddeev equations turns out to contain the same singularity as the previous one. In other words, these equations cannot be solved using standard numerical procedures. There is no proof of the compactness of the Faddeev equations when the attractive Coulomb interaction is involved.

A renormalization method based on screening [5,8] has been implemented successfully for the three-body problem when two particles are charged [24,25]. The method has been extended to two-fragment reactions in a system of three charged particles [26,25]. However, as mentioned earlier, further investigations showed that this might not fix all the problems regarding the compactness of the underlying equations [22,23], particularly when charges of opposite signs are involved, as they are in atomic and molecular physics. Though Dollard's time-dependent approach [2,3] is believed to be formally valid for arbitrary multichannel collisions including the three-body problem, it has not developed into a practical method for calculations. At the same time, no practical time-independent renormalization method exists that is valid for a system of three charged particles above the breakup threshold either. The problem is that above the threshold the Coulomb three-body system possesses essentially different types of singularities and the two-particle renormalization procedures are not sufficient to guarantee compactness of the equations [6,20,27]. Thus there are no compact integral equations yet known for collisions of more than two charged particles that are satisfactory above the breakup threshold [10]. Furthermore, there is no theoretical proof or practical evidence that a renormalization approach can be applied to the Faddeev equations for genuine three-body Coulomb problems. To make the situation even worse, as pointed out by Merkuriev and Faddeev [21], if one of the particles has a charge of opposite sign to others then in some so-called singular directions asymptotic forms for the Faddeev components cannot be formulated. This is a rather disturbing situation especially for three-body problems in atomic physics where all three particles are charged and where two of the pair interactions are always attractive.

From the theory point of view, several issues relating to a complete formal understanding of the breakup process remain open. One of them is the problem of adequate matching of the internal (scattering region) and the external (asymptotic region) solutions [28]. The key issue, however, is how to extract the scattering information from the wavefunction when the latter is available. To be more specific, in case of neutral particles the breakup amplitude is calculated using six-dimensional (or two-dimensional, if partial-wave expansion is used) volume integrals. This requires the knowledge of the total wavefunction everywhere in space, whereas the necessary information is contained in just the asymptotic part. Furthermore, for three charged particles the theory fails to give a formal post-form definition of the scattering amplitude in terms of the calculated total wavefunction with outgoing scattered-wave boundary conditions. This has been a long-standing problem. In its absence, the formula for the short-range case is often used. However, the short-range case definition of the breakup amplitude diverges when interactions are long-ranged.

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 the screening is removed. This leaves no choice but to invoke renormalization to fix unphysical results. Therefore, a new approach to Coulomb few-body problems that does not need renormalization is required. The variational approach [29] is a step forward in this direction. However, this approach leads to representations for the transition amplitudes which also contain oscillatory divergences but for different reasons. It was suggested that these divergences can be made to vanish using a "radius averaging" procedure [29]. The method has been extended to breakup in a system of three charged particles in [30]. Extension to a system of arbitrary number of charged particles is given in [74].

There are several sophisticated numerical approaches to solving three-body problems in nuclear physics with two charged particles [31–37]. Some of these are based on the framework of the Faddeev [18,21] and Alt–Grassberger–Sandhas equations [26,38]. Other methods tackle the same problem through direct numerical solution of the relevant SE for the scattering wavefunction [35,37] or using variational techniques [36]. The Coulomb interaction between the two protons has been fully included in the calculation of proton–deuteron breakup for the first time in [39]. However, due to formal problems mentioned earlier no such strict approach for breakup processes in nuclear three-body systems, when all particles are charged, has been developed. For this reason calculations of (e,ep), $(p,2p)$ and similar nuclear breakup reactions with three charged particles in the final state have been limited to high energies where distorted-wave Born-type approximations (DWBA) are applicable.

In atomic physics, despite the above-mentioned formal difficulties, surprising progress has been achieved in describing $(e,2e)$ processes via the exterior complex scaling (ECS) [40–43] and the convergent close coupling (CCC) [44–46] methods. The success of the ECS approach to Coulomb breakup problems in particular caused us to reexamine the underlying formal theory [47]. The amplitude is calculated from Peterkop's trial integral [48] that has phase ambiguity and divergence problems. In the CCC method, one of the electrons is treated using a square-integrable representation, and the breakup amplitude can be related to a particular form of Peterkop's trial integral. Despite the success of the computational methods, in describing the measured cross-sections, the traditional formal theory of scattering is unable to show how to calculate the breakup amplitude unambiguously and in a divergence-free manner. The conventional formal theory is also not capable of explaining the origin of the trial integral which is the cornerstone of the aforementioned methods.

One reason preventing the direct solution methods in atomic physics from extracting ionization amplitudes rigorously has been a lack of an ambiguity-free form of the asymptotic wavefunction for positive energies. The well-known Peterkop asymptotic wavefunction [49] has an ambiguous phase, and is not valid in all asymptotic domains relevant to the problem [50]. In part, because of this, it has been impossible to define the ionization amplitude in a divergence-free manner. The full and unambiguous asymptotic forms of the three-body scattered wavefunction have been given recently [50,51]. This allowed us to obtain an integral representation for the ionization amplitude which is free of ambiguity and divergence problems [47,52]. Our analysis has provided a formal justification of the cross-sections obtained in the approaches based on the Peterkop integral.

In this manuscript, we present a surface-integral approach to formulating scattering theory. We use the recently derived analytic forms of total scattering wavefunctions in asymptotic domains [51–53] to develop a well-defined prior and post forms of the breakup amplitude valid for short-range and Coulom-

bic potentials. All derivations are based on a surface-integral technique. Green's functions and formal solutions of the SE in integral form are not required. A short synopsis of the results presented here has been published in [54]. As a follow up to [54] in this manuscript, we present full details of the formalism.

Since our approach is completely different to what is adopted in the standard literature, we start in Section 2 by applying it to the well-formulated two-body problem (potential scattering) with short-range interactions. This will enable us to extend the potential scattering theory to nuclear plus Coulomb interactions without the use of screening and renormalization. Here we also briefly recapitulate the main results of [17] and generalize the potential scattering theory to long-range interactions. New definitions for the scattering amplitude valid for arbitrary interactions will be presented. For the Coulomb potential, the generalized amplitude will be shown to give the physical (on-shell) amplitude without recourse to a renormalization procedure. This section will also enable us to better understand the surface integrals emerging in different situations and prepare a proper platform for moving on to the three-body problem.

In Section 3, the three-body scattering problem is considered. After formulating the asymptotic boundary conditions, surface-integral representations for the breakup amplitude in a three-body system will be derived. We develop a well-defined post form of the breakup amplitude valid for arbitrary potentials. They will be shown to take surface-integral forms well suited for practical calculations. The surface-integral representations are extended to amplitudes of all other possible scattering processes taking place in an arbitrary three-body system. Different computational methods for extracting the scattering amplitudes are discussed. Generalized wave operators are given in Section 4. Section 5 contains discussion of the results.

2. Two-body scattering problem

In this section, a new formulation of potential scattering theory is presented. Essential feature of this alternative formulation is that it avoids the reference to the Green's function and formal solution for the scattering wavefunction in the integral form. This leads to new more general definitions for scattering amplitude and wave operators valid for arbitrary interactions including Coulombic long-range ones. We demonstrate that the SE for the scattering wavefunction with properly formulated asymptotic boundary conditions completely and unambiguously define all quantities necessary for the description of a scattering event. The considerations of this section will serve as a model for the three-body problem dealt with in the subsequent sections.

In scattering theory, we deal with functions which go beyond the Hilbert space. These wavefunctions belong to the so-called rigged Hilbert space [55]. Since these functions are not square-integrable (L^2) their scalar products can be unbounded. While this fact is not a problem on its own, nevertheless, non-L^2 functions do make certain integrals emerging in the theory divergent. In case of integrals containing the interaction potential a standard procedure, which ensures their existence, is limiting the range of the potential. However, this irreversibly distorts the nature of the problem. Throughout this work, we use a different approach to dealing with the aforementioned problem. We first formulate the scattering problem in a finite region of coordinate space and then extend it to the full space.

Our formulation heavily relies on surface integrals. This subject is new and has not been discussed in literature. Since some physicists question the very existence of surface integrals in scattering theory we start from discussing the surface integrals and circumstances under which they may, or may not, appear. We will continue this discussion progressively throughout the paper.

2.1. Surface integrals in the absence of interaction

To start with, let us consider an equation for free relative motion of two particles

$$(\epsilon - h_0)\phi_{\boldsymbol{k}}(\boldsymbol{r}) = 0, \tag{1}$$

where $h_0 = -\Delta_{\boldsymbol{r}}/2\mu$ is the free Hamiltonian operator, $\epsilon = k^2/2\mu$ is the energy of the relative motion, $\boldsymbol{r}$ is the relative coordinate of the particles 1 and 2 and $\boldsymbol{k}$ is their relative momentum, μ is the reduced mass.

We define an incomplete scalar product according to

$$\langle f_{\boldsymbol{k}'}|g_{\boldsymbol{k}}\rangle_{r_0} = \int_{r\leqslant r_0} d\boldsymbol{r} f^*_{\boldsymbol{k}'}(\boldsymbol{r}) g_{\boldsymbol{k}}(\boldsymbol{r}), \tag{2}$$

where the integration is limited to the volume of a sphere of radius r_0. Generally speaking, the full scalar product $\langle f_{\boldsymbol{k}'}|g_{\boldsymbol{k}}\rangle$ can be unbounded.

Let us now consider another free-wave equation but at different momentum

$$(\epsilon' - h_0)\phi_{\boldsymbol{k}'}(\boldsymbol{r}) = 0, \tag{3}$$

and investigate the following difference[1]:

$$\langle h_0\phi_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle_{r_0} - \langle \phi_{\boldsymbol{k}'}|h_0\phi_{\boldsymbol{k}}\rangle_{r_0}. \tag{4}$$

Using Green's theorem, this quantity given by two volume integrals can be transformed into a single surface integral as follows:

$$\begin{aligned}\langle h_0\phi_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle_{r_0} - \langle \phi_{\boldsymbol{k}'}|h_0\phi_{\boldsymbol{k}}\rangle_{r_0} &= \frac{1}{2\mu}\int_{r\leqslant r_0} d\boldsymbol{r}(\phi^*_{\boldsymbol{k}'}\Delta_{\boldsymbol{r}}\phi_{\boldsymbol{k}} - \phi_{\boldsymbol{k}}\Delta_{\boldsymbol{r}}\phi^*_{\boldsymbol{k}'}) \\ &= \left[\frac{1}{2\mu}r^2\int d\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}(\phi^*_{\boldsymbol{k}'}\nabla_{\boldsymbol{r}}\phi_{\boldsymbol{k}} - \phi_{\boldsymbol{k}}\nabla_{\boldsymbol{r}}\phi^*_{\boldsymbol{k}'})\right]_{r=r_0}.\end{aligned} \tag{5}$$

Then, obviously, we have

$$\left[\frac{1}{2\mu}r^2\int d\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}(\phi^*_{\boldsymbol{k}'}\nabla_{\boldsymbol{r}}\phi_{\boldsymbol{k}} - \phi_{\boldsymbol{k}}\nabla_{\boldsymbol{r}}\phi^*_{\boldsymbol{k}'})\right]_{r=r_0} = (\epsilon' - \epsilon)\langle\phi_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle_{r_0}. \tag{6}$$

As we can see, if free waves are on the same energy shell the above surface integral disappears for all r_0 because $\epsilon' = \epsilon$. If the waves are not on the same energy shell (i.e., $\epsilon' \neq \epsilon$) then the right-hand side (RHS) of Eq. (6) goes to 0 as $r_0 \to \infty$ because $\langle\phi_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle = \delta(\boldsymbol{k} - \boldsymbol{k}') = 0$. The conclusion is that if there is no interaction the surface integral vanishes. As we will see below, the situation is different if there is interaction between the particles.

2.2. Scattering via short-range interaction

Let us consider now a system of two interacting particles. The scattering state of this system is a solution to the SE

$$(\epsilon - h)\psi^{\pm}_{\boldsymbol{k}}(\boldsymbol{r}) = 0, \tag{7}$$

where $h = h_0 + V$ is the total two-body Hamiltonian of the system, V is a short-range interaction potential such that the asymptotic boundary conditions specified below are valid. The interaction potential can be local or non-local. However, we assume it to be real.

From all possible solutions to Eq. (7), we should choose the one satisfying, in the leading order, the asymptotic boundary condition

$$\psi^+_{\boldsymbol{k}}(\boldsymbol{r}) \overset{r\to\infty}{\sim} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f(\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{ikr}}{r}. \tag{8}$$

The second suitable solution $\psi^-_{\boldsymbol{k}}(\boldsymbol{r})$ can be found from the well-known relationship [56]

$$\psi^-_{\boldsymbol{k}}(\boldsymbol{r}) = \left[\psi^+_{-\boldsymbol{k}}(\boldsymbol{r})\right]^*. \tag{9}$$

The latter asymptotically behaves, in the leading order, like

$$\psi^-_{\boldsymbol{k}}(\boldsymbol{r}) \overset{r\to\infty}{\sim} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} + f^*(-\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{-ikr}}{r}. \tag{10}$$

[1] Note that $\langle A\phi_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle$ means $(\langle\phi_{\boldsymbol{k}'}|A)|\phi_{\boldsymbol{k}}\rangle$, while $\langle\phi_{\boldsymbol{k}'}|A\phi_{\boldsymbol{k}}\rangle$ stands for $\langle\phi_{\boldsymbol{k}'}|(A|\phi_{\boldsymbol{k}}\rangle)$, where A is a self-adjoint operator.

If we were following tradition we would need to introduce after Eq. (7) some definition of what is short range. Generally speaking, as used in standard literature such a definition involves convergence of a certain integral containing the wavefunction $\psi_{\boldsymbol{k}}^{\pm}$ and the potential V. Our approach presented below is based on partial inner products and does not require the short-rangeness as far as integrals are concerned. All integrals converge just because we are in a limited box. When we say that the SE has a solution and the solution has a certain asymptotic boundary condition we already impose all conditions on the potential. As the box size increases integrals have to converge if the SE for the wavefunction has a solution as we assumed. Therefore, without going into details, we simply assume the following definition of the short-rangeness: V is short-ranged so that the asymptotic boundary conditions are given by Eqs. (8) and (10).

We can separate $\psi_{\boldsymbol{k}}^{\pm}$ into the incident and the scattered parts according to

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}(\boldsymbol{r}) + \psi_{\boldsymbol{k}}^{\mathrm{sc}\pm}(\boldsymbol{r}), \tag{11}$$

where $\phi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ and $\psi_{\boldsymbol{k}}^{\mathrm{sc}\pm}$ asymptotically behave like

$$\psi_{\boldsymbol{k}}^{\mathrm{sc}+}(\boldsymbol{r}) \overset{r\to\infty}{\sim} f(\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{ikr}}{r}, \tag{12}$$

$$\psi_{\boldsymbol{k}}^{\mathrm{sc}-}(\boldsymbol{r}) \overset{r\to\infty}{\sim} f^{*}(-\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{-ikr}}{r}. \tag{13}$$

Then Eq. (7) can be written in the form

$$(\epsilon - h)\psi_{\boldsymbol{k}}^{\mathrm{sc}\pm}(\boldsymbol{r}) = (h-\epsilon)\phi_{\boldsymbol{k}}(\boldsymbol{r}). \tag{14}$$

Let us multiply Eq. (14) (for $\psi_{\boldsymbol{k}}^{\mathrm{sc}+}$) by $\psi_{\boldsymbol{k}'}^{-*}(\boldsymbol{r})$ from the left and integrate the result over the volume of a sphere of radius r_0:

$$\left\langle \psi_{\boldsymbol{k}'}^{-}|(\epsilon-h)\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle_{r_0} = \left\langle \psi_{\boldsymbol{k}'}^{-}|(h-\epsilon)\phi_{\boldsymbol{k}}\right\rangle_{r_0}, \tag{15}$$

where $\psi_{\boldsymbol{k}'}^{-}(\boldsymbol{r})$ is another solution of the SE at a different momentum but the same energy ϵ, i.e., $k' = k$. In other words, $\psi_{\boldsymbol{k}'}^{-}(\boldsymbol{r})$ is the eigenfunction of the operator $(\epsilon - h)$, therefore we also can write

$$\left\langle (\epsilon-h)\psi_{\boldsymbol{k}'}^{-}|\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle_{r_0} = 0. \tag{16}$$

Subtracting Eq. (16) from (15), we get

$$\left\langle \psi_{\boldsymbol{k}'}^{-}|(\epsilon-h)\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle_{r_0} - \left\langle (\epsilon-h)\psi_{\boldsymbol{k}'}^{-}|\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle_{r_0} = \left\langle \psi_{\boldsymbol{k}'}^{-}|(h-\epsilon)\phi_{\boldsymbol{k}}\right\rangle_{r_0}. \tag{17}$$

Canceling the terms containing $\epsilon - V$ (these terms are finite because we are in a limited space), we have

$$-\left\langle \psi_{\boldsymbol{k}'}^{-}|h_0\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle_{r_0} + \left\langle h_0\psi_{\boldsymbol{k}'}^{-}|\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle_{r_0} = \left\langle \psi_{\boldsymbol{k}'}^{-}|(h-\epsilon)\phi_{\boldsymbol{k}}\right\rangle_{r_0}. \tag{18}$$

The left-hand side (LHS) of Eq. (18) would vanish if the operator h_0 were Hermitian. We will return to the question of Hermicity of the operators later. At this stage, we let $r_0 \to \infty$ on both sides of the equation

$$\lim_{r_0\to\infty}\left[-\left\langle \psi_{\boldsymbol{k}'}^{-}|h_0\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle + \left\langle h_0\psi_{\boldsymbol{k}'}^{-}|\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right\rangle\right]_{r_0} = \lim_{r_0\to\infty}\left\langle \psi_{\boldsymbol{k}'}^{-}|(h-\epsilon)\phi_{\boldsymbol{k}}\right\rangle_{r_0}. \tag{19}$$

What does this equation represent? In order to establish its meaning, we calculate both sides of the equation independently. First, we investigate the limit on the LHS. For the LHS of Eq. (19), we have

$$\mathrm{LHS} = \lim_{r_0\to\infty}\int_{r\le r_0} d\boldsymbol{r}\left[\psi_{\boldsymbol{k}}^{\mathrm{sc}+}(\boldsymbol{r})h_0\psi_{\boldsymbol{k}'}^{-*}(\boldsymbol{r}) - \psi_{\boldsymbol{k}'}^{-*}(\boldsymbol{r})h_0\psi_{\boldsymbol{k}}^{\mathrm{sc}+}(\boldsymbol{r})\right] \tag{20}$$

$$= \lim_{r_0\to\infty}\left[-\frac{1}{2\mu}\int_{r\le r_0} d\boldsymbol{r}\left(\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\Delta_{\boldsymbol{r}}\psi_{\boldsymbol{k}'}^{-*} - \psi_{\boldsymbol{k}'}^{-*}\Delta_{\boldsymbol{r}}\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right)\right] \tag{21}$$

$$= \lim_{r_0\to\infty}\left[-\frac{1}{2\mu}r^2\int d\hat{\boldsymbol{r}}\,\hat{\boldsymbol{r}}\left(\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\nabla_{\boldsymbol{r}}\psi_{\boldsymbol{k}'}^{-*} - \psi_{\boldsymbol{k}'}^{-*}\nabla_{\boldsymbol{r}}\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\right)\right]_{r=r_0} \tag{22}$$

$$= \lim_{r_0\to\infty}\left[-\frac{1}{2\mu}r^2\int d\hat{\boldsymbol{r}}\left(\psi_{\boldsymbol{k}}^{\mathrm{sc}+}\frac{\partial\psi_{\boldsymbol{k}'}^{-*}}{\partial r} - \psi_{\boldsymbol{k}'}^{-*}\frac{\partial\psi_{\boldsymbol{k}}^{\mathrm{sc}+}}{\partial r}\right)\right]_{r=r_0}. \tag{23}$$

Above we used Green's theorem. Using Eq. (12) and differentiating we get, in the leading order,

$$\text{LHS} = \lim_{r_0\to\infty}\left[-\frac{1}{2\mu}r\int d\hat{\boldsymbol{r}} f(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}})e^{ikr}e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}}(-ik - i\boldsymbol{k}'\cdot\hat{\boldsymbol{r}})\right]_{r=r_0}. \tag{24}$$

Using the asymptotic form of the plane wave (see, e.g. [57])

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \overset{r\to\infty}{\sim} \frac{2\pi}{ikr}\left[e^{ikr}\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}}) - e^{-ikr}\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})\right], \tag{25}$$

we get from Eq. (24)

$$\text{LHS} = \lim_{r_0\to\infty}\left[-\frac{\pi}{\mu k'}\left(e^{i(k-k')r}f(\hat{\boldsymbol{k}}'\cdot\hat{\boldsymbol{k}})(k+k') - e^{i(k+k')r}f(-\hat{\boldsymbol{k}}'\cdot\hat{\boldsymbol{k}})(k-k')\right)\right]_{r=r_0}. \tag{26}$$

Taking into account the fact that $k = k\prime$, we finally have

$$\text{LHS} = -\frac{2\pi}{\mu}f(\hat{\boldsymbol{k}\prime}\cdot\hat{\boldsymbol{k}}). \tag{27}$$

Since the latter is simply the onshell T-matrix ($-2\pi/\mu f = t$) then we can write Eq. (19) as

$$t(\boldsymbol{k}',\boldsymbol{k}) = \lim_{r_0\to\infty}\langle\psi^-_{\boldsymbol{k}'}|(h-\epsilon)\phi_{\boldsymbol{k}}\rangle_{r_0}. \tag{28}$$

Thus we have obtained a definition for the on-shell transition matrix. We emphasize that, this definition has emerged as a result of a surface integral which has not vanished. In addition, in order to show this, there was no need to use a formal solution of the SE in the integral form as we did in [17].

We now consider Eq. (14) for $\psi^{sc-}_{\boldsymbol{k}'}$ and multiply it by $\psi^+_{\boldsymbol{k}}$ from the right. Integrating the result over the volume of a sphere of radius r_0, we have

$$\langle(\epsilon-h)\psi^{sc-}_{\boldsymbol{k}'}|\psi^+_{\boldsymbol{k}}\rangle_{r_0} = \langle(h-\epsilon)\phi_{\boldsymbol{k}'}|\psi^+_{\boldsymbol{k}}\rangle_{r_0}, \tag{29}$$

where again $k' = k$. We also consider

$$\langle\psi^{sc-}_{\boldsymbol{k}'}|(\epsilon-h)\psi^+_{\boldsymbol{k}}\rangle_{r_0} = 0, \tag{30}$$

which is valid for arbitrary r_0 due to Eq. (7). Subtracting Eq. (30) from (29), we get

$$\langle(\epsilon-h)\psi^{sc-}_{\boldsymbol{k}'}|\psi^+_{\boldsymbol{k}}\rangle_{r_0} - \langle\psi^{sc-}_{\boldsymbol{k}'}|(\epsilon-h)\psi^+_{\boldsymbol{k}}\rangle_{r_0} = \langle(h-\epsilon)\phi_{\boldsymbol{k}'}|\psi^+_{\boldsymbol{k}}\rangle_{r_0}. \tag{31}$$

This equation is similar to Eq. (17) 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 scattering amplitude

$$t(\boldsymbol{k}',\boldsymbol{k}) = \lim_{r_0\to\infty}\langle(h-\epsilon)\phi_{\boldsymbol{k}'}|\psi^+_{\boldsymbol{k}}\rangle_{r_0}. \tag{32}$$

We call Eqs. (28) and (32) the prior- and post-form definitions of the scattering amplitude, respectively. How do we know that the RHS of Eqs. (28) and (32) also converge? We return to this question after discussing the following point.

Eqs. (28) and (32) immediately suggest that the scattering amplitude can take surface-integral forms. Indeed, since

$$\langle(\epsilon-h)\psi^-_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle_{r_0} = 0, \tag{33}$$

from Eq. (28) we have

$$t^{\text{prior}}(\boldsymbol{k}',\boldsymbol{k}) = \lim_{r_0\to\infty}\left[\langle\psi^-_{\boldsymbol{k}'}|(h-\epsilon)\phi_{\boldsymbol{k}}\rangle + \langle(\epsilon-h)\psi^-_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle\right]_{r_0}, \tag{34}$$

$$= \lim_{r_0\to\infty}\left[\langle\psi^-_{\boldsymbol{k}'}|h_0\phi_{\boldsymbol{k}}\rangle - \langle h_0\psi^-_{\boldsymbol{k}'}|\phi_{\boldsymbol{k}}\rangle\right]_{r_0}, \tag{35}$$

$$= -\frac{1}{2\mu}\lim_{r_0\to\infty} r_0^2\int\hat{\boldsymbol{r}}d\hat{\boldsymbol{r}}\left[\psi^{-*}_{\boldsymbol{k}'}\nabla_{\boldsymbol{r}}\phi_{\boldsymbol{k}} - \phi_{\boldsymbol{k}}\nabla_{\boldsymbol{r}}\psi^{-*}_{\boldsymbol{k}'}\right]_{r_0}, \tag{36}$$

which can be written as

$$t^{\text{prior}}(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{2\mu}\lim_{r_0\to\infty} r_0^2 \int d\hat{\boldsymbol{r}}\left[\psi_{\boldsymbol{k}'}^{-*}\frac{\partial\phi_{\boldsymbol{k}}}{\partial r} - \phi_{\boldsymbol{k}}\frac{\partial\psi_{\boldsymbol{k}'}^{-*}}{\partial r}\right]_{r_0}. \tag{37}$$

At the same time using the fact that

$$\left\langle \phi_{\boldsymbol{k}'}|(h-\epsilon)\psi_{\boldsymbol{k}}^{+}\right\rangle_{r_0} = 0, \tag{38}$$

from Eq. (32) we also get

$$t^{\text{post}}(\boldsymbol{k}',\boldsymbol{k}) = \lim_{r_0\to\infty}\left[\left\langle h_0\phi_{\boldsymbol{k}'}|\psi_{\boldsymbol{k}}^{+}\right\rangle - \left\langle \phi_{\boldsymbol{k}'}|h_0\psi_{\boldsymbol{k}}^{+}\right\rangle\right]_{r_0}, \tag{39}$$

which transforms to

$$t^{\text{post}}(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{2\mu}\lim_{r_0\to\infty} r_0^2 \int d\hat{\boldsymbol{r}}\left[\psi_{\boldsymbol{k}}^{+}\frac{\partial\phi_{\boldsymbol{k}'}^{*}}{\partial r} - \phi_{\boldsymbol{k}'}^{*}\frac{\partial\psi_{\boldsymbol{k}}^{+}}{\partial r}\right]_{r_0}. \tag{40}$$

Thus the scattering T-matrix, conventionally given as a volume integral, can be written equivalently in surface-integral forms. We emphasize that in these forms the T-matrix depends only on the asymptotic behavior of the participating functions. Therefore, generally speaking, knowledge of the scattering wavefunction in the internal (non-asymptotic) region is not required. In addition, the surface-integral forms are readily expanded in partial waves leading to a simple result containing only the limiting procedure. Therefore, these forms are particularly suitable for practical calculations.

Returning to the question asked at the end of the previous paragraph, the same analysis as used above to calculate the LHS of Eq. (19) can be performed on the surface-integral representations (37) and (40) to yield $t(\boldsymbol{k}',\boldsymbol{k})$. This is a proof that the limits on the RHS of Eqs. (28) and (32) do exist. Therefore, from Eqs. (28) and (32), we get the general volume-integral prior and post forms of the scattering amplitude

$$t^{\text{prior}}(\boldsymbol{k}',\boldsymbol{k}) = \left\langle \psi_{\boldsymbol{k}'}^{-}|(h-\epsilon)\phi_{\boldsymbol{k}}\right\rangle, \tag{41}$$

$$t^{\text{post}}(\boldsymbol{k}',\boldsymbol{k}) = \left\langle (h-\epsilon)\phi_{\boldsymbol{k}'}|\psi_{\boldsymbol{k}}^{+}\right\rangle. \tag{42}$$

These forms are consistent with the conventional theory. Indeed, in the light of Eq. (1), we have

$$(h-\epsilon)\phi_{\boldsymbol{k}}(\boldsymbol{r}) = V\phi_{\boldsymbol{k}}(\boldsymbol{r}). \tag{43}$$

Therefore, the two forms given by Eqs. (28) and (32), respectively, are in fact identical to the standard prior and post forms of the T-matrix

$$t^{\text{prior}}(\boldsymbol{k}',\boldsymbol{k}) = \left\langle \psi_{\boldsymbol{k}'}^{-}|V|\phi_{\boldsymbol{k}}\right\rangle, \tag{44}$$

$$t^{\text{post}}(\boldsymbol{k}',\boldsymbol{k}) = \left\langle \phi_{\boldsymbol{k}'}|V|\psi_{\boldsymbol{k}}^{+}\right\rangle. \tag{45}$$

Though the volume-integral definitions can be written without the limit procedure, there are a number of reasons for keeping definitions of the T-matrix as in Eqs. (28) and (32). First of all, the latter with the explicit limit operation carry a clear message on how the T-matrix must be calculated in practice. The plane wave ϕ and scattering waves $\psi^{\pm}$ which define the T-matrix are rapidly oscillating functions of r. On the other hand, the T-matrix does not depend on r. Therefore, Eqs. (28) and (32) suggest that the scattering waves must be calculated in a reasonably large but limited space, then checked if r_0 was sufficiently large to make the T-matrix independent of r_0. Second, the surface-integral forms of the scattering amplitude naturally follow from definitions (28) and (32). We shall show in the following subsection that the T-matrices as written in Eqs. (28) and (32) are more general and valid for arbitrary interaction potentials provided the function on which the operator $(h-\epsilon)$ is applied is the leading-order incident wave.

Concluding the subsection, it is interesting to note the close resemblance of the new forms of the T-matrix to the representation of the number of scattered particles crossing the surface element $d\hat{\boldsymbol{r}}$ per unit time at large distance r_0. Taking into account Eq. (11), we can write Eqs. (37) and (40) in the following equivalent forms:

$$t^{\text{prior}}(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{2\mu}\lim_{r_0\to\infty} r_0^2 \int \hat{\boldsymbol{r}}d\hat{\boldsymbol{r}}\left[\psi_{\boldsymbol{k}'}^{\text{sc}-*}\nabla_{\boldsymbol{r}}\phi_{\boldsymbol{k}} - \phi_{\boldsymbol{k}}\nabla_{\boldsymbol{r}}\psi_{\boldsymbol{k}'}^{\text{sc}-*}\right]_{r_0} \tag{46}$$

$$= -\frac{1}{2\mu}\lim_{r_0\to\infty} r_0^2 \int d\hat{\boldsymbol{r}}\left[\psi_{\boldsymbol{k}'}^{\text{sc}-*}\frac{\partial\phi_{\boldsymbol{k}}}{\partial r} - \phi_{\boldsymbol{k}}\frac{\partial\psi_{\boldsymbol{k}'}^{\text{sc}-*}}{\partial r}\right]_{r_0}, \tag{47}$$

and

$$t^{\rm post}(\boldsymbol{k}',\boldsymbol{k}) = -\frac{1}{2\mu}\lim_{r_0\to\infty} r_0^2 \int \hat{\boldsymbol{r}} d\hat{\boldsymbol{r}} \left[\psi_{\boldsymbol{k}}^{\rm sc+}\nabla_{\boldsymbol{r}}\phi_{\boldsymbol{k}'}^{*} - \phi_{\boldsymbol{k}'}^{*}\nabla_{\boldsymbol{r}}\psi_{\boldsymbol{k}}^{\rm sc+}\right]_{r_0} \tag{48}$$

$$= -\frac{1}{2\mu}\lim_{r_0\to\infty} r_0^2 \int d\hat{\boldsymbol{r}} \left[\psi_{\boldsymbol{k}}^{\rm sc+}\frac{\partial\phi_{\boldsymbol{k}'}^{*}}{\partial r} - \phi_{\boldsymbol{k}'}^{*}\frac{\partial\psi_{\boldsymbol{k}}^{\rm sc+}}{\partial r}\right]_{r_0}. \tag{49}$$

In getting these results, we used Eq. (6) for $\epsilon\prime = \epsilon$. These can now be compared with the probability density flux which is written as

$$\boldsymbol{j} = -\frac{i}{2\mu}\left[\psi_{\boldsymbol{k}}^{\rm sc+*}\nabla_{\boldsymbol{r}}\psi_{\boldsymbol{k}}^{\rm sc+} - \psi_{\boldsymbol{k}}^{\rm sc+}\nabla_{\boldsymbol{r}}\psi_{\boldsymbol{k}}^{\rm sc+*}\right]_{r_0}. \tag{50}$$

Thus, the flux is proportional to the square of the magnitude of the scattering amplitude. While it is used for cross-section calculations, it cannot provide the full information about the scattering amplitude. This comparison also shows that the new definitions for the scattering amplitude obtained in this subsection make the physical meaning of the amplitude very transparent.

2.3. Scattering via coulomb-like interaction

Here we generalize the results of the previous subsection to the case of Coulombic long range interactions. To be more specific, we assume that interaction V consists of some short-range part $V^{\rm S}$ and the Coulomb potential $V^{\rm C} = z_1 z_2/r$, where z_1 and z_2 are the charges of the particles. A scattering state in a system of two Coulomb particles is still the solution to the SE (7). However, when the potential has the Coulomb tail the scattering wavefunction $\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ asymptotically behaves like the Coulomb-modified plane wave and a Coulomb-modified outgoing spherical wave

$$\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) \overset{r\to\infty}{\sim} e^{i\boldsymbol{k}\cdot\boldsymbol{r}+i\gamma\ln(kr-\boldsymbol{k}\cdot\boldsymbol{r})}[1+O(1/r)] + f(\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{ikr-i\gamma\ln(2kr)}}{r}[1+O(1/r)], \tag{51}$$

where $\gamma = z_1 z_2 \mu/k$ is the Sommerfeld parameter. The second suitable solution $\psi_{\boldsymbol{k}}^{-}(\boldsymbol{r})$ asymptotically behaves like the Coulomb-modified plane wave and a Coulomb-modified incoming spherical wave

$$\psi_{\boldsymbol{k}}^{-}(\boldsymbol{r}) \overset{r\to\infty}{\sim} e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\gamma\ln(kr+\boldsymbol{k}\cdot\boldsymbol{r})}[1+O(1/r)] + f^{*}(-\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{-ikr+i\gamma\ln(2kr)}}{r}[1+O(1/r)]. \tag{52}$$

Note that $\boldsymbol{k}\cdot\boldsymbol{r} \neq \pm kr$, respectively, for (51) and (52). If $\boldsymbol{k}\cdot\boldsymbol{r} = \pm kr$, 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 we have shown in [17], in the asymptotic sense for which Eqs. (51) and (52) are written these singularities merely distort δ-functions emerging from the forward/backward directions (see Eq. (25)). Consequently, in the asymptotic region the distorted plane waves can be treated much like the ordinary plane wave.

We could separate $\psi_{\boldsymbol{k}}^{\pm}$ into the incident and the scattered parts according to

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = \tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) + \tilde{\psi}_{\boldsymbol{k}}^{\rm sc\pm}(\boldsymbol{r}), \tag{53}$$

where $\tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})$ and $\tilde{\psi}_{\boldsymbol{k}}^{\rm sc\pm}$ asymptotically behave like the first and the second terms of Eq. (51) and (52), respectively. The unscattered wave is the plane wave, Coulomb-modified to all orders of magnitude, and given as [10]

$$\tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}e^{\pi\gamma/2}U(\mp i\gamma, 1, \pm ikr - i\boldsymbol{k}\cdot\boldsymbol{r}), \tag{54}$$

where U is the confluent hypergeometric function of the second kind. This splitting follows from the fact that functions $\tilde{\phi}_{\boldsymbol{k}}^{\pm}$ and $\tilde{\psi}_{\boldsymbol{k}}^{\rm sc\pm}$ satisfy the first and the second parts of the asymptotic conditions (51) and (52). However, (for the pure Coulomb interaction) $\tilde{\phi}_{\boldsymbol{k}}^{\pm}$ alone is a solution to the original SE

$$(\epsilon - h)\tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = 0. \tag{55}$$

Consequently, the corresponding scattered wave $\tilde{\psi}^{\mathrm{sc}\pm}_{\boldsymbol{k}}$ is a solution as well. At the same time, since $\tilde{\phi}^{\pm}_{\boldsymbol{k}}$ and $\tilde{\psi}^{\mathrm{sc}\pm}_{\boldsymbol{k}}$ are both irregular solutions they are not eigenfunctions of the Hamiltonian h. Thus, as a result of separation (53) the original SE for $\psi^{\pm}_{\boldsymbol{k}}$ splits into two equations making it impossible to single out uniquely the important surface-integral components in the full solution. Therefore representation (53) is not a satisfactory starting point. It also leads to other anomalies associated with the Coulomb problem. In particular, using Eq. (55) one can demonstrate that the Coulomb wave function is a solution to a homogeneous Lippmann–Schwinger equation [58].

On the other hand, as the form of Eqs. (51) and (52) suggest, the leading order terms in the asymptotic region already contain 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 $\psi^{\mathrm{sc}\pm}_{\boldsymbol{k}}$. Therefore, let us denote the leading-order incident wave in Eqs. (51) and (52) as

$$\phi^{(0)\pm}_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}\pm i\gamma\ln(kr\mp\boldsymbol{k}\cdot\boldsymbol{r})}, \tag{56}$$

and single it out in $\psi^{\pm}_{\boldsymbol{k}}$ according to

$$\psi^{\pm}_{\boldsymbol{k}}(\boldsymbol{r}) = \phi^{(0)\pm}_{\boldsymbol{k}}(\boldsymbol{r}) + \psi^{\mathrm{sc}\pm}_{\boldsymbol{k}}(\boldsymbol{r}). \tag{57}$$

It is sufficient to know that $\psi^{\mathrm{sc}+}_{\boldsymbol{k}}$ and $\psi^{\mathrm{sc}-}_{\boldsymbol{k}}$ asymptotically behave as

$$\psi^{\mathrm{sc}+}_{\boldsymbol{k}}(\boldsymbol{r}) \overset{r\to\infty}{\sim} O\left(\phi^{(0)+}_{\boldsymbol{k}}(\boldsymbol{r})/r\right) + f(\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{ikr-i\gamma\ln(2kr)}}{r}[1+O(1/r)] \tag{58}$$

and

$$\psi^{\mathrm{sc}-}_{\boldsymbol{k}}(\boldsymbol{r}) \overset{r\to\infty}{\sim} O\left(\phi^{(0)-}_{\boldsymbol{k}}(\boldsymbol{r})/r\right) + f^{*}(-\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}})\frac{e^{-ikr+i\gamma\ln(2kr)}}{r}[1+O(1/r)]. \tag{59}$$

Thus, the splitting according to Eq. (57) 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.

With these prerequisites repeating the algebra of the previous subsection, we get

$$t^{\mathrm{prior}}(\boldsymbol{k}',\boldsymbol{k}) = \lim_{r_0\to\infty}\left\langle \psi^{-}_{\boldsymbol{k}'}|(h-\epsilon)\phi^{(0)+}_{\boldsymbol{k}}\right\rangle_{r_0}, \tag{60}$$

$$t^{\mathrm{post}}(\boldsymbol{k}',\boldsymbol{k}) = \lim_{r_0\to\infty}\left\langle (h-\epsilon)\phi^{(0)-}_{\boldsymbol{k}'}|\psi^{+}_{\boldsymbol{k}}\right\rangle_{r_0}. \tag{61}$$

Here, as in Eqs. (17) and (18), the two integrals containing $\epsilon - V$ cancel 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.

Another difference is that while evaluating integrals similar to those we had in Eq. (24), we use an asymptotic form of the distorted plane waves $\phi^{(0)\pm}_{\boldsymbol{k}}(\boldsymbol{r})$ [17]:

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}\pm i\gamma\ln(kr\mp\boldsymbol{k}\cdot\boldsymbol{r})} \overset{r\to\infty}{\to} \frac{2\pi}{ikr}\left[e^{ikr-i\gamma\ln(2kr)}\delta(\widehat{\boldsymbol{k}}-\widehat{\boldsymbol{r}}) - e^{-ikr+i\gamma\ln(2kr)}\delta(\widehat{\boldsymbol{k}}+\widehat{\boldsymbol{r}})\right]. \tag{62}$$

The physical meaning of this replacement is quite obvious: the distorted plane waves correspond to two different fluxes of particles; two particles approaching each other are represented by the incoming wave and particles going away from each other are described by the outgoing wave. In the absence of the long-range distortion Eq. (62) transforms to the familiar asymptotic form of the plane wave (Eq. (25)). We will address the question of the usage of the replacement in Section 5.

Are the results given above 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 $r\to\infty$ [$\gamma = 0$ in Eqs. (51) and (52)], so that

$$\phi^{(0)\pm}_{\boldsymbol{k}}(\boldsymbol{r}) \to \phi_{\boldsymbol{k}}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}. \tag{63}$$

Therefore, our results transform to Eqs. (28) and (32) which, in the light of Eqs. (1) and (43), further reduce to Eqs. (44) and (45) in agreement with the standard definitions of the T-matrix. Obviously, when interaction V has a tail which does not disappear at infinity, $\phi_{\boldsymbol{k}}^{(0)+}$ does not satisfy the Helmholtz Eq. (1), and consequently Eq. (43) is not valid. As a result, conventional definitions become invalid for Coulomb–like potentials.

On the other hand, when the interaction is purely Coulomb ($V^S = 0$), we can proceed further with analytical methods. Then we have

$$(h-\epsilon)\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}) = \frac{\gamma^2 k}{\mu r(kr \mp \boldsymbol{k}\cdot\boldsymbol{r})}\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}). \tag{64}$$

Therefore, Eqs. (60) and (61) transform to

$$t^{\text{prior}}(\boldsymbol{k}',\boldsymbol{k}) = \left\langle \psi_{\boldsymbol{k}'}^{-}\left|\frac{\gamma^2 k}{\mu r(kr-\boldsymbol{k}\cdot\boldsymbol{r})}\right|\phi_{\boldsymbol{k}}^{(0)+}\right\rangle, \tag{65}$$

$$t^{\text{post}}(\boldsymbol{k}',\boldsymbol{k}) = \left\langle \phi_{\boldsymbol{k}'}^{(0)-}\left|\frac{\gamma^2 k}{\mu r(kr+\boldsymbol{k}\cdot\boldsymbol{r})}\right|\psi_{\boldsymbol{k}}^{+}\right\rangle. \tag{66}$$

Here, $\psi_{\boldsymbol{k}}^{\pm}$ are the well-known Coulomb waves (see, e.g. [10])

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}e^{-\pi\gamma/2}\Gamma(1\pm i\gamma)\,{}_1F_1(\mp i\gamma,1,\pm ikr - i\boldsymbol{k}\cdot\boldsymbol{r}), \tag{67}$$

with ${}_1F_1$ being the usual confluent hypergeometric function. The matrix elements in Eqs. (65) and (66) have been evaluated in [59] in closed form and lead to

$$t^{\text{prior}}(\boldsymbol{k}',\boldsymbol{k}) \equiv t^{past}(\boldsymbol{k}',\boldsymbol{k}) = \frac{4\pi z_1 z_2}{|\boldsymbol{k}'-\boldsymbol{k}|^2}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\left[\frac{4k^2}{|\boldsymbol{k}'-\boldsymbol{k}|^2}\right]^{i\gamma}, \tag{68}$$

which is the well-known on-shell Coulomb T-matrix. This gives additional support for the new definitions of the T-matrix.

2.4. Surface integrals in the off-shell case

Before moving to the three-body problem let us investigate the surface integrals in the off-shell case. When $\epsilon \neq \epsilon'$ subtraction of Eq. (16) from (15) gives

$$\left\langle \psi_{\boldsymbol{k}'}^{-}\right|(\epsilon-h)\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle_{r_0} - \left\langle (\epsilon'-h)\psi_{\boldsymbol{k}'}^{-}\right|\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle_{r_0} = \left\langle \psi_{\boldsymbol{k}'}^{-}\right|(h-\epsilon)\phi_{\boldsymbol{k}}\rangle_{r_0}, \tag{69}$$

which can be written as

$$(\epsilon-\epsilon')\left\langle \psi_{\boldsymbol{k}'}^{-}\right|\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle_{r_0} - \left[\left\langle \psi_{\boldsymbol{k}'}^{-}\right|h_0\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle_{r_0} - \left\langle h_0\psi_{\boldsymbol{k}'}^{-}\right|\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle_{r_0}\right] = \left\langle \psi_{\boldsymbol{k}'}^{-}\right|(h-\epsilon)|\phi_{\boldsymbol{k}}\rangle_{r_0}. \tag{70}$$

If we let $r_0 \to \infty$ on both sides of the equation the term on the RHS would represent an off-shell extension of $t(\boldsymbol{k}',\boldsymbol{k})$ according to our definition (28). The second term on the LHS can be written as a surface integral. It has been evaluated as $r_0 \to \infty$ and shown to reduce to (26). Consider the first term. Using Eq. (11), we can write it as

$$(\epsilon-\epsilon')\lim_{r_0\to\infty}\left\langle \psi_{\boldsymbol{k}'}^{-}\right|\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle_{r_0} = (\epsilon-\epsilon')\lim_{r_0\to\infty}\left\langle \psi_{\boldsymbol{k}'}^{-}\right|\psi_{\boldsymbol{k}}^{+}-\phi_{\boldsymbol{k}}\rangle_{r_0} = (\epsilon'-\epsilon)\lim_{r_0\to\infty}\left\langle \psi_{\boldsymbol{k}'}^{-}\right|\phi_{\boldsymbol{k}}\rangle_{r_0}. \tag{71}$$

The fact that $\lim_{r_0\to\infty}\langle\psi_{\boldsymbol{k}'}^{-}|\psi_{\boldsymbol{k}}^{+}\rangle_{r_0} = 0$ when $\epsilon \neq \epsilon'$ becomes evident when Eq. (9) is referred to. As we can see, the first term on the LHS of Eq. (70) is proportional to the Fourier transformation of $\psi_{\boldsymbol{k}'}^{-*}(\boldsymbol{r})$ as $r_0 \to \infty$.

The conclusion is that in the off-shell case the amplitude cannot take a purely surface-integral form, though some part of the amplitude can still be written as a surface integral. The term $[\langle\psi_{\boldsymbol{k}'}^{-}|h_0\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle - \langle h_0\psi_{\boldsymbol{k}'}^{-}|\psi_{\boldsymbol{k}}^{\text{sc}+}\rangle]$ which is the $r_0 \to \infty$ limit of the term in the square brackets in Eq. (70), may seem a"ghost" surface integral (i.e., equal to zero). However, Eq. (26) suggests that this integral does exist. Since $k \neq k'$ it becomes an infinitely oscillatory function as $r_0 \to \infty$. Therefore, if this surface-integral part comes inside another (external) integral over $\boldsymbol{k}'$, like it does in the integral equation or the formal solution for the wavefunction, then it kills the integral everywhere except at the point of

the singularity (the on-shell point) while itself transforming into the physical scattering amplitude at the singularity. In other cases such an external integral can only survive at a point where the integrand has a stationary phase, if there is any.

In this connection we also emphasize that if off-shell surface integrals are used in the Trojan Horse method in nuclear physics they are capable of nullifying the final result. This and other related points are discussed elsewhere [60].

3. Three-body scattering problem

3.1. Asymptotic boundary conditions

Let us consider a system of three particles of mass m_α and charge z_α, $\alpha = 1,2,3$. We use a system of Jacobi coordinates where $\boldsymbol{r}_\alpha$ is the relative coordinate, and $\boldsymbol{k}_\alpha$ is the relative momentum, between particles β and γ, $\boldsymbol{\rho}_\alpha$ is the relative coordinate of the center of mass of the pair (β,γ) and particle α, with $\boldsymbol{q}_\alpha$ 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 and throughout the paper, $\beta,\gamma = 1,2,3$, $\alpha \neq \beta \neq \gamma$. In addition, we use n and m to specify a full set of quantum numbers of a state in a particular grouping (arrangement). For further reference, we note that

$$\boldsymbol{r}_\beta = -\frac{\mu_\alpha}{m_\gamma}\boldsymbol{r}_\alpha - \epsilon_{\beta\alpha}\boldsymbol{\rho}_\alpha, \quad \rho_\beta = \epsilon_{\beta\alpha}\frac{\mu_\beta}{M_\alpha}\boldsymbol{r}_\alpha - \frac{\mu_\beta}{m_\gamma}\boldsymbol{\rho}_\alpha \tag{72}$$

and

$$\boldsymbol{k}_\beta = -\frac{\mu_\beta}{m_\gamma}\boldsymbol{k}_\alpha - \epsilon_{\beta\alpha}\frac{\mu_\alpha}{M_\beta}\boldsymbol{q}_\alpha, \quad \boldsymbol{q}_\beta = \epsilon_{\beta\alpha}\boldsymbol{k}_\alpha - \frac{\mu_\alpha}{m_\gamma}\boldsymbol{q}_\alpha, \tag{73}$$

where $\epsilon_{\beta\alpha} = -\epsilon_{\alpha\beta}$ is the antisymmetric symbol, with $\epsilon_{\beta\alpha} = 1$ for $(\beta\alpha)$ being a cyclic permutation of $(1,2,3)$, and $\epsilon_{\alpha\alpha} = 0$.

We introduce a hyperradius in the six-dimensional configurations space according to

$$R = \left(\frac{\mu_\alpha}{\mu}r_\alpha^2 + \frac{M_\alpha}{\mu}\rho_\alpha^2\right)^{1/2}, \tag{74}$$

where μ is an arbitrary mass constant introduced for convenience so that the hyperradius has units of length,[2] and a five-dimensional hyperangle

$$\omega = (\widehat{\boldsymbol{r}}_\alpha, \widehat{\boldsymbol{\rho}}_\alpha, \varphi_\alpha) \tag{75}$$

with

$$\varphi_\alpha = \arctan\left[\left(\frac{\mu_\alpha}{M_\alpha}\right)^{1/2}\frac{r_\alpha}{\rho_\alpha}\right], \quad 0 \leqslant \varphi_\alpha \leqslant \pi/2. \tag{76}$$

Consider now scattering of particle α with incident momentum $\boldsymbol{q}_{\alpha n}$ off a bound pair (β,γ) in initial state $\phi_{\alpha n}(\boldsymbol{r}_\alpha)$ 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. Thus we are interested in

$$\alpha + (\beta,\gamma) \to \begin{cases} \alpha + (\beta,\gamma), \\ \beta + (\gamma,\alpha), \\ \alpha + \beta + \gamma, \end{cases} \tag{77}$$

which we call $2 \to 3$ processes. Note that there are two possible rearrangement channels $(\beta + (\gamma,\alpha))$. 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

[2] As it will be seen later, the final results do not depend on this complementary constant.

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. In order to specify these boundary conditions, we should first define 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 SE

$$(E - H)\Psi^+_{\alpha n}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \tag{78}$$

with outgoing-wave boundary conditions, where $H = H_0 + V$ is the three-body Hamiltonian, and where $H_0 = -\Delta_{\mathbf{r}_\alpha}/2\mu_\alpha - \Delta_{\rho_\alpha}/2M_\alpha$ is the free Hamiltonian and $V = v + V_\alpha(\mathbf{r}_\alpha) + V_\beta(\mathbf{r}_\beta) + V_\gamma(\mathbf{r}_\gamma)$ is the full interaction, including the possibility of a three-body interaction potential v. We write the pair potentials as

$$V_\alpha(\mathbf{r}_\alpha) = V^S_\alpha(\mathbf{r}_\alpha) + V^C_\alpha(\mathbf{r}_\alpha), \quad V^C_\alpha(\mathbf{r}_\alpha) = \frac{Z_\beta Z_\gamma}{r_\alpha}, \tag{79}$$

with V^C_α (V^S_α) being the Coulomb (short-range) interaction between particles β and γ. $E = E_{\alpha n} + q^2_{\alpha n}/2M_\alpha = k^2_\alpha/2\mu_\alpha + q^2_\alpha/2M_\alpha$ is the total energy of the system.

Index αn of the total wavefunction $\Psi^+_{\alpha n}$ is referring to the fact that the wavefunction is developed from the initial two-fragment channel αn. It is convenient to split the wavefunction $\Psi^+_{\alpha n}$ into the initial-channel wave $\Phi^+_{\alpha n}$ and scattered wave $\Psi^{sc+}_{\alpha n}$:

$$\Psi^+_{\alpha n}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \Phi^+_{\alpha n}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + \Psi^{sc+}_{\alpha n}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{80}$$

where the initial-channel wave is also separable and given by

$$\Phi^+_{\alpha n}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \chi^+_{\alpha n}(\boldsymbol{\rho}_\alpha)\phi_{\alpha n}(\mathbf{r}_\alpha). \tag{81}$$

The two-body bound state in the initial channel is determined from

$$\left(\frac{1}{2\mu_\alpha}\Delta_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha) + E_{\alpha n}\right)\phi_{\alpha n}(\mathbf{r}_\alpha) = 0. \tag{82}$$

The wavefunction describing the relative motion of two clusters in the initial channel is given by[3]

$$\chi^+_{\alpha n}(\boldsymbol{\rho}_\alpha) = e^{i\mathbf{q}_{\alpha n}\cdot\boldsymbol{\rho}_\alpha + i\bar{\eta}_\alpha/q_{\alpha n}\ln(q_{\alpha n}\rho_\alpha - \mathbf{q}_{\alpha n}\cdot\boldsymbol{\rho}_\alpha)}[1 + O(1/\rho_\alpha)], \tag{83}$$

where

$$\bar{\eta}_\alpha = z_\alpha(z_\beta + z_\gamma)M_\alpha. \tag{84}$$

[3] Often in the literature this wavefunction is taken as the scattering state of two clusters in the initial channel satisfying the equation

$$\left(\frac{1}{2M_\alpha}\Delta_{\rho_\alpha} - U_\alpha(\boldsymbol{\rho}_\alpha) + \frac{q^2_{\alpha n}}{2M_\alpha}\right)\chi^+_{\alpha n}(\boldsymbol{\rho}_\alpha) = 0,$$

with the outgoing-wave boundary condition. Here, $U_\alpha(\boldsymbol{\rho}_\alpha)$ describes the interaction of the incident particle α with the c.m. of the bound subsystem (β, γ) and is written as

$$U_\alpha(\boldsymbol{\rho}_\alpha) = V_\beta(\boldsymbol{\rho}_\alpha) + V_\gamma(\boldsymbol{\rho}_\alpha).$$

This is an attempt to give to $\chi^+_{\alpha n}(\boldsymbol{\rho}_\alpha)$ more meaning than it is supposed to have. In order to make our point clear, let us assume that there is no Coulomb interaction between the cluster. Then for their relative motion we would use the simple plane wave rather than the scattering state. Though for the purpose of derivations given in the subsequent sections this choice is inessential, it may affect calculations of the total wavefunction in direct numerical methods. Therefore, the scattering amplitudes extracted from it may change unless the surface-integral representations given in the following sections of this work are used.

The complete and unambiguous asymptotic conditions for the solution of Eq. (78) with outgoing waves have been derived in [50,51]. In Ω_0, the scattered wave $\Psi_{\alpha n}^{\mathrm{sc}+}$ should satisfy the following asymptotic boundary conditions[4]:

$$\Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\overset{\Omega_0}{\to}\frac{1}{(2\pi)^{5/2}}\frac{(\mu_\alpha M_\alpha)^{3/2}}{\mu^2}T\left(\frac{\mu_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\alpha,\frac{M_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{\rho}_\alpha\right)\frac{\kappa^{3/2}}{R^{5/2}}e^{i\kappa R-i\lambda_0\ln(2\kappa R)-i\sigma_0+i\pi/4}, \tag{85}$$

where T is the amplitude for breakup of bound state αn (see [51]), $\kappa=(2\mu E)^{1/2}$ and

$$\lambda_0=\frac{1}{\kappa}\sum_{v=1,2,3}\left(\frac{\mu}{\mu_v}\right)^{1/2}\frac{\eta_v}{\sin\varphi_v}, \tag{86}$$

$$\sigma_0=\frac{2}{\kappa}\sum_{v=1,2,3}\left(\frac{\mu}{\mu_v}\right)^{1/2}\frac{\eta_v\ln(\sin\varphi_v)}{\sin\varphi_v}, \tag{87}$$

$$\eta_\alpha=z_\beta z_\gamma\mu_\alpha. \tag{88}$$

In Ω_α, we have [51]

$$\begin{aligned}\Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)&\overset{\Omega_\alpha}{\to}\frac{1}{(2\pi)^{5/2}}\\&\times\frac{(\mu_\alpha M_\alpha)^{3/2}}{\mu^2}T\left(\frac{\mu_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\alpha,\frac{M_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{\rho}_\alpha\right)\frac{\kappa^{3/2}}{R^{5/2}}\psi_\alpha^-\left(\frac{\mu_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\alpha,\boldsymbol{r}_\alpha\right)e^{i\kappa R-i\lambda_\alpha\ln(2\kappa R)-i\sigma_\alpha+i\pi/4}\\&-\frac{M_\alpha}{2\pi}\sum_m F(q_{\alpha m}\widehat{\boldsymbol{\rho}}_\alpha,\boldsymbol{q}_{\alpha n})\frac{e^{iq_{\alpha m}\rho_\alpha}}{\rho_\alpha}e^{-i\bar{\eta}_\alpha/q_{\alpha m}\ln(2q_{\alpha m}\rho_\alpha)}\phi_{\alpha m}(\boldsymbol{r}_\alpha),\end{aligned} \tag{89}$$

where F is the amplitude for transition from channel αn into another two-fragment channel state αm within the same arrangement (elastic scattering and direct excitation),

$$\lambda_\alpha=\frac{1}{\kappa}\sum_{v=\beta,\gamma}\left(\frac{\mu}{\mu_v}\right)^{1/2}\frac{\eta_v}{\sin\varphi_v}, \tag{90}$$

$$\sigma_\alpha=\frac{2}{\kappa}\sum_{v=\beta,\gamma}\left(\frac{\mu}{\mu_v}\right)^{1/2}\frac{\eta_v\ln(\sin\varphi_v)}{\sin\varphi_v}. \tag{91}$$

The wavefunction $\psi_\alpha^-(\boldsymbol{k}_\alpha,\boldsymbol{r}_\alpha)$ satisfies the equation

$$\left[\frac{1}{2\mu_\alpha}\Delta_{\boldsymbol{r}_\alpha}+i\frac{1}{\mu_\alpha}\boldsymbol{k}_\alpha\nabla_{\boldsymbol{r}_\alpha}-V_\alpha(\boldsymbol{r}_\alpha)\right]\psi_\alpha^-(\boldsymbol{k}_\alpha,\boldsymbol{r}_\alpha)=0. \tag{92}$$

In other words, $\{\phi_{\alpha n}(\boldsymbol{r}_\alpha),e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha}\psi_\alpha^-(\boldsymbol{k}_\alpha,\boldsymbol{r}_\alpha)\}$ is a complete orthonormal set of wavefunctions describing the state of the pair of particles β and γ, interacting via the potential given by the sum of the Coulomb and short-range potentials $V_\alpha=V_\alpha^C+V_\alpha^S$. We emphasize that the continuum part $e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha}\psi_\alpha^-(\boldsymbol{k}_\alpha,\boldsymbol{r}_\alpha)$ has the incoming-wave boundary condition. The momentum of the scattered particle α relative to the bound pair (β,γ) in state m is given by

$$q_{\alpha m}=[2M_\alpha(E-E_{\alpha m})]^{1/2}. \tag{93}$$

In Ω_β, we have [51]

$$\begin{aligned}\Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)&\overset{\Omega_\beta}{\to}\frac{1}{(2\pi)^{5/2}}\frac{(\mu_\beta M_\beta)^{3/2}}{\mu^2}T\left(\frac{\mu_\beta}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\beta,\frac{M_\beta}{\mu}\frac{\kappa}{R}\boldsymbol{\rho}_\beta\right)\frac{\kappa^{3/2}}{R^{5/2}}\psi_\beta^-\left(\frac{\mu_\beta}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\beta,\boldsymbol{r}_\beta\right)e^{i\kappa R-i\lambda_\beta\ln(2\kappa R)-i\sigma_\beta+i\pi/4}\\&-\frac{M_\beta}{2\pi}\sum_m G(q_{\beta m}\widehat{\boldsymbol{\rho}}_\beta,\boldsymbol{q}_{\alpha n})\frac{e^{iq_{\beta m}\rho_\beta}}{\rho_\beta}e^{-i\bar{\eta}_\beta/q_{\beta m}\ln(2q_{\beta m}\rho_\beta)}\phi_{\beta m}(\boldsymbol{r}_\beta),\end{aligned} \tag{94}$$

[4] Here we give only the leading-order terms without three-body correlation and multiple scattering effects which are of higher order. In principle, all the derivations can be done with these terms included, however this does not change the final results.

where G is the amplitude for transition from channel αn into two-fragment channel state βm with rearrangement.

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

$$\alpha+\beta+\gamma\to\begin{cases}\alpha+(\beta,\gamma),\\ \beta+(\gamma,\alpha),\\ \alpha+\beta+\gamma,\end{cases} \tag{95}$$

which we call a $3\to 3$ scattering. The wavefunction Ψ_0^- describing this process is also an eigenstate of the same Hamiltonian H, i.e.,

$$(E-H)\Psi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)=0, \tag{96}$$

but with incoming scattered-wave boundary conditions.

In the total wavefunction $\Psi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)$, we separate the part describing the unscattered state of three free particles, denoted $\Phi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)$ and which Ψ_0^- is developed to (in the absence of the Coulomb interaction this would simply be the three-body plane wave)

$$\Psi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)=\Phi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)+\Psi_0^{\mathrm{sc}-}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha). \tag{97}$$

The unscattered Coulomb-distorted three-body state $\Phi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)$ in Ω_0 was given by [61] and has the form of the three-body plane wave distorted by the long-range Coulomb interaction between all three pairs of particles:

$$\Phi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\overset{\Omega_0}{\to}e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha+i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\prod_{\nu=1,2,3}e^{-i\eta_\nu/k_\nu\ln\zeta(\boldsymbol{k}_\nu,\boldsymbol{r}_\nu)}, \tag{98}$$

where

$$\zeta(\boldsymbol{k}_\alpha,\boldsymbol{r}_\alpha)=k_\alpha r_\alpha+\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha. \tag{99}$$

In this domain, the scattered part of the total wavefunction $\Psi_0^{\mathrm{sc}-}$ has the following boundary condition [52]:

$$\Psi_0^{\mathrm{sc}-}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\overset{\Omega_0}{\to}\frac{1}{(2\pi)^{5/2}}\frac{(\mu_\alpha M_\alpha)^{3/2}}{\mu^2}\widetilde{T}\left(\frac{\mu_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\alpha,\frac{M_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{\rho}_\alpha\right)\frac{\kappa^{3/2}}{R^{5/2}}e^{-i\kappa R+i\lambda_0\ln(2\kappa R)+i\sigma_0-i\pi/4}, \tag{100}$$

where $\widetilde{T}$ is the amplitude of $3\to 3$ scattering.

In Ω_α, domain the incident three-body state Φ_0^- is written [53], in the leading order, as[5]

$$\Phi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\overset{\Omega_\alpha}{\to}e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha+i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\psi_\alpha^-(\boldsymbol{k}_\alpha,\boldsymbol{r}_\alpha)\prod_{\nu=\beta,\gamma}e^{-i\eta_\nu/k_\nu\ln\zeta(\boldsymbol{k}_\nu,\boldsymbol{r}_\nu)} \tag{101}$$

and

$$\begin{aligned}\Psi_0^{\mathrm{sc}-}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\to^{\Omega_\alpha}&\frac{1}{(2\pi)^{5/2}}\frac{(\mu_\alpha M_\alpha)^{3/2}}{\mu^2}\widetilde{T}\left(\frac{\mu_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\alpha,\frac{M_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{\rho}_\alpha\right)\frac{\kappa^{3/2}}{R^{5/2}}\psi_\alpha^-\left(\frac{\mu_\alpha}{\mu}\frac{\kappa}{R}\boldsymbol{r}_\alpha,\boldsymbol{r}_\alpha\right)e^{-i\kappa R+i\lambda_\alpha\ln(2\kappa R)+i\sigma_\alpha-i\pi/4}\\ &-\frac{M_\alpha}{2\pi}\sum_n\widetilde{F}(q_{\alpha n}\widehat{\boldsymbol{\rho}}_\alpha)\frac{e^{-iq_{\alpha n}\rho_\alpha}}{\rho_\alpha}e^{i\bar{\eta}_\alpha/q_{\alpha n}\ln(2q_{\alpha n}\rho_\alpha)}\phi_{\alpha n}(\boldsymbol{r}_\alpha),\end{aligned} \tag{102}$$

where $\widetilde{F}$ is the amplitude for recombination of three free particles into a two-fragment channel state αn [52].

In the Ω_β domain, the unscattered three-body state Φ_0^- and the scattered part $\Psi_0^{\mathrm{sc}-}$ have the asymptotic forms similar to (101) and (102), with index α replaced by β.

[5] For more detailed wavefunctions with higher-order terms, see [53,62,63].

Thus we have fully specified two total scattering wavefunctions corresponding to outgoing and incoming-wave boundary conditions $\Psi^+_{\alpha n}$ and Ψ^-_0 and have given their asymptotic forms in each asymptotic domain. The remaining two wavefunctions $\Psi^-_{\alpha m}$ and $\Psi^-_{\beta m}$ both having incoming-wave boundary condition should develop to final states αm and βm, respectively. Therefore, they are obtained from $\Psi^+_{\alpha n}$ with complex conjugation and simultaneous reversal of all momenta [56] (similar to Eq. (9)). We obtain various asymptotic forms of $\Psi^-_{\alpha m}$ and $\Psi^-_{\beta m}$ from the corresponding forms of $\Psi^+_{\alpha n}$ in the same way.

A comment about the different scattering wavefunctions used in this work is appropriate. As mentioned above, wavefunctions Ψ^-_0 and $\Psi^+_{\alpha n}$ are in fact two forms of the total scattering wavefunction of the three-body system, having two different starting points (boundary conditions). However, for breakup, it is particularly important to clearly understand the differences in the continuum parts of the asymptotic forms of the total scattering wavefunctions $\Psi^+_{\alpha n}$ and Ψ^-_0. Often in the literature the asymptotic form of $\Psi^{sc+}_{\alpha n}$ in Ω_0, that is the scattered part of $\Psi^+_{\alpha n}$, and wavefunction Φ^-_0, which is the unscattered part of Ψ^-_0 are called two versions (the plane-wave and spherical-wave) of "one asymptotic wavefunction" as if they were equivalent or represented the same function. Peterkop [64] claimed that asymptotically they should coincide. This is not right. Function Φ^-_0 represents the initial unscattered state of the three "free" (unbound) Coulomb particles, i.e., the Coulomb-modified three-body plane wave. Apart from the modification of the plane wave due to the long-range Coulomb interaction between the three pairs, there is no scattering information in this wavefunction. It is a state where the total scattering wavefunction Ψ^-_0 ends up developing to in the time reversed picture. In contrast, wavefunction $\Phi^{sc+}_{\alpha n}$ is formed when the scattering takes place and describes the breakup event. Therefore, by definition, it should carry information about the breakup of the initial bound state and has a form of the outgoing spherical scattered wave. From Eqs. (100) and (102), we see that Ψ^-_0 also has a spherical scattered part (containing information about the $3 \to 3$ process) of the same order as in the asymptotic form of $\Psi^{sc+}_{\alpha n}$, however it is suppressed by the stronger continuum term Φ^-_0. In other words, Φ^-_0 and the asymptotic form of $\Phi^+_{\alpha n}$ in Ω_0 are completely different functions. Therefore, an attempt to unify the three-body plane wave and the spherical scattered wave carrying away the information about what happened during the collision is not justified.

3.2. Coulomb breakup amplitude in prior form

In this section, we use $\Psi^+_{\alpha n}$ and Ψ^-_0 as starting points to derive amplitudes for different scattering processes. For this, we need an incomplete inner product in the six-dimensional configuration space. An 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 is written as a six-dimensional volume integral

$$\langle \Psi_f | \Psi_i \rangle = \int d\mathbf{r}_\alpha \, d\boldsymbol{\rho}_\alpha \, \Psi^*_f(\mathbf{r}_\beta, \boldsymbol{\rho}_\beta) \Psi_i(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha). \tag{103}$$

As in the case of the two-body problem in scattering with three particles, we deal with non-square-integrable functions. Therefore, the inner product defined above can be unbounded. In order to avoid difficulties associated with this fact, let us introduce an incomplete inner product according to

$$\langle \Psi_f | \Psi_i \rangle_{R_0} = \int_{R \leqslant R_0} d\mathbf{r}_\alpha d\boldsymbol{\rho}_\alpha \Psi^*_f(\mathbf{r}_\beta, \boldsymbol{\rho}_\beta) \Psi_i(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{104}$$

where the integration is limited to the volume of a six-dimensional hypersphere of radius R_0.

Taking into account Eq. (80), we can write Eq. (78) as

$$(E - H) \Psi^{sc+}_{\alpha n}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = (H - E) \Phi^+_{\alpha n}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha). \tag{105}$$

Let us multiply Eq. (105) by $\Psi^{-*}_0(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ from the left and integrate the result over the volume of a hypersphere of radius R_0:

$$\langle \Psi^-_0 | (E - H) \Psi^{sc+}_{\alpha n} \rangle_{R_0} = \langle \Psi^-_0 | (H - E) \Phi^+_{\alpha n} \rangle_{R_0}. \tag{106}$$

We also have

$$\left\langle (E-H)\Psi_0^- | \Psi_{\alpha n}^{\mathrm{sc}+} \right\rangle_{R_0} = 0, \tag{107}$$

which is true for any R_0 simply due to Eq. (96). Now, we subtract Eq. (107) from (106) to get

$$\left\langle \Psi_0^- | (E-H)\Psi_{\alpha n}^{\mathrm{sc}+} \right\rangle_{R_0} - \left\langle (E-H)\Psi_0^- | \Psi_{\alpha n}^{\mathrm{sc}+} \right\rangle_{R_0} = \left\langle \Psi_0^- | (H-E)\Phi_{\alpha n}^+ \right\rangle_{R_0}. \tag{108}$$

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

$$-\left\langle \Psi_0^- | H_0 \Psi_{\alpha n}^{\mathrm{sc}+} \right\rangle_{R_0} + \left\langle H_0 \Psi_0^- | \Psi_{\alpha n}^{\mathrm{sc}+} \right\rangle_{R_0} = \left\langle \Psi_0^- | (H-E)\Phi_{\alpha n}^+ \right\rangle_{R_0}. \tag{109}$$

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

$$\lim_{R_0\to\infty} \left[-\left\langle \Psi_0^- | H_0 \Psi_{\alpha n}^{\mathrm{sc}+} \right\rangle + \left\langle H_0 \Psi_0^- | \Psi_{\alpha n}^{\mathrm{sc}+} \right\rangle \right]_{R_0} = \lim_{R_0\to\infty} \left\langle \Psi_0^- | (H-E)\Phi_{\alpha n}^+ \right\rangle_{R_0}. \tag{110}$$

What does $\lim_{R_0\to\infty} \langle \Psi_0^- | (H-E)\Phi_{\alpha n}^+ \rangle_{R_0}$ on the RHS of Eq. (110) represent? 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. (110) 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. For this integral, the knowledge of the wavefunctions anywhere inside the surface is not required. Then it can be evaluated using the asymptotic forms of the wavefunctions, given in the previous subsection, in the corresponding asymptotic domain.

Let us start from Ω_0 domain. If $R_0 \to \infty$ in Ω_0 then for the LHS of Eq. (110) we have

$$\begin{aligned}
\mathrm{LHS} &= \lim_{R_0\to\infty} \int_{R\leqslant R_0} d\boldsymbol{r}_\alpha d\boldsymbol{\rho}_\alpha \left[-\Psi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) H_0 \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) + \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) H_0 \Psi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \right] \\
&= \frac{\mu^3}{(\mu_\alpha M_\alpha)^{3/2}} \lim_{R_0\to\infty} R_0^5 \int d\hat{\boldsymbol{r}}_\alpha d\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} d\varphi_\alpha \sin^2\varphi_\alpha \cos^2\varphi_\alpha \\
&\quad \times \frac{1}{2\mu} \left[\Psi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) - \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \right]_{R=R_0}.
\end{aligned} \tag{111}$$

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 using Eq. (85) for $\Psi_{\alpha n}^{\mathrm{sc}+}$ and Eqs. (97), (98) and (100) for Ψ_0^- and performing differentiation we get from Eq. (111), in the leading order,

$$\begin{aligned}
\mathrm{LHS} &= \frac{1}{2} \frac{\mu^2}{(\mu_\alpha M_\alpha)^{3/2}} \lim_{R_0\to\infty} R_0^5 \int d\hat{\boldsymbol{r}}_\alpha d\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} d\varphi_\alpha \sin^2\varphi_\alpha \cos^2\varphi_\alpha \left[\Phi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \right. \\
&\quad - \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Phi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) + \Psi_0^{\mathrm{sc}-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) - \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_0^{\mathrm{sc}-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \left. \right]_{R=R_0} \\
&= \frac{1}{2} \frac{\mu^2}{(\mu_\alpha M_\alpha)^{3/2}} \lim_{R_0\to\infty} R_0^5 \int d\hat{\boldsymbol{r}}_\alpha d\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} d\varphi_\alpha \sin^2\varphi_\alpha \cos^2\varphi_\alpha \left[i\left(\kappa + \sqrt{\frac{\mu}{\mu_\alpha}} \boldsymbol{k}_\alpha \cdot \hat{\boldsymbol{r}}_\alpha \sin\varphi_\alpha \right. \right. \\
&\quad \left. \left. + \sqrt{\frac{\mu}{M_\alpha}} \boldsymbol{q}_\alpha \cdot \hat{\boldsymbol{\rho}}_\alpha \cos\varphi_\alpha \right) \Phi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) + i(\kappa - \kappa) \Psi_0^{\mathrm{sc}-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \right]_{R=R_0}.
\end{aligned} \tag{112}$$

For brevity in the last equation, we kept the short notations for the wavefunctions, however, here their asymptotic forms are assumed. As we can see, the second term in the square brackets disappears. For the two plane waves present in Φ_0^-, we use their asymptotic forms. Then we have

$$
\begin{aligned}
\mathrm{LHS} = {} & \frac{2\pi^2}{ik_\alpha q_\alpha}\frac{\mu}{(\mu_\alpha M_\alpha)}\lim_{R_0\to\infty} R_0^3\int_0^{\pi/2} d\varphi_\alpha \sin\varphi_\alpha\cos\varphi_\alpha\Bigg\{\left(\kappa+\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha\sin\varphi_\alpha+\sqrt{\frac{\mu}{M_\alpha}}q_\alpha\cos\varphi_\alpha\right)\\
& \times\exp\left[-i\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha R_0\sin\varphi_\alpha - i\sqrt{\frac{\mu}{M_\alpha}}q_\alpha R_0\cos\varphi_\alpha\right]\prod_{v=1,2,3}\exp\left[\frac{i\eta_v}{k_v}\ln\zeta(\boldsymbol{k}_v,\sqrt{\frac{\mu}{\mu_v}}R_0\sin\phi_v\hat{\boldsymbol{k}}_v)\right]\\
& \times\Psi^{\mathrm{sc}+}_{\alpha n}\left(\sqrt{\frac{\mu}{\mu_\alpha}}R_0\sin\varphi_\alpha\hat{\boldsymbol{k}}_\alpha,\sqrt{\frac{\mu}{M_\alpha}}R_0\cos\varphi_\alpha\hat{\boldsymbol{q}}_\alpha\right)+\left(\kappa-\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha\sin\varphi_\alpha-\sqrt{\frac{\mu}{M_\alpha}}q_\alpha\cos\varphi_\alpha\right)\\
& \times\exp\left[i\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha R_0\sin\varphi_\alpha + i\sqrt{\frac{\mu}{M_\alpha}}q_\alpha R_0\cos\varphi_\alpha\right]\prod_{v=1,2,3}\exp\left[\frac{i\eta_v}{k_v}\ln\zeta(\boldsymbol{k}_v,-\sqrt{\frac{\mu}{\mu_v}}R_0\sin\phi_v\hat{\boldsymbol{k}}_v)\right]\\
& \times\Psi^{\mathrm{sc}+}_{\alpha n}\left(-\sqrt{\frac{\mu}{\mu_\alpha}}R_0\sin\varphi_\alpha\hat{\boldsymbol{k}}_\alpha,-\sqrt{\frac{\mu}{M_\alpha}}R_0\cos\varphi_\alpha\hat{\boldsymbol{q}}_\alpha\right)+\left(\kappa+\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha\sin\varphi_\alpha-\sqrt{\frac{\mu}{M_\alpha}}q_\alpha\cos\varphi_\alpha\right)\\
& \times\exp\left[-i\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha R_0\sin\varphi_\alpha + i\sqrt{\frac{\mu}{M_\alpha}}q_\alpha R_0\cos\varphi_\alpha\right]\prod_{v=1,2,3}\exp\left[\frac{i\eta_v}{k_v}\ln\zeta(\boldsymbol{k}_v,\sqrt{\frac{\mu}{\mu_v}}R_0\sin\phi_v\hat{\boldsymbol{k}}_v)\right]\\
& \times\Psi^{\mathrm{sc}+}_{\alpha n}\left(\sqrt{\frac{\mu}{\mu_\alpha}}R_0\sin\varphi_\alpha\hat{\boldsymbol{k}}_\alpha,-\sqrt{\frac{\mu}{M_\alpha}}R_0\cos\varphi_\alpha\hat{\boldsymbol{q}}_\alpha\right)+\left(\kappa-\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha\sin\varphi_\alpha+\sqrt{\frac{\mu}{M_\alpha}}q_\alpha\cos\varphi_\alpha\right)\\
& \times\exp\left[i\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha R_0\sin\varphi_\alpha - i\sqrt{\frac{\mu}{M_\alpha}}q_\alpha R_0\cos\varphi_\alpha\right]\prod_{v=1,2,3}\exp\left[\frac{i\eta_v}{k_v}\ln\zeta(\boldsymbol{k}_v,-\sqrt{\frac{\mu}{\mu_v}}R_0\sin\phi_v\hat{\boldsymbol{k}}_v)\right]\\
& \times\Psi^{\mathrm{sc}+}_{\alpha n}\left(-\sqrt{\frac{\mu}{\mu_\alpha}}R_0\sin\varphi_\alpha\hat{\boldsymbol{k}}_\alpha,\sqrt{\frac{\mu}{M_\alpha}}R_0\cos\varphi_\alpha\hat{\boldsymbol{q}}_\alpha\right)\Bigg\}. \qquad (113)
\end{aligned}
$$

This is an extremely (in fact – infinitely) oscillatory integral as $R_0\to\infty$ and therefore, only points of stationary phase in φ_α, if there are any, should contribute to the integral. The first two terms within the braces have a common stationary-phase point at $\sin\varphi_\alpha=\sqrt{\mu/\mu_\alpha}k_\alpha/\kappa$ where $\cos\varphi_\alpha=\sqrt{\mu/M_\alpha}q_\alpha/\kappa$. However, the second term is identically zero at the stationary point. The third and fourth terms of the integrand have no stationary points and, therefore, do not contribute to the integral. Thus we have to evaluate

$$
\begin{aligned}
\mathrm{LHS} = {} & \frac{1}{ik_\alpha q_\alpha}\frac{1}{2\sqrt{2\pi}}\frac{(\mu_\alpha M_\alpha)^{1/2}}{\mu}\kappa^{3/2}\lim_{R_0\to\infty}R_0^{1/2}\int_0^{\pi/2}d\varphi_\alpha\sin\varphi_\alpha\cos\varphi_\alpha e^{i\kappa R_0 - i\lambda_0\ln(2\kappa R_0)-i\sigma_0+i\pi/4}\\
& \times\left(\kappa+\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha\sin\varphi_\alpha+\sqrt{\frac{\mu}{M_\alpha}}q_\alpha\cos\varphi_\alpha\right)\exp\left[-i\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha R_0\sin\varphi_\alpha - i\sqrt{\frac{\mu}{M_\alpha}}q_\alpha R_0\cos\varphi_\alpha\right]\\
& \times\prod_{v=1,2,3}\exp\left[\frac{i\eta_v}{k_v}\ln\left(2\sqrt{\frac{\mu}{\mu_v}}R_0\sin\phi_v k_v\right)\right]T\left(\sqrt{\frac{\mu_\alpha}{\mu}}\kappa\sin\varphi_\alpha\hat{\boldsymbol{k}}_\alpha,\sqrt{\frac{M_\alpha}{\mu}}\kappa\cos\varphi_\alpha\hat{\boldsymbol{q}}_\alpha\right), \qquad (114)
\end{aligned}
$$

where we used Eq. (85). Calculating the remaining integral by means of the stationary-phase method [65], we arrive at

$$
\begin{aligned}
\mathrm{LHS} = {} & \frac{1}{i\sqrt{2\pi}}T(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)\kappa^{1/2}\lim_{R_0\to\infty}R_0^{1/2}e^{i\kappa R_0+i\pi/4}\int_0^{\pi/2}d\varphi_\alpha\\
& \times\exp\left[-i\sqrt{\frac{\mu}{\mu_\alpha}}k_\alpha R_0\sin\varphi_\alpha - i\sqrt{\frac{\mu}{M_\alpha}}q_\alpha R_0\cos\varphi_\alpha\right]\\
= {} & \frac{1}{i\sqrt{2\pi}}T(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)\kappa^{1/2}\lim_{R_0\to\infty}R_0^{1/2}e^{i\kappa R_0+i\pi/4}\sqrt{\frac{2\pi}{\kappa R_0}}e^{-i\kappa R_0+i\pi/4}\\
= {} & T(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha). \qquad (115)
\end{aligned}
$$

Thus we get that the LHS of Eq. (110) is in fact equal to $T(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)$. Therefore, at least in Ω_0 domain Eq. (110) is written as

$$
T(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)=\lim_{R_0\to\infty}\left\langle\Psi_0^-|(H-E)\Phi^+_{\alpha n}\right\rangle_{R_0}. \qquad (116)
$$

In other words, if scattering takes place into Ω_0 domain then expression $\lim_{R_0\to\infty}\langle\Psi_0^-|(H-E)\Phi^+_{\alpha n}\rangle_{R_0}$ 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 $\lim_{R_0\to\infty}\langle\Psi_0^-|(H-E)\Phi_{\alpha n}^+\rangle$ again represents the breakup amplitude. Thus, Eq. (116) defines the breakup amplitude in all asymptotic domains.

3.3. Amplitudes for direct and rearrangement scattering in prior form

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 the 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. (105) by $\Psi_{\alpha m}^{-*}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ from the left and integrate the result over the volume of a hypersphere of radius R_0:

$$\left\langle\Psi_{\alpha m}^-|(E-H)\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle_{R_0}=\left\langle\Psi_{\alpha m}^-|(H-E)\Phi_{\alpha n}^+\right\rangle_{R_0}. \tag{117}$$

We also need

$$\left\langle(E-H)\Psi_{\alpha m}^-|\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle_{R_0}=0. \tag{118}$$

Now we subtract Eq. (118) from (117)

$$\left\langle\Psi_{\alpha m}^-|(E-H)\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle_{R_0}-\left\langle(E-H)\Psi_{\alpha m}^-|\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle_{R_0}=\left\langle\Psi_{\alpha m}^-|(H-E)\Phi_{\alpha n}^+\right\rangle_{R_0}, \tag{119}$$

which, for the same reasons as Eq. (108), reduces to

$$-\left\langle\Psi_{\alpha m}^-|H_0\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle_{R_0}+\left\langle H_0\Psi_{\alpha m}^-|\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle_{R_0}=\left\langle\Psi_{\alpha m}^-|(H-E)\Phi_{\alpha n}^+\right\rangle_{R_0}. \tag{120}$$

We will again investigate the limit of this equation as $R_0\to\infty$:

$$\lim_{R_0\to\infty}\left[-\left\langle\Psi_{\alpha m}^-|H_0\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle+\left\langle H_0\Psi_{\alpha m}^-|\Psi_{\alpha n}^{\mathrm{sc}+}\right\rangle\right]_{R_0}=\lim_{R_0\to\infty}\left\langle\Psi_{\alpha m}^-|(H-E)|\Phi_{\alpha n}^+\right\rangle_{R_0}. \tag{121}$$

Since this time $R_0\to\infty$ in Ω_α then for the LHS of Eq. (121) we have

$$\begin{aligned}\mathrm{LHS}&=\lim_{R_0\to\infty}\int_{R\leqslant R_0}d\mathbf{r}_\alpha\,d\boldsymbol{\rho}_\alpha\left[-\Psi_{\alpha m}^{-*}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)H_0\Psi_{\alpha n}^{\mathrm{sc}+}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)+\Psi_{\alpha n}^{\mathrm{sc}+}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)H_0\Psi_{\alpha m}^{-*}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]\\&=\frac{1}{2M_\alpha}\lim_{R_0\to\infty}R_0^2\int d\mathbf{r}_\alpha\,d\hat{\boldsymbol{\rho}}_\alpha\left[\Psi_{\alpha m}^{-*}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Psi_{\alpha n}^{\mathrm{sc}+}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)-\Psi_{\alpha n}^{\mathrm{sc}+}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Psi_{\alpha m}^{-*}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{\rho_\alpha=R_0}.\end{aligned} \tag{122}$$

Here we transformed only one of the volume integrals into the surface integral (the other two-body space is limited).

As we mentioned earlier the asymptotic forms of the wavefunction $\Psi_{\alpha m}^-$ are obtained from those of $\Psi_{\alpha n}^+$ with complex conjugation and simultaneous reversal of directions of all momenta. In particular, the unscattered part of $\Psi_{\alpha m}^-$ (we split $\Psi_{\alpha m}^-$ according to $\Psi_{\alpha m}^-=\Phi_{\alpha m}^-+\Psi_{\alpha m}^{\mathrm{sc}-}$) is given as

$$\Phi_{\alpha m}^-(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)=\chi_{\alpha m}^-(\boldsymbol{\rho}_\alpha)\phi_{\alpha m}(\mathbf{r}_\alpha). \tag{123}$$

Using the asymptotic forms of the wavefunctions and performing differentiation we get from Eq. (122), in the leading order,

$$\begin{aligned}\mathrm{LHS}=\frac{1}{2M_\alpha}\lim_{R_0\to\infty}R_0^2\int d\mathbf{r}_\alpha\,d\hat{\boldsymbol{\rho}}_\alpha\Bigg[&-\chi_{\alpha m}^{-*}(\boldsymbol{\rho}_\alpha)\phi_{\alpha m}^*(\mathbf{r}_\alpha)\frac{\partial}{\partial\rho_\alpha}\frac{M_\alpha}{2\pi}\sum_l F(q_{\alpha l}\hat{\boldsymbol{\rho}}_\alpha,\mathbf{q}_{\alpha n})\frac{e^{iq_{\alpha l}\rho_\alpha}}{\rho_\alpha}e^{-i\eta_{\alpha l}/q_{\alpha l}\ln(2q_{\alpha l}\rho_\alpha)}\phi_{\alpha l}(\mathbf{r}_\alpha)\\&+\frac{M_\alpha}{2\pi}\sum_l F(q_{\alpha l}\hat{\boldsymbol{\rho}}_\alpha,\mathbf{q}_{\alpha n})\frac{e^{iq_{\alpha l}\rho_\alpha}}{\rho_\alpha}e^{-i\eta_{\alpha l}/q_{\alpha l}\ln(2q_{\alpha l}\rho_\alpha)}\phi_{\alpha l}(\mathbf{r}_\alpha)\frac{\partial}{\partial\rho_\alpha}\chi_{\alpha m}^{-*}(\boldsymbol{\rho}_\alpha)\phi_{\alpha m}^*(\mathbf{r}_\alpha)\Bigg]_{\rho_\alpha=R_0}.\end{aligned} \tag{124}$$

Taking into account the orthogonality of the two-particle bound state wavefunctions, we arrive at

$$\begin{aligned}\text{LHS} &= \frac{1}{4\pi}\lim_{R_0\to\infty} R_0 \int d\hat{\boldsymbol{\rho}}_\alpha \left[\chi^{-*}_{\alpha m}(\boldsymbol{\rho}_\alpha) F(q_{\alpha m}\hat{\boldsymbol{\rho}}_\alpha, \boldsymbol{q}_{\alpha n}) e^{iq_{\alpha m}\rho_\alpha - i\eta_{\alpha m}/q_{\alpha m}\ln(2q_{\alpha m}\rho_\alpha)}(-iq_{\alpha n} + i\boldsymbol{q}_{\alpha m}\cdot\hat{\boldsymbol{\rho}}_\alpha)\right]_{\rho_\alpha=R_0} \\ &= F(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}). \end{aligned} \tag{125}$$

In the last step, we used Eq. (62) for the Coulomb-modified plane wave $\chi^-_{\alpha m}$ to evaluate the remaining integral. Thus we have established that Eq. (121) is in fact written as

$$F(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) = \lim_{R_0\to\infty} \left\langle \Psi^-_{\alpha m} | (H-E)\Phi^+_{\alpha n}\right\rangle_{R_0}. \tag{126}$$

In other words, we have obtained 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 channel channel β) and calculating the LHS of Eq. (121), we get a definition for the amplitude of the rearrangement scattering

$$G(\boldsymbol{q}_{\beta m}, \boldsymbol{q}_{\alpha n}) = \lim_{R_0\to\infty} \left\langle \Psi^-_{\beta m} | (H-E)\Phi^+_{\alpha n}\right\rangle_{R_0}. \tag{127}$$

Calculations leading to this result are similar to those which lead to Eq. (126).

3.4. Scattering and breakup amplitudes for a Coulomb three-body system in post form

In this section, we derive amplitudes for various processes in the so-called post form. Taking into account Eq. (97), we can write Eq. (96) as

$$(E-H)\Psi^{sc-}_0(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = (H-E)\Phi^-_0(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha). \tag{128}$$

Let us take the complex conjugate of Eq. (128) and multiply it by $\Psi^+_{\alpha n}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha)$ from right. Then integrating the result over the volume of a hypersphere of radius R_0, we get

$$\left\langle (E-H)\Psi^{sc-}_0 | \Psi^+_{\alpha n}\right\rangle_{R_0} = \left\langle (E-H)\Phi^-_0 | \Psi^+_{\alpha n}\right\rangle_{R_0}. \tag{129}$$

We also consider

$$\left\langle \Psi^{sc-}_0 | (E-H)\Psi^+_{\alpha n}\right\rangle_{R_0} = 0, \tag{130}$$

which is again valid for any R_0 due to Eq. (78). Now we subtract Eq. (130) from (129)

$$\left\langle (E-H)\Psi^{sc-}_0 | \Psi^+_{\alpha n}\right\rangle_{R_0} - \left\langle \Psi^{sc-}_0 | (E-H)\Psi^+_{\alpha n}\right\rangle_{R_0} = \left\langle (E-H)\Phi^-_0 | \Psi^+_{\alpha n}\right\rangle_{R_0}, \tag{131}$$

which reduces to

$$-\left\langle H_0\Psi^{sc-}_0 | \Psi^+_{\alpha n}\right\rangle_{R_0} + \left\langle \Psi^{sc-}_0 | H_0\Psi^+_{\alpha n}\right\rangle_{R_0} = (\left\langle \Phi^-_0 | (H-E)\right)\Psi^+_{\alpha n}\rangle_{R_0}. \tag{132}$$

We again investigate the limit of this equation as $R_0 \to \infty$

$$\lim_{R_0\to\infty}\left[-(\left\langle \Psi^{sc-}_0 | H_0\right)|\Psi^+_{\alpha n}\right\rangle + \left\langle \Psi^{sc-}_0 | H_0 | \Psi^+_{\alpha n}\right\rangle\Big]_{R_0} = \lim_{R_0\to\infty}\left\langle (E-H)\Phi^-_0 | \Psi^+_{\alpha n}\right\rangle_{R_0}. \tag{133}$$

Calculations of the limit of the LHS of Eq. (133) are similar to those of Eq. (110) leading to Eqs. (116), (126) and (127). Therefore, we skip the details and simply give the final answer. Depending on whether the $R_0 \to \infty$ limit is taken in domains Ω_0, Ω_α or Ω_β, we have

$$T(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \lim_{R_0\to\infty}\left\langle (E-H)\Phi^-_0 | \Psi^+_{\alpha n}\right\rangle_{R_0}, \tag{134}$$

$$F(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) = \lim_{R_0\to\infty}\left\langle (E-H)\Phi^-_{\alpha m} | \Psi^+_{\alpha n}\right\rangle_{R_0}, \tag{135}$$

$$G(\boldsymbol{q}_{\beta m}, \boldsymbol{q}_{\alpha n}) = \lim_{R_0\to\infty}\left\langle (E-H)\Phi^-_{\beta m} | \Psi^+_{\alpha n}\right\rangle_{R_0}, \tag{136}$$

respectively. Thus we get alternative representations for the breakup, scattering and rearrangement amplitudes. These are called the post forms of the amplitudes. In particular, the definition given in Eq. (134) resolves the long-standing problem about the post form of the breakup amplitude mentioned earlier.

3.5. Surface-integral forms for the scattering amplitudes

Let us consider the post form of the breakup amplitude $T^{\rm post}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)$ given by Eq. (134). Using Eq. (78), which is valid for any R_0, we can write this as

$$\begin{aligned} T^{\rm post}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha) &= \lim_{R_0\to\infty}\left[\langle (E-H)\Phi_0^-|\Psi_{\alpha n}^+\rangle + \langle \Phi_0^-|(E-H)\Psi_{\alpha n}^+\rangle\right]_{R_0} \\ &= \lim_{R_0\to\infty}\left[\langle H_0\Phi_0^-|\Psi_{\alpha n}^+\rangle - \langle \Phi_0^-|H_0\Psi_{\alpha n}^+\rangle\right]_{R_0} \\ &= \lim_{R_0\to\infty}\int_{R\leqslant R_0} d\boldsymbol{r}_\alpha d\boldsymbol{\rho}_\alpha\left[\Psi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)H_0\Phi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) - \Phi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)H_0\Psi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]. \end{aligned} \tag{137}$$

Transforming the volume integral into a surface integral, we get

$$\begin{aligned} T^{\rm post}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha) = &-\frac{\mu^2}{2(\mu_\alpha M_\alpha)^{3/2}}\lim_{R_0\to\infty} R_0^5\int d\hat{\boldsymbol{r}}_\alpha d\hat{\boldsymbol{\rho}}_\alpha\int_0^{\pi/2} d\varphi_\alpha \sin^2\varphi_\alpha \\ &\times\cos^2\varphi_\alpha\left[\Psi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial R}\Phi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) - \Phi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial R}\Psi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{R=R_0}. \end{aligned} \tag{138}$$

Thus, the breakup amplitude in the post form is written as a five-dimensional surface integral. In the prior form of this amplitude and also both in the post and prior forms of scattering and rearrangement amplitudes only one of the three-dimensional volume integrals can be transformed into a (two-dimensional) surface integral. Consider, for instance, the prior form of the breakup amplitude. Using Eq. (96), we get from Eq. (116)

$$\begin{aligned} T^{\rm prior}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha) &= \lim_{R_0\to\infty}\left[\langle \Psi_0^-|(H-E)\Phi_{\alpha n}^+\rangle + \langle (E-H)\Psi_0^-|\Phi_{\alpha n}^+\rangle\right]_{R_0} \\ &= \lim_{R_0\to\infty}\left[\langle \Psi_0^-|H_0\Phi_{\alpha n}^+\rangle - \langle H_0\Psi_0^-|\Phi_{\alpha n}^+\rangle\right]_{R_0} \\ &= \lim_{R_0\to\infty}\int_{R\leqslant R_0} d\boldsymbol{r}_\alpha d\boldsymbol{\rho}_\alpha\left[\Psi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)H_0\Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) - \Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)H_0\Psi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]. \end{aligned} \tag{139}$$

This can be written as

$$T^{\rm prior}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha) = -\frac{1}{2M_\alpha}\lim_{R_0\to\infty} R_0^2\int d\boldsymbol{r}_\alpha d\hat{\boldsymbol{\rho}}_\alpha\left[\Psi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) - \Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Psi_0^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{\rho_\alpha=R_0}. \tag{140}$$

Above we took into account the fact that the surface integral in the other two-body space is zero as $r_\alpha\to\infty$ (the function $\Phi_{\alpha n}^+$ falls off exponentially in this variable). Similarly, we get

$$\begin{aligned} F^{\rm prior}(\boldsymbol{q}_{\alpha m},\boldsymbol{q}_{\alpha n}) &= \lim_{R_0\to\infty}\left[\langle \Psi_{\alpha m}^-|H_0\Phi_{\alpha n}^+\rangle - \langle H_0\Psi_{\alpha m}^-|\Phi_{\alpha n}^+\rangle\right]_{R_0} \\ &= -\frac{1}{2M_\alpha}\lim_{R_0\to\infty} R_0^2\int d\boldsymbol{r}_\alpha d\hat{\boldsymbol{\rho}}_\alpha\left[\Psi_{\alpha m}^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) - \Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Psi_{\alpha m}^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{\rho_\alpha=R_0}, \end{aligned} \tag{141}$$

$$\begin{aligned} G^{\rm prior}(\boldsymbol{q}_{\beta m},\boldsymbol{q}_{\alpha n}) &= \lim_{R_0\to\infty}\left[\left\langle \Psi_{\beta m}^-|H_0|\Phi_{\alpha n}^+\right\rangle - (\left\langle \Psi_{\beta m}^-|H_0)|\Phi_{\alpha n}^+\right\rangle\right]_{R_0} \\ &= -\frac{1}{2M_\alpha}\lim_{R_0\to\infty} R_0^2\int d\boldsymbol{r}_\alpha d\hat{\boldsymbol{\rho}}_\alpha\left[\Psi_{\beta m}^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) - \Phi_{\alpha n}^+(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Psi_{\beta m}^{-*}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{\rho_\alpha=R_0}, \end{aligned} \tag{142}$$

and in post forms

$$F^{\rm post}(\boldsymbol{q}_{\alpha m},\boldsymbol{q}_{\alpha n}) = \lim_{R_0\to\infty}\left[\langle H_0\Phi^-_{\alpha m}|\Psi^+_{\alpha n}\rangle - \langle\Phi^-_{\alpha m}|H_0\Psi^+_{\alpha n}\rangle\right]_{R_0}$$
$$= -\frac{1}{2M_\alpha}\lim_{R_0\to\infty}R_0^2\int d\boldsymbol{r}_\alpha d\hat{\boldsymbol{\rho}}_\alpha\left[\Psi^+_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Phi^{-*}_{\alpha m}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) - \Phi^{-*}_{\alpha m}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Psi^+_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{\rho_\alpha=R_0}, \tag{143}$$

$$G^{\rm post}(\boldsymbol{q}_{\beta m},\boldsymbol{q}_{\alpha n}) = \lim_{R_0\to\infty}\left[\left\langle H_0\Phi^-_{\beta m}|\Psi^+_{\alpha n}\right\rangle - \left\langle\Phi^-_{\beta m}|H_0\Psi^+_{\alpha n}\right\rangle\right]_{R_0}$$
$$= -\frac{1}{2M_\beta}\lim_{R_0\to\infty}R_0^2\int d\boldsymbol{r}_\beta d\hat{\boldsymbol{\rho}}_\beta\left[\Psi^+_{\alpha n}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta)\frac{\partial}{\partial\rho_\beta}\Phi^{-*}_{\beta m}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta) - \Phi^{-*}_{\beta m}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta)\frac{\partial}{\partial\rho_\beta}\Psi^+_{\alpha n}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta)\right]_{\rho_\alpha=R_0}. \tag{144}$$

3.6. Conventional forms of the scattering and breakup amplitudes

Here, we show consistency of the new definitions for the scattering and breakup amplitudes with the conventional forms. In the previous subsection, we gave the prior and post forms of the breakup amplitude in surface-integral forms. The surface integrals in Eqs. (138) and (140) are similar to those calculated in Sections 3.2 and 3.4. They can be calculated using the same analysis and shown to yield the same result, i.e., the breakup amplitude. This is the proof that Eqs. (110) and (133) are identities and that both sides of these equations represent the breakup amplitude. The same is true for the surface-integral representations of the direct scattering and rearrangement amplitudes. Therefore, Eqs. (116), (126) and (127) can in fact be written as

$$T^{\rm prior}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha) = \langle\Psi^-_0|(H-E)\Phi^+_{\alpha n}\rangle, \tag{145}$$
$$F^{\rm prior}(\boldsymbol{q}_{\alpha m},\boldsymbol{q}_{\alpha n}) = \langle\Psi^-_{\alpha m}|(H-E)\Phi^+_{\alpha n}\rangle, \tag{146}$$
$$G^{\rm prior}(\boldsymbol{q}_{\beta m},\boldsymbol{q}_{\alpha n}) = \left\langle\Psi^-_{\beta m}|(H-E)\Phi^+_{\alpha n}\right\rangle, \tag{147}$$

and Eqs. (134)–(136) as

$$T^{\rm post}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha) = \langle(E-H)\Phi^-_0|\Psi^+_{\alpha n}\rangle, \tag{148}$$
$$F^{\rm post}(\boldsymbol{q}_{\alpha m},\boldsymbol{q}_{\alpha n}) = \langle(E-H)\Phi^-_{\alpha m}|\Psi^+_{\alpha n}\rangle, \tag{149}$$
$$G^{\rm post}(\boldsymbol{q}_{\beta m},\boldsymbol{q}_{\alpha n}) = \left\langle(E-H)\Phi^-_{\beta m}|\Psi^+_{\alpha n}\right\rangle. \tag{150}$$

We note that when the interactions between all three pairs are short ranged then

$$\Phi^\pm_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\to e^{i\boldsymbol{q}_{\alpha n}\cdot\boldsymbol{\rho}_\alpha}\phi_{\alpha n}(\boldsymbol{r}_\alpha). \tag{151}$$

This state satisfies the equation

$$(H_0+V_\alpha-E)e^{i\boldsymbol{q}_{\alpha n}\cdot\boldsymbol{\rho}_\alpha}\phi_{\alpha n}(\boldsymbol{r}_\alpha) = 0. \tag{152}$$

At the same time, if we have three particles in the final channel then

$$\Phi^-_0(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\to e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha+i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}, \tag{153}$$

which is the solution to

$$(H_0-E)e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha+i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} = 0. \tag{154}$$

Then, in view of Eqs. (152) and (154), we would have

$$(H-E)\Phi^-_0(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = Ve^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha+i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}, \tag{155}$$
$$(H-E)\Phi^\pm_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = \overline{V}_\alpha e^{i\boldsymbol{q}_{\alpha n}\cdot\boldsymbol{\rho}_\alpha}\phi_{\alpha n}(\boldsymbol{r}_\alpha), \tag{156}$$
$$(H-E)\Phi^-_{\beta m}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta) = \overline{V}_\beta e^{i\boldsymbol{q}_{\beta m}\cdot\boldsymbol{\rho}_\beta}\phi_{\beta m}(\boldsymbol{r}_\beta). \tag{157}$$

where $\overline{V}_\alpha = V - V_\alpha$. Therefore, Eqs. (155)–(157) reduce the new generalized forms of the amplitudes (145)–(150) to the standard definitions

$$T^{\rm prior}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \left\langle \Psi_0^- | \overline{V}_\alpha | \phi_{\alpha n}, \boldsymbol{q}_{\alpha n} \right\rangle, \tag{158}$$

$$F^{\rm prior}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) = \left\langle \Psi_{\alpha m}^- | \overline{V}_\alpha | \phi_{\alpha n}, \boldsymbol{q}_{\alpha n} \right\rangle, \tag{159}$$

$$G^{\rm prior}(\boldsymbol{q}_{\beta m}, \boldsymbol{q}_{\alpha n}) = \left\langle \Psi_{\beta m}^- | \overline{V}_\alpha | \phi_{\alpha n}, \boldsymbol{q}_{\alpha n} \right\rangle, \tag{160}$$

and

$$T^{\rm post}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \left\langle \boldsymbol{q}_\alpha, \boldsymbol{k}_\alpha | V | \Psi_{\alpha n}^+ \right\rangle, \tag{161}$$

$$F^{\rm post}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) = \left\langle \boldsymbol{q}_{\alpha m}, \phi_{\alpha m} | \overline{V}_\alpha | \Psi_{\alpha n}^+ \right\rangle, \tag{162}$$

$$G^{\rm post}(\boldsymbol{q}_{\beta m}, \boldsymbol{q}_{\alpha n}) = \left\langle \boldsymbol{q}_{\beta m}, \phi_{\beta m} | \overline{V}_\beta | \Psi_{\alpha n}^+ \right\rangle. \tag{163}$$

When the interactions have the Coulomb tail, Eqs. (155)–(157) are not satisfied. For this reason, the standard definitions (158)–(163) become invalid.

In computation, we suggest the usage of the scattering amplitudes as defined in Eqs. (116, (126), (127), (134)–(136)), even in case of short-range potentials. Since these contain explicit limit operations they indicate how the amplitudes can be calculated in practice. The various asymptotic channel wavefunctions and scattered waves which define the relevant amplitudes are oscillatory functions of R_0. In some cases these waves can even be divergent. On the other hand the amplitudes do not depend on R_0. Therefore, the limiting procedure indicates that in practical calculations the scattered waves are calculated at reasonably large but limited space. When R_0 is sufficiently large the required amplitude becomes independent of R_0. Also, the surface-integral forms of the scattering amplitudes obtained in the previous section naturally follow from the forms containing the limits.

3.7. Computational methods for extracting the scattering amplitudes

If we want to calculate the amplitude of $2 \to 3$ breakup process then it is natural to extract it from the scattering wavefunction $\Psi_{\alpha n}^+$ which describes this process, though the same can be extracted from Ψ_0^- describing the time reversed process. The same is true for direct and rearrangement scattering amplitudes. In other words, the post form represents a more natural choice. Therefore, let us make a few comments of practical relevance about the post forms. Since when $r_\alpha \to \infty$ the incident part of $\Psi_{\alpha n}^+$ disappears, Eq. (138) can be written as

$$T^{\rm post}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = -\frac{\mu^2}{2(\mu_\alpha M_\alpha)^{3/2}} \lim_{R_0 \to \infty} R_0^5 \int d\hat{\boldsymbol{r}}_\alpha d\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} d\varphi_\alpha \sin^2 \varphi_\alpha \times \cos^2 \varphi_\alpha \left[\Psi_{\alpha n}^{{\rm sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Phi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) - \Phi_0^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial R} \Psi_{\alpha n}^{{\rm sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \right]_{R=R_0}. \tag{164}$$

We also can write

$$F^{\rm post}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) = -\frac{1}{2M_\alpha} \lim_{R_0 \to \infty} R_0^2 \int d\boldsymbol{r}_\alpha d\hat{\boldsymbol{\rho}}_\alpha \times \left[\Psi_{\alpha n}^{{\rm sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial \rho_\alpha} \Phi_{\alpha m}^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) - \Phi_{\alpha m}^{-*}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \frac{\partial}{\partial \rho_\alpha} \Psi_{\alpha n}^{{\rm sc}+}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \right]_{\rho_\alpha = R_0}, \tag{165}$$

$$G^{\rm post}(\boldsymbol{q}_{\beta m}, \boldsymbol{q}_{\alpha n}) = -\frac{1}{2M_\beta} \lim_{R_0 \to \infty} R_0^2 \int d\boldsymbol{r}_\beta d\hat{\boldsymbol{\rho}}_\beta \times \left[\Psi_{\alpha n}^{{\rm sc}+}(\boldsymbol{r}_\beta, \boldsymbol{\rho}_\beta) \frac{\partial}{\partial \rho_\beta} \Phi_{\beta m}^{-*}(\boldsymbol{r}_\beta, \boldsymbol{\rho}_\beta) - \Phi_{\beta m}^{-*}(\boldsymbol{r}_\beta, \boldsymbol{\rho}_\beta) \frac{\partial}{\partial \rho_\beta} \Psi_{\alpha n}^{{\rm sc}+}(\boldsymbol{r}_\beta, \boldsymbol{\rho}_\beta) \right]_{\rho_\alpha = R_0}. \tag{166}$$

However, the reason why the incident wave part of $\Psi_{\alpha n}^+$ does not contribute here is different. First of all, as $R_0 \to \infty$, due to the orthogonality of bound state wavefunctions present in the incident waves $\Phi_{\alpha n}^+$ and $\Phi_{\alpha m}^-$, the momenta describing relative motion of the clusters sit on the energy shell. Then,

according to the results of Section 2.1, the surface integral of two plane waves of the same energy is zero. It is not difficult to show the same to be the case if we have Coulomb-modified plane waves instead. For similar reasons, we can replace Ψ_0^-, $\Psi_{\alpha m}^-$ and $\Psi_{\beta m}^+$ by $\Psi_0^{\mathrm{sc}-}$, $\Psi_{\alpha m}^{\mathrm{sc}-}$ and $\Psi_{\beta m}^{\mathrm{sc}-}$ in Eqs. (140)–(142), respectively. These replacements are not valid in volume-integral forms where all parts of the space contribute.[6]

What is the advantage of the surface-integral representations over the volume-integral forms? As we can see from the surface-integral forms for the amplitudes, they are ideal for full practical calculations in partial waves. For example, let us expand the wavefunctions in bipolar spherical harmonics of a pair of unit vectors $\widehat{\boldsymbol{r}}_\alpha$ and $\widehat{\boldsymbol{\rho}}_\alpha$:

$$\Psi_{\alpha n}^{\mathrm{sc}+}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)=\sum_\lambda \mathcal{R}_\lambda^+(r_\alpha,\rho_\alpha)\mathcal{Y}_\lambda(\widehat{\boldsymbol{r}}_\alpha,\widehat{\boldsymbol{\rho}}_\alpha), \tag{167}$$

$$\Phi_0^-(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)=\sum_{\lambda,\lambda'} \mathcal{R}_{\lambda,\lambda'}^-(k_\alpha,q_\alpha;r_\alpha,\rho_\alpha)\mathcal{Y}_{\lambda'}^*(\widehat{\boldsymbol{k}}_\alpha,\widehat{\boldsymbol{q}}_\alpha)\mathcal{Y}_\lambda(\widehat{\boldsymbol{r}}_\alpha,\widehat{\boldsymbol{\rho}}_\alpha), \tag{168}$$

where we used a combination notation $\lambda=\{l_\alpha,L_\alpha,J,K\}$. The bipolar spherical harmonics are defined as [66]

$$\mathcal{Y}_{l_\alpha,L_\alpha,J,K}(\widehat{\boldsymbol{r}}_\alpha,\widehat{\boldsymbol{\rho}}_\alpha)=\sum_{m_\alpha,M_\alpha} C^{JK}_{l_\alpha m_\alpha L_\alpha M_\alpha} Y_{l_\alpha,m_\alpha}(\widehat{\boldsymbol{r}}_\alpha)Y_{L_\alpha,M_\alpha}(\widehat{\boldsymbol{\rho}}_\alpha), \tag{169}$$

where $C^{JK}_{l_\alpha m_\alpha L_\alpha M_\alpha}$ are the Clebsch–Gordan coefficients, l_α is the angular momentum of the pair (β,γ), L_α is the angular momentum corresponding to the relative motion of particle α relative to the pair (β,γ) and J is the total angular momentum, m_α, M_α and K are their projections, respectively. For convenience, one can set $K=0$.

Then we immediately get an expansion for the breakup amplitude:

$$T^{\mathrm{post}}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)=\sum_\lambda \mathcal{T}_\lambda(k_\alpha,q_\alpha)\mathcal{Y}_\lambda^*(\widehat{\boldsymbol{k}}_\alpha,\widehat{\boldsymbol{q}}_\alpha), \tag{170}$$

where $\mathcal{T}_\lambda$ are the partial breakup amplitudes defined as

$$\begin{aligned}\mathcal{T}_\lambda(k_\alpha,q_\alpha)=&-\frac{\mu^2}{2(\mu_\alpha M_\alpha)^{3/2}}\lim_{R_0\to\infty}R_0^5\int_0^{\pi/2}d\varphi_\alpha\sin^2\varphi_\alpha\cos^2\varphi_\alpha\Big[\mathcal{R}_\lambda^+(r_\alpha,\rho_\alpha)\frac{\partial}{\partial R}\mathcal{R}_{\lambda,\lambda}^{-*}(k_\alpha,q_\alpha;r_\alpha,\rho_\alpha)\\&-\mathcal{R}_{\lambda,\lambda}^{-*}(k_\alpha,q_\alpha;r_\alpha,\rho_\alpha)\frac{\partial}{\partial R}\mathcal{R}_\lambda^+(r_\alpha,\rho_\alpha)\Big]_{R=R_0}.\end{aligned} \tag{171}$$

Expansion (167) transforms Eq. (105) into an infinite set of two-dimensional second-order partial differential equations for radial waves $\mathcal{R}_\lambda^+$. Then the infinite set is truncated and solved in a two-dimensional (r_α,ρ_α) lattice, e.g. using standard numerical techniques like finite-element or finite-difference methods, imposing proper boundary conditions specified earlier. Thus, the radial coefficients $\mathcal{R}_\lambda^+(r_\alpha,\rho_\alpha)$ come from the solution of the SE. How about radial functions $\mathcal{R}_{\lambda,\lambda}^-(k_\alpha,q_\alpha;r_\alpha,\rho_\alpha)$? These are the partial waves of the three-body plane wave. When there is no Coulomb interaction they take a simple form

$$\mathcal{R}_{\lambda,\lambda}^-(k_\alpha,q_\alpha;r_\alpha,\rho_\alpha)=(4\pi)^2 i^{l_\alpha+L_\alpha}j_{l_\alpha}(k_\alpha r_\alpha)j_{L_\alpha}(q_\alpha\rho_\alpha), \tag{172}$$

where $j_l(kr)$ is the spherical Bessel function. When there is the Coulomb interaction the corresponding partial waves have been given in [52]. They have a complicated form. However, the main advantage of the surface forms is that the asymptotic channel state wavefunctions Φ_0^-, $\Phi_{\alpha m}^-$ and $\Phi_{\beta m}^-$ necessary for the breakup, scattering and rearrangement amplitudes, respectively, do not have to be exact. Moreover, they can be replaced by other suitable functions making sure that *magnitudes* of the amplitudes are still calculated exactly. The phase parts can be inserted afterwards, if necessary [67,68].

As we have emphasized, the main benefit from using the surface-integral forms for the scattering amplitudes is that they depend only on the asymptotic behavior of the relevant wavefunctions but not

[6] For example, it is incorrect to write $T^{\mathrm{post}}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)=\langle(E-H)\Phi_0^-|\Psi_{\alpha n}^{\mathrm{sc}+}\rangle$.

on their values anywhere in the limited space. Though the scattering wave $\Psi^+_{\alpha n}$ is obtained in a numerical form, in their surface-integral forms the scattering amplitudes are calculated from this wave at asymptotically large distances. At these distances, $\Psi^+_{\alpha n}$ actually takes the asymptotic forms (but, of course, in numerical representation) specified in Section 3.1 and the amplitudes are in fact factorized. Therefore, by projecting the numerical wavefunction at large distances on a suitable trial function, we can get rid of all other factors except the amplitudes. This is of course only possible due to ambiguity-free asymptotic wavefunctions given in Section 3.1. Thus, the asymptotic channel state wavefunctions Φ^-_0, $\Phi^-_{\alpha m}$ and $\Phi^-_{\beta m}$ necessary for the breakup, scattering and rearrangement amplitudes, respectively, do not have to be exact. The question is what kind of properties trial functions, capable of replacing the aforementioned three functions, should posses?

Let us assume that as a result of solving the SE scattering wave $\Psi^+_{\alpha n}$ (or $\Psi^{sc+}_{\alpha n}$) became available. First, consider the way of extracting the direct scattering amplitude. According to Eq. (143) (or Eq. (165)), in order to extract this amplitude we need $\Phi^-_{\alpha m}$ of Eq. (123), or its partial waves. Consider the following trial surface integral instead

$$F_{R_0}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) \equiv \left[\left\langle H_0 \Phi_{\alpha m} | \Psi^+_{\alpha n}\right\rangle - \left\langle \Phi_{\alpha m} | H_0 \Psi^+_{\alpha n}\right\rangle\right]_{R_0}, \tag{173}$$

(here and below we use this short volume integral as a schematic representation of the surface integral which immediately follows it after using Green's theorem as in Eq. (143)) where

$$\Phi_{\alpha m} = e^{i\boldsymbol{q}_{\alpha m}\boldsymbol{\rho}_\alpha}\phi_{\alpha m}(\boldsymbol{r}_\alpha). \tag{174}$$

After some algebra similar to what we have used in the previous section, we arrive at

$$\lim_{R_0\to\infty} F_{R_0}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) = F(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) \lim_{R_0\to\infty} \exp\left[-i\eta_{\alpha m}/q_{\alpha m}\ln(2q_{\alpha m}R_0)\right], \tag{175}$$

with a divergent phase. From this result, we conclude that

$$|\lim_{R_0\to\infty} F_{R_0}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n})| = |F(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n})|. \tag{176}$$

Similarly, for the magnitude of the rearrangement amplitude, we get

$$|G(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n})| = |\lim_{R_0\to\infty} G_{R_0}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n})|, \tag{177}$$

where

$$G_{R_0}(\boldsymbol{q}_{\alpha m}, \boldsymbol{q}_{\alpha n}) \equiv \left[\left\langle H_0 \Phi_{\beta m} | \Psi^+_{\alpha n}\right\rangle - \left\langle \Phi_{\beta m} | H_0 \Psi^+_{\alpha n}\right\rangle\right]_{R_0} \tag{178}$$

and

$$\Phi_{\beta m} = e^{i\boldsymbol{q}_{\beta m}\cdot\boldsymbol{\rho}_\beta}\phi_{\beta m}(\boldsymbol{r}_\beta). \tag{179}$$

Finally, we consider breakup. The breakup amplitude in terms of $\Psi^+_{\alpha n}$ is given by Eq. (134) as a volume integral and Eq. (138) as a surface integral. These forms require Φ^-_0. Though the latter is known, its partial waves have complicated analytical form [52]. Therefore, we consider the following surface integral:

$$I_{R_0}(\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha) = \left[\left\langle H_0 \widetilde{\Phi}_0 | \Psi^+_{\alpha n}\right\rangle - \left\langle \widetilde{\Phi}_0 | H_0 \Psi^+_{\alpha n}\right\rangle\right]_{R_0}, \tag{180}$$

where $\widetilde{\Phi}_0$ is a trial function. The trial function can be the three-body plane wave or any other function containing the three-body plane wave as a leading term at large distances. Another requirement is that it must be easily expandable in partial waves. Consider the case when

$$\widetilde{\Phi}_0(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha + i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}. \tag{181}$$

Then we get, after some algebra [47,52],

$$\lim_{R_0\to\infty} I_{R_0}(\boldsymbol{q}_\alpha, \boldsymbol{q}_\alpha) = T(\boldsymbol{q}_\alpha, \boldsymbol{q}_\alpha) \lim_{R_0\to\infty} \exp\left[-i\lambda_0\ln(2\kappa R_0) - i\sigma_0\right]. \tag{182}$$

The phase factor on the RHS diverges logarithmically as $R_0 \to \infty$. However, we can again write that

$$|\lim_{R_0\to\infty} I_{R_0}(\boldsymbol{q}_\alpha,\boldsymbol{q}_\alpha)| = |T(\boldsymbol{q}_\alpha,\boldsymbol{q}_\alpha)|. \tag{183}$$

Thus, in order to extract the *magnitude* of the scattering amplitudes, it is not necessary to use the exact asymptotic state. The same can be done using much simpler trial functions. And that is the main advantage of the surface-integral representations.

A similar approach to atomic ionization problem is known as the Peterkop effective-charge formalism [48,69,70]. Peterkop introduced a trial integral

$$I_{z_1,z_2}(\boldsymbol{q}_\alpha,\boldsymbol{q}_\alpha) = \left\langle (H-E)\Phi^-_{z_1,z_2}|\Psi^+_{\alpha n}\right\rangle, \tag{184}$$

where $\Phi^-_{z_1,z_2}$ is a trial function taken as a product of two Coulomb waves of effective charges z_1 and z_2:

$$\Phi_{z_1,z_2}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = \psi^-_{z_1}(\boldsymbol{r}_\alpha)\psi^-_{z_2}(\boldsymbol{r}_\beta). \tag{185}$$

Eq. (184), which is identical to Eq. (180) after transformation into the surface integral, is known as the Peterkop integral. For this integral, Peterkop obtained a relationship similar to Eq. (182) with a divergent phase factor on the right-hand side. He also showed that provided the effective charges satisfy a certain dynamic condition [48] the divergent phase simply disappears. Since the Peterkop condition turned out to be impossible to satisfy in practice, for almost four decades the Peterkop formalism had looked like an elaborate theory without practical implications. A breakthrough came in the form of ECS method [71]. These authors practically demonstrated that there was no need to satisfy the Peterkop condition and one can directly proceed to Eq. (183). Moreover, they showed that for calculations of the breakup amplitude using integral representation of Eq. (180) it is more convenient to choose the trial function Φ_{z_1,z_2} as a combination of two two-particle scattering states. In the hydrogen ionization problem, this corresponds to taking $z_1 = z_2 = 1$ in Eq. (185). Since these two-particle scattering states are orthogonal to bound-state wavefunctions of the relevant pair of particles, this lead to faster convergence of the resulting integral [71]. Notice, however, that Eq. (183) is valid for the full amplitude only while the ECS calculations are made in partial waves. Generalization of Eq. (183) to partial-wave amplitudes is given in [52].

In more general case, the ECS-type choice of the trial function would correspond to

$$\widetilde{\Phi}_0(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = \psi^-_{\boldsymbol{k}_\alpha}(\boldsymbol{r}_\alpha)\psi^-_{\boldsymbol{k}_\beta}(\boldsymbol{r}_\beta), \tag{186}$$

where $\psi^-_{\boldsymbol{k}}$ satisfies Eq. (7) but with $V = V^S + V^C$. However, this choice is suitable only when one of the particles is significantly heavier than the other two. Otherwise, it would demand the whole approach to the problem be formulated in so-called V-coordinates (in contrast to Jacobian T-coordinates we use in this work). However, in the general case of three particles with arbitrary masses, such a formulation would lead to significantly more complicated asymptotic wavefunctions due to artificially created so-called non-direct interaction potentials. When one of the particles is infinitely heavier, such non-direct interactions disappear.

The CCC method [45], another successful approach to atomic breakup problem, takes start from a representation similar to the Peterkop trial integral, though it does not use the surface-integral technique for calculating the breakup amplitude. The CCC choice of effective potentials correspond to $z_1 = 0$ for more energetic of the electrons and $z_2 = 1$ for the other (before the antisymmetrization).

Thus, the new post form of the breakup amplitude given in Eq. (148) in particular explains the origin of the Peterkop integral, a cornerstone of the highly successful ECS and CCC approaches to Coulomb breakup problems in atomic physics. Comparison of Eq. (184) with Eq. (148) shows that the Peterkop integral is simply an approximation to the exact breakup amplitude in its post form, where the exact three-body state Φ^-_0 is replaced by the trial function Φ_{z_1,z_2}. Remarkably, it turns out that with any choice of the effective charges, the difference between the breakup amplitude and Peterkop's integral reduces to a phase factor which does not affect the calculated cross-sections [47,52], provided $\Psi^+_{\alpha n}$ is accurate and R_0 is asymptotically large.

When R_0 is large, for reasons explained in the very beginning of this subsection the total wavefunction $\Psi^+_{\alpha n}$ in the trial surface integrals (173), (178) and (180) can be replaced by $\Psi^{sc+}_{\alpha n}$. With this, the final working expressions for calculating the magnitudes of the scattering amplitudes read

$$|F^{\rm post}(\boldsymbol{q}_{\alpha m},\boldsymbol{q}_{\alpha n})| = \frac{1}{2M_\alpha}\left|\lim_{R_0\to\infty} R_0^2\int d\boldsymbol{r}_\alpha\, d\hat{\rho}_\alpha\left[\Psi^{\rm sc+}_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Phi^*_{\alpha m}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right.\right.$$
$$\left.\left.-\Phi^*_{\alpha m}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial\rho_\alpha}\Psi^{\rm sc+}_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{\rho_\alpha=R_0}\right|, \tag{187}$$

$$|G^{\rm post}(\boldsymbol{q}_{\beta m},\boldsymbol{q}_{\alpha n})| = \frac{1}{2M_\beta}\left|\lim_{R_0\to\infty} R_0^2\int d\boldsymbol{r}_\beta\, d\hat{\rho}_\beta\left[\Psi^{\rm sc+}_{\alpha n}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta)\frac{\partial}{\partial\rho_\beta}\Phi^*_{\beta m}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta)\right.\right.$$
$$\left.\left.-\Phi^*_{\beta m}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta)\frac{\partial}{\partial\rho_\beta}\Psi^{\rm sc+}_{\alpha n}(\boldsymbol{r}_\beta,\boldsymbol{\rho}_\beta)\right]_{\rho_\alpha=R_0}\right|, \tag{188}$$

$$|T^{\rm post}(\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha)| = \frac{\mu^2}{2(\mu_\alpha M_\alpha)^{3/2}}\left|\lim_{R_0\to\infty} R_0^5\int d\hat{\boldsymbol{r}}_\alpha d\hat{\rho}_\alpha\int_0^{\pi/2} d\varphi_\alpha \sin^2\varphi_\alpha\cos^2\varphi_\alpha\left[\Psi^{\rm sc+}_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial R}\widetilde{\Phi}^*_0(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right.\right.$$
$$\left.\left.-\widetilde{\Phi}^*_0(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\frac{\partial}{\partial R}\Psi^{\rm sc+}_{\alpha n}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)\right]_{R=R_0}\right|, \tag{189}$$

for direct scattering, rearrangement and breakup, respectively.

4. Generalized wave operators

In our derivations in the preceding sections, we did not refer to the Green function and the formal solution of the SE in the integral form. Therefore, in order to derive definitions for the scattering amplitudes, we did not have to know anything about complicated analytic structure and the asymptotic behavior of the two-body and three-body Green's functions. In particular, this can be considered as another confirmation of the result obtained in [17] for the two-body case based on the formal solution of the SE in an integral form. In addition to definitions of the scattering amplitudes in [17], generalized definitions of wave operators have also been given. It has been established that the generalized wave operators are defined according to

$$\omega^{\pm} = 1 + g(\epsilon \pm i0)(h-\epsilon), \tag{190}$$

where $g = (\epsilon \pm i0 - h)^{-1}$ is the resolvent operator which defines the total two-particle Green's function. Operators $\omega^{\pm}$ transform the incident wave into the scattering wave. When they act on the plane wave, the generalized wave operators introduced above act exactly like the usual Möller (M) ones:

$$\omega^{\rm M\pm} = 1 + g(\epsilon \pm i0)V. \tag{191}$$

In the three-body case, the conventional wave operator depends on the initial state and is written as

$$\Omega^{\rm M\pm}_\alpha = 1 + G(E \pm i0)\overline{V}_\alpha, \tag{192}$$

if the wave operator is supposed to act on a two-fragment channel, and

$$\Omega^{\rm M\pm}_0 = 1 + G(E \pm i0)V, \tag{193}$$

if in the initial state we have three free particles. Here, $G = (E \pm i0 - H)^{-1}$ is the resolvent operator corresponding to the total three-body Green's function. These definitions are channel dependent. However, using Eqs. (80), (105), (97) and (128), we can write formal solutions to Eqs. (78) and (96) as

$$\Psi^{\pm} = \Phi^{\pm} + G(E \pm i0)(H-E)\Phi^{\pm}. \tag{194}$$

From this result, we can read that the three-body wave operators should be defined according to

$$\Omega^{\pm} = 1 + G(E \pm i0)(H-E). \tag{195}$$

We emphasize that they are independent of the state on which they are acting and independent of the fact whether the interactions are short-ranged or long-ranged. It is not difficult to see that $\Omega^{\pm}$ can be

written as $\Omega_\alpha^{M\pm}$ and $\Omega_0^{M\pm}$ provided the interactions are short-ranged and the initial arrangement of particles is known. This is another satisfying outcome of the present formulation.

5. Discussion

All the results presented in this work rely on the asymptotic forms of the plane wave and the Coulomb-distorted plane waves given by Eqs. (25) and (62), respectively. While Eq. (25) is correct, strictly speaking Eq. (62) is just a replacement. This is because the latter is obtained assuming convergence of the partial-wave expansions for the scattering amplitude and the scattering wave in the presence of the Coulomb interaction. It is well known that such expansions are divergent if considered in the sense of ordinary functions. However, Taylor [72] has shown that these expansions converge as distributions. Following Taylor, let us introduce auxiliary functions $\varphi^{\pm}(z)$ according to

$$\varphi^{\pm} \in C^2[-1,+1] \quad \text{and} \quad \varphi^{-}(-1)=0, \;\; \varphi^{+}(+1)=0, \tag{196}$$

where $z=\widehat{\boldsymbol{k}}\cdot\widehat{\boldsymbol{r}}$. In other words, functions $\varphi^{\pm}(z)$ are twice continuously differentiable on $[-1,+1]$. In addition, function $\varphi^{+}(z)$ vanishes in the forward direction and $\varphi^{-}(z)$ does so in the backward direction. Mathematically, these requirements are made to ensure convergence of the partial-wave expansions in the presence of the Coulomb interaction. Physically, according to Taylor, the requirements correspond to the well-known fact that in Coulomb scattering it is impossible to measure a meaningful forward cross-section. This corresponds to backward cross-section in the time-reversal picture.

Let us indicate by the symbols $D^{\pm}$ that distributions are meant in the above sense. Then, instead of Eq. (62), we obtain two separate equations

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\gamma\ln(kr+\boldsymbol{k}\cdot\boldsymbol{r})} \overset{r\to\infty}{\sim} \frac{2\pi}{ikr} e^{ikr-i\gamma\ln(2kr)}\delta(\widehat{\boldsymbol{k}}-\widehat{\boldsymbol{r}}), \quad D^{-} \tag{197}$$

and

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}+i\gamma\ln(kr-\boldsymbol{k}\cdot\boldsymbol{r})} \overset{r\to\infty}{\sim} -\frac{2\pi}{ikr} e^{-ikr+i\gamma\ln(2kr)}\delta(\widehat{\boldsymbol{k}}+\widehat{\boldsymbol{r}}), \quad D^{+}. \tag{198}$$

Now, if we use Eqs. (197) and (198), respectively, whenever the asymptotic forms of $e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\gamma\ln(kr+\boldsymbol{k}\cdot\boldsymbol{r})}$ and $e^{i\boldsymbol{k}\cdot\boldsymbol{r}+i\gamma\ln(kr-\boldsymbol{k}\cdot\boldsymbol{r})}$ are required in the derivations of the earlier chapters, we arrive at the same results. It is remarkable that when we use Eq. (62) in deriving the amplitudes in the post form only the term given by Eq. (197) contributes. Alternatively, when deriving the amplitudes in the prior form only the term given by Eq. (198) contributes. Contributions from the corresponding second terms simply vanish on the energy shell and, in addition, due to the absence of stationary-phase points in integrals of infinitely-oscillatory functions in the three-body case. In other words, the notorious forward/backward logarithmic singularities cancel out before they cause any problems. Thus, the auxiliary functions introduced above merely regularize problems in parts of the configuration space which ultimately do not contribute. This justifies the use of replacement (62) for Eqs. (197) and (198). For this reason, we can claim that in the present approach the aforementioned partial-wave expansions can be considered convergent without introducing the auxiliary functions.[7] In order to highlight this remarkable feature of the present formalism, we opted to use Eq. (62) in this work. Also, by using Eq. (62), there was no need to give a separate proof of the results for short-range interactions as, in this case, Eqs. (197) and (198) combined give exactly Eq. (25). Nevertheless, from a mathematical point of view, Eq. (62) must always be understood in the sense of Eqs. (197) and (198). From a practical point of view, the bottom line is that such a mathematically strict treatment does not change the results given in this paper.

Another essential feature of the formulation presented in this work is that it avoids any reference to Green's function and a formal solution of the SE for the scattering wavefunction in an integral form. This leads to more general definitions for the scattering amplitude and wave operators valid for both sort-range and Coulombic long-range interactions. Not surprsingly, the SE for the scattering wavefunction with properly formulated asymptotic boundary conditions completely and unambiguously

[7] Whether or not these partial-wave expansions can always be considered convergent is a separate question and goes beyond the framework of this paper.

define all quantities necessary for the description of the collision process. We emphasise that in our approach the non-Hermitian operator $(H - E)$ defines the scattering amplitude instead of the Hermitian operator V. On the surface, this looks at odds with one of the general principles of quantum mechanics which states that all operators leading to physical observables are Hermitian. So is the transition operator V (interaction potential) used in the standard scattering theory. But there is a subtle point here. The Hermicity of good operators in physics is required in the Hilbert space. The wavefunctions we deal with in scattering theory do not belong to the Hilbert space. Rather, they belong to the so-called rigged Hilbert space[55]. Strictly speaking operators leading to scattering do not have to be Hermitian. The operator $(H - E)$ is Hermitian only when used in the Hilbert space.

Solving a scattering problem is twofold. First, one has to find the total wavefunction describing the scattering process. The second part consists in the extraction of the necessary scattering amplitudes for the purpose of calculating the cross-sections. In this work, we have resolved some outstanding problems of scattering theory related to extracting the information about the scattering event. When the total scattering wavefunction is available the scattering amplitudes can be reliably extracted from it using the new definitions regardless the long-range nature of the interactions. Once the amplitudes are available calculations of corresponding cross-sections are straightforward (see, e.g. [1,73]).

As to the first part of the problem, there are sophisticated numerical methods which can provide reliable numerical solution to the SE in special cases. However, in the case of three distinguishable particles where rearrangement is possible the SE cannot provide a unique answer. This is because of the fact that it is impossible to specify all asymptotic boundary conditions using one set of the Jacobi variables. To overcome this difficulty, Faddeev suggested a set of equations which incorporates all the required asymptotic boundary conditions. However, as mentioned earlier in the case of charged particles, the Faddeev equations become non-compact. In other words, they cannot be solved using standard numerical techniques though non-compactness generally does not exclude existence of analytic solutions. At the same time, the present work shows that problems with the Faddeev equations are more serious than non-compactness. Equivalent sets of the Faddeev equations can be written for the wavefunction, resolvent of Green's function or T-matrix. Let us take the equations for components of the three-body T-matrix. The starting point for these equations are Eqs. (158)–(163) which are not correct for charged particles. This implies that any results derived from Eqs. (158)–(163) are valid strictly for short-range potentials. For the Coulombic potentials, they might be simply incorrect. Thus, the Faddeev equations in the presence of long-range Coulomb interactions require careful inspection. We believe it may be possible to formulate the Faddeev equations in a form that would not require screening and renormalization along the lines of the formalism presented in this manuscript. We are currently working on this problem.

6. Summary

The conventional formulation of scattering theory is only valid for short-range interactions. In this paper, we have given a general formalism of scattering theory which is applicable to two-body and three-body systems with long-range interactions with Coulombic tails. 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 a Coulombic potential, these generalized definitions of the amplitude give the physical on-shell amplitude without recourse to a renormalization procedure. We have derived prior and post forms of the breakup amplitude for a three-body system that are valid for both short-range and Coulombic potentials.The latter, in particular, resolves a long-standing problem about the conventional post form of the breakup amplitude for the long-range Coulombic interactions. The new forms for the potential scattering and breakup amplitudes have equivalent surface-integral forms well suited for practical calculations. The surface-integral representations are extended to amplitudes of direct and rearrangement scattering processes taking place in an arbitrary three-body system. Different practical methods of calculations are suggested. Finally, we emphasize that the formalism presented in this manuscript has developed from the analysis of the extraordinarily successful ECS and CCC methods used for solving breakup problems in atomic physics.

Acknowledgements

This work was supported by the Australian Research Council and the U.S. Department of Energy under Grant No. DE-FG02-93ER40773.

References

[1] R.G. Newton, Scattering Theory of Waves and Particles, second ed., Springer, New York, 1982.
[2] J.D. Dollard, J. Math. Phys. 5 (6) (1964) 729–738.
[3] J.D. Dollard, J. Math. 1 (1971) 5.
[4] V.G. Gorshkov, Zh. Eksp. Teor. Fiz. 40 (1961) 1481–1490; Sov. Phys. JETP 13 (1961) 1037.
[5] J.D. Dollard, J. Math. Phys. 9 (4) (1968) 620–624.
[6] A.M. Veselova, Teor. Mat. Fiz. 3 (1970) 326–331; Theor. Math. Phys. 3 (1970) 542–546.
[7] A.G. Gibson, C. Chandler, J. Math. Phys. 15 (1974) 1633.
[8] M.D. Semon, J.R. Taylor, Nuovo Cim. A 26 (1975) 48.
[9] J. Zorbas, J. Math. Phys. 17 (1976) 498.
[10] H. van Haeringen, Charged-particle Interactions, Coulomb Press Leyden, Leiden, 1985.
[11] S. Okubo, D. Feldman, Phys. Rev. 117 (1) (1960) 292–306.
[12] J. Schwinger, J. Math. Phys. 5 (1964) 1606.
[13] W.F. Ford, Phys. Rev. 133 (1964) B1616–B1621.
[14] J. Nuttall, W. Stagat, Phys. Rev. A 31 (1970) 1355.
[15] K. Dettman, Z. Phys. 244 (1971) 86.
[16] H. van Haeringen, J. Math. Phys. 17 (1976) 995–1000.
[17] A.S. Kadyrov, I. Bray, A.M. Mukhamedzhanov, A.T. Stelbovics, Phys. Rev. A 72 (3) (2005) 032712.
[18] L.D. Faddeev, Zh. Eksp. Teor. Fiz. 39 (1960) 1459–1467; Sov. Phys.-JETP 12 (1961) 1014–1019.
[19] L.D. Faddeev, Tr. Mat. Inst. Akad. Nauk SSSR 69 (1963) 1; Mathematical aspects of the three-body problem in the quantum scattering, Israel Program for Scientific Translations, Jerusalem, 1965.
[20] S.P. Merkuriev, Ann. Phys. 130 (1980) 395–426.
[21] S.P. Merkuriev, L.D. Faddeev, Nauka, Moscow, 1985.; L.D. Faddeev, S.P. Merkuriev, Quantum Scattering Theory for Several Particle Systems, Kluwer Academic Publishers, Dordrecht, 1993.
[22] A.M. Mukhamedzhanov, E.O. Alt, G.V. Avakov, Phys. Rev. C 61 (2000) 064006.
[23] A.M. Mukhamedzhanov, E.O. Alt, G.V. Avakov, Phys. Rev. C 63 (2001) 044005.
[24] E.O. Alt, W. Sandhas, H. Ziegelmann, Phys. Rev. C 17 (1978) 1981–2005.
[25] E.O. Alt, W. Sandhas, Collision theory for two- and three-particle systems interacting via short-range and coulomb forces, in: F.S. Levin, D. Micha (Eds.), Coulomb Interactions in Nuclear and Atomic Few-Body Collisions, Plenum Press, New York, 1996, pp. 1–95.
[26] E.O. Alt, W. Sandhas, Phys. Rev. C 21 (1980) 1733–1745.
[27] S.P. Merkuriev, Teor. Mat. Fiz. 32 (1977) 187–207; Theor. Math. Phys. 32 (1977) 680.
[28] T. Sawada, K. Thushima, Prog. Theor. Phys. 76 (2) (1986) 440–459.
[29] L. Rosenberg, Phys. Rev. D 8 (1973) 1833–1843.
[30] L. Rosenberg, Phys. Scr. 77 (1) (2008) 015305.
[31] E.O. Alt, A.M. Mukhamedzhanov, M.M. Nishonov, A.I. Sattarov, Phys. Rev. C 65 (6) (2002) 064613.
[32] E.O. Alt, L.D. Blokhintsev, A.M. Mukhamedzhanov, A.I. Sattarov, Phys. Rev. C 75 (5) (2007) 054003.
[33] A. Deltuva, A.C. Fonseca, P.U. Sauer, Phys. Rev. C 71 (5) (2005) 054005.
[34] W. Glockle, H. Witala, D. Huber, H. Kamada, J. Golak, Phys. Rep. 274 (3–4) (1996) 107–285.
[35] N. Austern, Y. Iseri, M. Kamimura, M. Kawai, G. Rawitscher, M. Yahiro, Phys. Rep. 154 (3) (1987) 125–204.
[36] A. Kievsky, S. Rosati, M. Viviani, Phys. Rev. Lett. 82 (1999) 3759.
[37] J.A. Tostevin, F.M. Nunes, I.J. Thompson, Phys. Rev. C 63 (2) (2001) 024617.
[38] E.O. Alt, P. Grassberger, W. Sandhas, Nucl. Phys. B 2 (1967) 167–180.
[39] A. Deltuva, A.C. Fonseca, P.U. Sauer, Phys. Rev. Lett. 95 (9) (2005) 092301.
[40] T.N. Rescigno, M. Baertschy, W.A. Isaacs, C.W. McCurdy, Science 286 (1999) 2474–2479.
[41] M. Baertschy, T.N. Rescigno, C.W. McCurdy, Phys. Rev. A 64 (2001) 022709.
[42] P.L. Bartlett, A.T. Stelbovics, I. Bray, J. Phys. B 37 (2004) L69.
[43] P.L. Bartlett, J. Phys. B 39 (22) (2006) R379–R424.
[44] I. Bray, A.T. Stelbovics, Phys. Rev. Lett. 69 (1992) 53–56.
[45] I. Bray, Phys. Rev. Lett. 89 (2002) 273201.
[46] A.T. Stelbovics, I. Bray, D.V. Fursa, K. Bartschat, Phys. Rev. A 71 (2005) 052716(13).
[47] A.S. Kadyrov, A.M. Mukhamedzhanov, A.T. Stelbovics, I. Bray, Phys. Rev. Lett. 91 (2003) 253202.
[48] R.K. Peterkop, Opt. Spektrosk. 13 (1962) 153;
Opt. Spectrosc. 13 (1962) 87.
[49] R.K. Peterkop, Izv. Akad. Nauk Latv. SSR Riga 9 (1960) 79.
[50] A.S. Kadyrov, A.M. Mukhamedzhanov, A.T. Stelbovics, Phys. Rev. A 67 (2003) 024702.
[51] A.S. Kadyrov, A.M. Mukhamedzhanov, A.T. Stelbovics, I. Bray, F. Pirlepesov, Phys. Rev. A 68 (2003) 022703.
[52] A.S. Kadyrov, A.M. Mukhamedzhanov, A.T. Stelbovics, I. Bray, Phys. Rev. A 70 (5) (2004) 062703.
[53] E.O. Alt, A.M. Mukhamedzhanov, Phys. Rev. A 47 (3) (1993) 2004–2022.
[54] A.S. Kadyrov, I. Bray, A.M. Mukhamedzhanov, A.T. Stelbovics, Phys. Rev. Lett. 101 (23) (2008) 230405.
[55] I.M. Gel'fand, N.Y. Vilenkin, Generalized Functions, vol. 4, Academic Press, New York, 1964.

[56] L.D. Landau, E.M. Lifshitz, Quantum Mechanics (Non-relativistic Theory), third ed., Vol. 3 of Course of Theoretical Physics, Pergamon Press, Oxford, 1985.
[57] A. Messiah, Quantum Mechanics, vol. 2, North-Holland, Amsterdam, 1965.
[58] G.B. West, J. Math. Phys. 8 (1967) 942–953.
[59] R.O. Barrachina, J. Macek, J. Math. Phys. 30 (1989) 2581–2584.
[60] A.M. Mukhamedzhanov, L.D. Blokhintsev, B.F. Irgaziev, A.S. Kadyrov, M. La Cognata, C. Spitaleri, R.E. Tribble, J. Phys. G 35 (2008) 014016.
[61] P.J. Redmond (unpublished), see [29].
[62] A.M. Mukhamedzhanov, M. Lieber, Phys. Rev. A 54 (4) (1996) 3078–3085.
[63] A.M. Mukhamedzhanov, A.S. Kadyrov, F. Pirlepesov, Phys. Rev. A 73 (1) (2006) 012713.
[64] R. Peterkop, J. Phys. B 15 (1982) L751–L754.
[65] N. Bleistein, R.A. Handelsman, Asymptotic Expansions of Integrals, Dover, New York, 1986.
[66] D.A. Varshalovich, A.N. Moskalev, V.K. Khersonskii, Quantum Theory of Angular Momentum, first ed., World Scientific, Philadelphia, 1988.
[67] P.L. Bartlett, I. Bray, S. Jones, A.T. Stelbovics, A.S. Kadyrov, K. Bartschat, G. ver Steeg, M.P. Scott, P.G. Burke, Phys. Rev. A 68 (2003) 020702(R).
[68] T.N. Rescigno, M. Baertschy, C.W. McCurdy, Phys. Rev. A 68 (2003) 020701(R).
[69] M.R.H. Rudge, Rev. Mod. Phys. 40 (1968) 564–590.
[70] R.K. Peterkop, Teoriya Ionizatsii Atomov Elektronnym Udarom, Zinatne, Riga, 1971 [Theory of Ionization of Atoms by Electron Impact, Colorado Associated University Press, Boulder, 1977].
[71] C.W. McCurdy, D.A. Horner, T.N. Rescigno, Phys. Rev. A 63 (2001) 022711.
[72] J.R. Taylor, Nuovo Cim. B 23 (1974) 313–334.
[73] R.G. Newton, Ann. Phys. 74 (1972) 324–351.
[74] L. Rosenberg, J. Phys. B 41 (2008) 155203.