ASYMPTOTIC SCATTERING WAVE FUNCTION FOR THREE CHARGED PARTICLES AND ASTROPHYSICAL CAPTURE PROCESSES

A Dissertation

by

FAKHRIDDIN PIRLEPESOV

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

May 2005

Major Subject: Physics

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ABSTRACT

Asymptotic Scattering Wave Function for Three Charged Particles and Astrophysical Capture Processes. (May 2005)

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The asymptotic behavior of the wave functions of three charged particles has been investigated. There are two different types of three-body scattering wave functions. The first type of scattering wave function evolves from the incident three-body wave of three charged particles in the continuum. The second type of scattering wave function evolves from the initial two-body incident wave. In this work the asymptotic three-body incident wave has been derived in the asymptotic regions where two particles are close to each other and far away from the third particle. This wave function satisfies the Schrödinger equation up to terms $O(1/\rho_\alpha^3)$, where ρ_α is the distance between the center of mass of two particles and the third particle. The derived asymptotic three-body incident wave transforms smoothly into Redmond's asymptotic incident wave in the asymptotic region where all three particles are well separated. For the scattering wave function of the second type the asymptotic three-body scattered wave has been derived in all the asymptotic regions. In the asymptotic region where all three particles well separated, the derived asymptotic scattered wave coincides with the Peterkop asymptotic wave. In the asymptotic regions where two particles are close to each other and far away from the third one, this is a new expression which is free of the logarithmically diverging phase factors that appeared in the Peterkop approach. The derived asymptotic scattered wave resolves a long-standing phase-amplitude ambiguity. Based on these results the expressions for the exact prior and post breakup amplitudes have been obtained. The post breakup amplitude for charged particles has not been known and has been derived for the first time directly from the prior form. It turns out that the post form of the breakup amplitude is given by a surface integral in the six dimensional hyperspace, rather than a volume integral, with the transition operator expressed in terms of the interaction potentials. We also show how to derive a generalized distorted-wave-Born approximation amplitude (DWBA) from the exact prior form of the breakup amplitude. It is impossible to derive the DWBA amplitude from the post form. The three-body Coulomb incident wave is used to calculate the reaction rates of $^7Be(ep,e)^8B$ and $^7Be(pp,p)^8B$ nonradiative triple collisions in stellar environments.

To my parents Shukurzhan, Orazymbet, my wife Adolat and my daughters

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CHAPTER I

INTRODUCTION

A. Three-body scattering wave function in the presence of the Coulomb interactions. General information

The inclusion of the Coulomb interaction into the scattering theory is a long standing and still unsolved problem in modern few-body physics. The simplicity of the Coulomb potential and the possibility to get results analytically is one of the reasons why the unscreened Coulomb interaction is preferable. However, the infinite range of the Coulomb interaction causes problems for formal scattering and reaction theories. Introduction of the screened Coulomb potential does not help. The final result should not depend on the screening radius. For the two-body scattering problem the screening procedure does not cause any troubles: the screening factor is well known analytically and can be easily singled out [1]. However, the effect of the screening procedure on the observables for three-body cases is unknown.

The Coulomb modification of the wave operator theory has been realized by Dollard [2]. He showed that the long range Coulomb interaction generates an additional exponential factor in the wave operator, which depends logarithmically on time. In the momentum space it means that interacting particles are never free, even at infinity. Hence, a conventional scattering theory based on the concept of "in" and "out" asymptotic states should be modified in the presence of Coulomb interactions. Eventually, the stationary scattering problem can be reduced to the calculation of the differential Schrödinger equation or equivalent integral equations. The uniqueness of the solution of the differential Schrödinger equation is provided by imposing

This dissertation follows the style of Physical Review A.

proper boundary conditions. Since particles are not free even when they are far away from each other the boundary conditions are Coulomb modified. Determination of the proper boundary conditions became a main problem in the formulation of the few-body scattering theory with Coulomb interations. The boundary conditions for the three-body systems have not yet been found for all the cases. Under specific conditions the asymptotic forms of the wave functions are enough to calculate the amplitudes of different processes involving three particles in the initial or final states. Examples of such conditions include triple collisions in a stellar medium or breakup processes.

There are two different types of three-body scattering wave functions [3]. The first type evolves from the initial three-body incident wave describing the collision of three incident particles in the continuum. The second type evolves from the initial two-body scattering wave describing the collision of the bound-state and the third particle.

The first goal of this work is to find all the asymptotic terms of the three-body incident wave of the scattering wave function of the first type in the presence of the Coulomb interactions, up to highest order without explicit solution of the three-body Schrödinger equation in the asymptotic regions where two particles are close to each other and far away from the third particle. This derivation will provide the asymptotic behavior of the three-body scattering wave function of the first type in leading order without explicit solution of the Schrödinger equation, in all the asymtotic regions where any two particles are close to each other and far away from the third particle. There is another unsolved problem in the three-body scattering theory with Coulomb interactions: the asymptotic behavior of the outgoing three-body scattered wave describing breakup/ionization processes is not known in the asymptotic regions where two particles are close to each other and far away from the third particle. This scattered wave is one of the asymptotic terms of the scattering wave function of the second type. Knowledge of the three-body scattered wave is imperative for a formulation and solution of the breakup problem in general, based on the direct solution of the Schrödinger equation (so-called "ab-initio" calculations in the continuum).

The second goal of this work is to find the asymptotic behavior of the three-body scattered wave in the asymptotic regions, where two particles are close to each other and far away from the third particle. To solve this problem we use the spectral decomposition of the three-body Green's function in terms of the scattering wave functions of the first type. This derivation will provide complete asymptotic behavior of the three-body scattering wave function of the second type in the appropriate asymptotic regions. The derived asymptotic wave function transforms smoothly into the corresponding leading asymptotic term of the three-body scattered wave in the asymptotic region where all particles are well separated.

The third goal of this work is to formulate the breakup reaction theory with charged particles in terms of surface integrals. First of all the post form exact breakup amplitude will be derived from the prior form. It will be demonstrated that to reformulate correctly the theory of the breakup reactions with charged particles one needs to know the leading asymptotic terms of the three-body incident wave of the scattering wave function of the first type and the three-body scattered wave of the scattering wave function of the second type. These results pave the way for determination of the breakup amplitude using direct solution of the Schrödinger equation ("ab-initio" calculations in continuum).

The fourth goal of this work is to apply the leading asymptotic term of the three-body incident wave for the calculation of reaction rates of nonradiative triple collisions in stellar matter. There are two essential differences between the nuclear reactions caused by binary and triple collisions. They can be considered as kinematical or dynamical. The former are related to selection rules while the later come from the inter-dependence of different nuclear processes. For example, some binary reactions are suppressed by angular momentum, parity and isospin conservation laws. But these suppression mechanisms can be modified by the presence of a third particle. Therefore, the three-body mechanism which is less restricted kinematically, may play a role in the nuclear burning in the stellar environment, when the probability of triple collisions can be higher due to high density and high temperature. In this work we have estimated the reaction rates of nonradiative triple collisions ${}^7Be(ep, e)^8B$ and ${}^7Be(pp, p)^8B$ in different stellar environments.

This thesis is organized as follows. General information about the three-body scattering wave functions with Coulomb interactions is presented in Chapter II. In Chapter III we give the derivation of the leading asymptotic terms of the three-body incident wave in all the asymptotic regions. In Chapter IV the asymptotic scattered wave, describing breakup processes of 2 particles $\rightarrow$ 3 particles for general masses and charges, has been derived in all four asymptotic regions. In Chapter V a new formulation of the theory of breakup processes is given. It includes also consideration of the distorted wave Born approximation. Chapter VI is devoted to calculations of reaction rates for the triple collisions ${}^7Be(ep, e)^8B$ and ${}^7Be(pp, p)^8B$.

CHAPTER II

GENERAL INFORMATION

In this Chapter we present general information on three charged particle scattering. The Chapter is set as following. In Sec. A we give general information for the three-body scattering wave function in the presence of the Coulomb interactions. In Sections B and C we present general information on the three-body Coulomb scattering wave functions evolved from the initial three-body and two-body incident waves, respectively.

A. Three-body scattering wave function in the presence of the Coulomb interactions

The knowledge of the scattering wave function describing three charged particles is important to reaction theory. There are two types of three-body scattering wave functions: the wave function which evolves from the initial incident wave of the three particles in the continuum, and the wave function which evolves from the initial two-body scattering state [3]. Both types of wave functions satisfy the same three-body Schrödinger equation and are orthogonal to each other. Hence to form a complete set of wave functions describing the three-body system, we have to include the three-body bound-state wave functions and all the types of scattering wave functions. In what follows we will concentrate only on the scattering wave functions. To get a unique solution to the Schrödinger equation, one has to impose proper boundary conditions. The scattering wave function which evolves from the initial incident wave of the three particles in the continuum is necessary for the analysis of reactions containing three particles in the continuum of the initial or final states (prior form). As examples we point to breakup/ionization processes or triple collisions in stellar or condensed matter. However, the second type of wave function which evolve from the initial two-body scattering state also can be used for the analysis of breakup/ionization processes (post form). In what follows we concentrate on the stationary approach, which is equivalent to the nonstationary one.

For the three-body case the problem of imposing the proper boundary conditions is not as straightforward as for the two-body problem. The reason is that there are four different asymptotic regions for the three-body particles in the continuum in contrast to the two-body case, where one has only one asymptotic region. Let us introduce these asymptotic regions:

$$\Omega_0 : r_\alpha \sim r_\beta \sim r_\gamma \to \infty; \tag{2.1}$$

$$\Omega_\nu : \ \rho_\nu \to \infty, \quad r_\nu/\rho_\nu \to 0, \qquad \nu = \alpha,\, \beta,\, \gamma. \tag{2.2}$$

Here $(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha)$ is the set of two Jacobian variables: $\mathbf{r}_\alpha$ is the radius vector connecting particles β and γ, and $\boldsymbol{\rho}_\alpha$ is the radius vector connecting particle α and the center of mass (c.m.) of the system $\beta+\gamma$. The set $(\mathbf{k}_\alpha,\, \mathbf{q}_\alpha)$ is the set of Jacobian momenta conjugate to the Jacobian coordinate set $(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha)$. Evidently the three different Jacobian sets with $\nu = \alpha,\, \beta, \gamma$ are equivalent. $\mathbf{k}_\alpha$ is the relative momentum of particles β and γ and is invariant under Galilean transformations:

$$\mathbf{k}_\alpha = \frac{m_\beta\, \mathbf{q}_\gamma - m_\gamma\, \mathbf{q}_\beta}{m_{\beta\,\gamma}}. \tag{2.3}$$

Besides in the c.m. of the three-body system

$$\mathbf{q}_\alpha + \mathbf{q}_\beta + \mathbf{q}_\gamma = 0. \tag{2.4}$$

Here $\mathbf{q}_\nu$ is the momentum of particle ν and m_ν is the mass of particle ν, $m_{\nu\,\sigma} = m_\nu + m_\sigma$.

In each asymptotic region with three particles in the continuum, the boundary conditions are different. The existence of the four different asymptotic regions does not allow us to replace one Schrödinger differential equation by one integral Lippmann-Schwinger type equation. A possible solution of the problem lies in using the coupled Faddeev equations [3]. But in the presence of Coulomb interactions, the Faddeev integral equations approach leads to technical problems [4, 5], even for repulsive Coulomb interactions. The differential Schrödinger equation also can be rewritten in the form of coupled Faddeev differential equations, which can be solved after imposing the proper boundary conditions in all the asymptotic regions [3]. However, such boundary conditions until recently were known only in the asymptotic region Ω_0, where all three particles are well separated [3, 6, 7, 8]. We note that there is one more important difference between the two- and three-body cases. In the two-body case the energy spectrum consists of the negative discrete part, if it exists, corresponding to the bound states and the positive continuum part. Thus the sign of the energy uniquely determines the boundary conditions. This is not the case the three-body systems. A negative eigenvalue for three-body systems does not necessarily correspond to the discrete spectrum. For example, consider a three-body system $\alpha + (\beta\,\gamma)$, where $(\beta\,\gamma)$ is a bound state of β and γ. The total energy of this system in the c.m. system can be written as

$$E = E^{\alpha} - \varepsilon_{\beta\,\gamma}, \tag{2.5}$$

where $\varepsilon_{\beta\,\gamma}$ is the binding energy of the bound state $(\beta\,\gamma)$. E^{α} is the kinetik energy of the three-body system $\alpha + (\beta\,\gamma)$ and given by

$$E^{\alpha} = \frac{q_{\alpha}^2}{2\,M_{\alpha}}, \tag{2.6}$$

where M_{α}, and M are their reduced and total masses, respectively, given by

$$M_{\alpha} = \frac{m_{\alpha}\,m_{\beta\,\gamma}}{M}, \tag{2.7}$$

$$M = m_\alpha + m_\beta + m_\gamma. \tag{2.8}$$

If $E^\alpha < \varepsilon_{\beta\gamma}$ the total energy of the three-body system is negative. Thus the sign of the total energy does not determine the state of the three-body system. For a given total energy of the three-body system E, all three particles can be in the continuum or any two particles can be in a bound state and the third particle in the continuum. This results in the existence of four different energy spectra branches in the three-body system. In the latter case we assume, for simplcity, that each bound pair $(\nu\,\sigma)$ has only one bound state with the bindig energy $\varepsilon_{\nu\,\sigma}$.

B. Three-body Coulomb scattering wave function evolved from the three-body incident wave

The first energy spectrum branch for the three-body scattering problem consists of the discrete negative spectrum, corresponding to the bound states of the three-body system, and the positive continuum $(0, \infty)$, corresponding to three particles in the continuum. The scattering wave function corresponding to the continuum is the scattering wave function of the first type. In leading orders asymptotically, it behaves as [3, 9, 10, 11]

$$\Psi^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} = \tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} + \sum_{\nu=\alpha,\,\beta,\,\gamma} \Phi^{(\nu)(+)}_{\mathrm{two-body\,scattered\,wave}} + \Phi_{\mathrm{three-body\,scattered\,wave}}. \tag{2.9}$$

The first term in Eq. (2.9), $\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ is the three-body incident Coulomb distorted wave. The second term is given by the sum of the two-body Coulomb distorted outgoing waves corresponding to all allowed processes for 3 *particles* $\rightarrow$ 2 *particles*.

Finally the third term describes the three-body Coulomb distorted outgoing 3 *particle* $\rightarrow$ 3 *particle* scattered wave.

1. Leading asymptotic term of the incident wave in Ω_0

The shape of the incident wave depends on the asymptotic region. The leading asymptotic term of the three-body incident wave in the asymptotic region Ω_0 has been derived by Redmond [6, 7]:

$$\Psi^{(0)(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\, e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} \prod_{\nu=\alpha,\,\beta,\,\gamma} e^{i\,\eta_\nu \ln \zeta_\nu}, \tag{2.10}$$

where

$$\zeta_\nu = k_\nu\, r_\nu - \mathbf{k}_\nu \cdot \mathbf{r}_\nu. \tag{2.11}$$

$$\eta_\alpha = \frac{z_\beta\, z_\gamma\, e^2\, \mu_\alpha}{k_\alpha} \tag{2.12}$$

is the Coulomb parameter of particles β and γ, $z_\alpha\, e$ is the charge of particle α and μ_α is the reduced mass of particles β and γ. In what follows we use the system of units in which $\hbar = c = 1$. Eq. (2.10) represents the three-body Coulomb distorted plane wave. Since the Coulomb interaction is long range, charged particles are not free, even asymptotically. Their asymptotic motion is distorted by the presence of other charged particles. The Coulomb distortion is represented by the three exponential logarithmic phase factors, one for each interacting pair. The asymptotic form (2.10) is valid only in those directions of the asymptotic domain Ω_0, where each $|\zeta_\nu| \to \infty$, $\nu = \alpha,\ \beta,\ \gamma$. Directions, for which one or more $|\zeta_\nu| < C$ for $r_\nu \to \infty$, $\nu = \alpha,\ \beta,\ \gamma$, are called singular directions. For practical applications Redmond's three-body Coulomb distorted plane wave is replaced by the Redmond-Merkuriev asymptotic term [3, 6, 7], which is also known as 3C [12, 13]:

$$\Psi^{(3C)(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\, e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} \prod_{\nu=\alpha,\,\beta,\,\gamma} F_\nu(\zeta_\nu), \tag{2.13}$$

where

$$F_\nu(\zeta_\nu) = N_\nu\, {}_1F_1(-i\,\eta_\nu,\, 1; i\,\zeta_\nu), \tag{2.14}$$

${}_1F_1(-i\,\eta_\nu,\,1;i\,\zeta_\nu)$ is the confluent hypergeometric function and

$$N_\nu = e^{-\pi\,\eta_\nu/2}\,\Gamma(1+i\,\eta_\nu) \tag{2.15}$$

is the normalization factor containing a Gamma function. Note that

$$\psi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) = e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\,F_\nu(\zeta_\nu) \tag{2.16}$$

is the Coulomb scattering wave function of particles β and γ moving with the relative momentum $\mathbf{k}_\alpha$.

The 3C function has been used in [12, 13, 14] for electron-atom ionization processes. However it is important to underscore that $\Psi^{(3C)(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ satisfies the Schrödinger equation only in the leading and the first order terms in the asymptotic region Ω_0.

2. Leading asymptotic term of the incident wave in Ω_α

An asymptotic wave function valid in Ω_α has been proposed in [15], however, only for partial waves, for monopole and monopole-plus-dipole electron-electron interactions. A formal scheme which would yield the desired asymptotic solution of the Schrödinger equation was suggested in [3] but no concrete realization leading to an analytical wave function was attempted.

The asymptotic wave function for three charged particles in Ω_α is well established now. The decisive breakthrough to get the leading asymptotic term of the incident wave function in the asymptotic domain Ω_α, where the distance between particles β and γ is much smaller than the distance from their c.m. to particle α, has been achieved in [16] where the so-called local momentum has been introduced. This asymptotic wave function smoothly transforms into Redmond's three-body Coulomb distorted plane wave [6, 7] which is valid in the Ω_0 region where all three interparticle distances are large. However, in [16] only the leading asymptotic term of the asymptotic solution in Ω_α was derived. This asymptotic term has been further improved in [17]. Mukhamedzhanov and Lieber [17] derived all the terms of the asymptotic solution in Ω_α up to $O(1/\rho_\alpha^2)$. The improved asymptotic wave function also smoothly transforms into Redmond's three-body Coulomb distorted plane wave [6, 7]. According to [3] the general asymptotic behavior of the three-body scattering wave function, evolved from the initial three-body incident wave, has the following form, which can be considered as a boundary condition:

$$\Psi^{(+)} = \tilde{\Psi}^{(+)} + \sum_{\nu=\alpha,\,\beta,\,\gamma} \varphi_\nu(\mathbf{r}_\nu) \frac{\mathcal{M}^{(\nu)}_{3\to 2}}{\rho_\nu}\, e^{i\,q_\nu\,\rho_\nu - i\overline{\eta}_\nu \ln(2q_\nu\,\rho_\nu)} + \frac{\mathcal{M}_{3\to 3}}{R^{5/2}}\, e^{i\kappa R - i\Pi\,\ln(2\kappa\,R) + iW}. \tag{2.17}$$

Here $\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ is the three-body incident wave. Its leading term in Ω_0 is given by the Redmond three-body Coulomb distorted plane wave [6, 7]. The leading asymptotic terms of $\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ in the asymptotic region $\Omega_\nu,\ \nu = \alpha,\,\beta,\,\gamma$ have been derived in [17] up to order $O(1/\rho_\alpha^2)$. These asymptotic terms contain the terms $O(1)$ and $O(1/\rho_\alpha)$ corresponding to plane and single scattering eikonals. However, terms of the next order, $O(1/\rho_\alpha^2)$, corresponding to double scattering eikonals, have not yet been found in the asymptotic regions Ω_ν. The second term in Eq. (2.17) describes the two-body outgoing scattering wave and corresponds to the processes $\alpha + \beta + \gamma \to$ two-body state. $\mathcal{M}^{(\nu)}_{3\to 2}$ is the 3 *particle* $\to$ 2 *particle* synthesis amplitude corresponding to the process which is the inverse of the breakup process $2 \to 3$. For example, for $\nu = \alpha,\ \mathcal{M}^{(\alpha)}_{3\to 2}$ is the amplitude of the process $\alpha + \beta + \gamma \to \alpha + (\beta\,\gamma)$. There are three different possible two-body final states: $\alpha + (\beta\,\gamma)$, $\beta + (\alpha\,\gamma)$ and $\gamma + (\alpha\,\beta)$. We note that, for simplicity, we allow only one bound state for each couple. Evidently in the asymptotic region Ω_0, where all the interparticle distances $r_\nu \to \infty$ the second term can be neglected in Ω_0 due to the exponential decay of the bound-state wave functions $\varphi_\nu(\mathbf{r}_\nu)$ of the couple $\nu = (\sigma\,\tau)$. Finally the third term describing the three-body outgoing scattering wave corresponds to the scattering process in the system of three particles. In the third term, R is the hyperradius, Π is the Coulomb parameter, and W is the phase-factor due to the Coulomb distortion. $\mathcal{M}_{3\to3}$ is the $3\,particle \to 3\,particle$ scattering amplitude.

It is evident from Eq. (2.17) that if we are able to find the next order terms, $O(1/\rho_\alpha^2)$, in the asymptotic behavior of the incident wave $\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ in Ω_ν we will have all available leading asymptotic terms of the three-body Coulomb scattering wave function $\Psi^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ in Ω_ν up to terms $O(1/\rho_\alpha^3)$. It does not make sense to find the higher order terms in $\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ because they will be the next order terms compared to the three-body outgoing scattered wave, which is $O(1/R^{5/2})$. Derivation of all the terms up to $O(1/\rho_\alpha^3)$ in the incident three-body Coulomb wave $\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ in Ω_ν is the first main problem of this work. The derived incident wave will contain all the zeroth-, first- and second-order terms and should satisfy the Schrödinger equation in Ω_α up to terms $O(1/\rho_\alpha^3)$. We note that terms $O(1/\rho_\alpha^2)$ are the highest order terms which can be derived without a direct solution of the three-body Schrödinger equation. The next order terms of the asymptotic solution in Ω_α, including the outgoing three-body scattered wave $O(1/\rho_\alpha^{5/2})$, and higher order terms can be found only by a direct solution of the Schrödinger equation .

C. The three-body Coulomb scattering wave evolved from the inital two-body incident wave

The are three other energy spectra branches covering the intervals $(-\varepsilon_{\beta\gamma},\,\infty)$, $(-\varepsilon_{\alpha\gamma},\,\infty)$ and $(-\varepsilon_{\alpha\beta},\,\infty)$. Each interval corresponds to the eigenfunctions which asymptotically behave as the incident two-body Coulomb distorted plane wave plus outgoing two-body scattering waves and three-body scattered wave. For example, the eigenfunction corresponding to the interval $(-\varepsilon_{\beta\gamma},\, \infty)$ with the eigenvalue

$$E = \frac{q_i^2}{2\,M_\alpha} - \varepsilon_{\beta\gamma}, \tag{2.18}$$

where $E_i = q_i^2/(2\,M_\alpha)$ is the relative kinetic energy of the scattering particles α and $(\beta\,\gamma)$ in the intial state, asymptotically behaves as

$$\Psi^{(+)}_{\mathbf{q}_i} = \varphi_\alpha\, \chi^{(+)}_{\mathbf{q}_i} + \sum_{\nu=\beta,\,\gamma} \varphi_\nu(\mathbf{r}_\nu) \frac{\mathcal{M}^{(\nu\,\alpha)}}{\rho_\nu}\, e^{i\, q_\nu\, \rho_\nu - i\overline{\eta}_\nu\, \ln(2q_\nu\, \rho_\nu)} + \frac{\mathcal{M}_{2\to 3}}{R^{5/2}}\, e^{i\kappa R - i\Pi\, \ln(2\kappa\, R) + i\, W} \tag{2.19}$$

in the leading orders. Here, φ_α is the bound-state wave function of the pair $(\beta\,\gamma)$, $\chi^{(+)}_{\mathbf{q}_i}$ is scattering wave function for particles $\alpha + (\beta\,\gamma)$ with the relative momentum $\mathbf{q}_i$. The second term is the two-body outgoing scattered wave describing the rearrangement process $\alpha + (\beta\,\gamma) \to \beta + (\alpha\,\gamma)$ or $\alpha + (\beta\,\gamma) \to \gamma + (\alpha\,\beta)$. $\mathcal{M}^{(\nu\,\alpha)}$ is the corresponding rearrangement reaction amplitude. The third term is the three-body outgoing scattered wave describing the breakup process $\alpha + (\beta\,\gamma) \to \alpha + \beta + \gamma$. $\mathcal{M}_{2\to 3}$ is the corresponding breakup amplitude. $\overline{\eta}_\nu$ and Π are Coulomb parameters. W is the phase factor due to the Coulomb distortion of the outgoing three-body spherical wave.

Determination of the phase factor in all the asymptotic regions has been the main problem in the invesitgation of the asymptotic behavior of the three-body scattered wave.

The asymptotic form of the three-body outgoing scattered wave was found more than four decades ago by Peterkop for electron-impact ionization of hydrogen in the case when all interparticle distances are large (asymptotic region Ω_0) [8]. The knowledge of the asymptotic form of the three-body scattered wave opens up the possibility to find the breakup/ionization amplitude by a direct numerical solution of the three-body Schrödinger equation in the configuration space and matching the computer output with the imposed boundary conditions or by using the integral representation of the breakup amplitude as a surface integral in the six-dimensional hyperspace when the hyperradius $R \to \infty$ [18, 19, 20, 21, 22, 23, 24]. Such methods, in principle, require knowledge of the asymptotic behaviour of the scattered wave function in all asymptotic regions of the configuration space. This is because asymptotic wave functions are used directly as boundary conditions in solving the differential equation, or for extracting the scattering amplitudes from integral expressions involving the full scattering wave function. Despite the progress in high-performance computing, this approach has not yet been successfully implemented.

One reason is that Peterkop's asymptotic wave function is invalid when the two electrons are close to each other or when one of the electrons is close to the proton. Thus Peterkop's asymptotic wave function is invalid in the asymptotic regions Ω_ν. In these asymptotic regions the phase factor, W, found by Peterkop [8] logarithmically diverges. For full-scale numerical calculations, an asymptotic representation of the three-body scattered wave describing breakup/ionization in all the asymptotic regions is necessary.

A second reason for the lack of implementation is the so-called phase-amplitude ambiguity. Peterkop used six-dimensional hyperspherical coordinates, which effectively transform the Schrödinger equation describing the development of the system into a Hamilton-Jacobi type equation as the asymptotic motion of the particles becomes classical. For this reason, the Peterkop asymptotic wave suffers from an amplitude-phase ambiguity problem, since some part of the hyperspherical ionization amplitude can be moved to the phase factor and the resulting wavefunction is still a solution to the original Hamilton-Jacobi equation [8]. Accordingly, the remainder amplitude can equally well be called an breakup/ionization amplitude. Thus, generally speaking, the hyperspherical approach is not capable of uniquely identifying the breakup/ionization amplitude. This amplitude-phase ambiguity has caused problems in the formal theory of breakup reactions at a very fundamental level.

Finally, a full knowledge of the asymptotic behavior of the scattered wave forms the basis for the Kohn variational approach to breakup scattering. Any trial function used in the variational approach should have currect asymptotic behavior in all asymptotic regions. Thus a knowledge of the asymptotic behavior of the three-body scattered wave in all regions of the configuration space is crucial in calculations of atomic and nuclear breakup processes.

The second main problem, which is addressed in the present work, is the determination of the asymptotic behavior of the three-body scattered wave in Eq. (5.28) in all the asymptotic regions for the general case of arbitrary masses and charges of particles α, β and γ. The resulting phase factor should coincide with the phase factor found by Peterkop in Ω_0 [8] in the limiting case of electon-hydrogen ionization. A general approach used in this work will allow us to resolve the phase-ambiguity problem. Knowledge of the asymptotic behavior of the three-body scattered wave allows us to correctly formulate the breakup problem with Coulomb interactions and opens up the possibility to apply a direct numerical solution of the Schrödinger equation to determine the breakup problem.

CHAPTER III

ASYMPTOTIC SCATTERING WAVE FUNCTION FOR THREE CHARGED PARTICLES IN THE CONTINUUM

In this chapter we consider the asymptotic behavior of the three-body scattering wave function, which evolves from the initial three-body incident wave describing three incident particles in the continuum. The quantum mechanical dynamics of three charged particles is described by Schrödinger's equation which should be suplemented by proper boundary conditions. Merkuriev and Fadeev [3] claimed that the solution of this equation exists and is unique if the boundary conditions are known in all asymptotic regions. Three-body scattering theory introduces new challenges compared to the two-body case.

The chapter is organized in the following way. In Sec. A, we introduce the three-body nomenclature and the statement of the problem. In Sec. B we recall some of the important relations from two-body scattering. In Sections C and D we present asymptotic solutions of the three-body Schrödineger's equation in all orders which can be obtained with the asymptotic method. The last Section, E, concludes the chapter.

A. Statement of the problem

We consider a nonrelativistic three-body problem for three charged particles of mass m_α and charge z_α, $\alpha = 1, 2, 3$ in the continuum state. We use the Greek letter α in several ways, as any one of the three particles as in $\alpha = 1, 2, 3$ or just the particle α while we define the other two as β, γ. In the conventional few-body notation, α stands for the pair of other two particles β, γ. The following conventional notations for the two body quantities are used: $A_\alpha \equiv A_{\beta\gamma}$, where $\alpha \neq \beta \neq \gamma$. This will be clear from the context.

We use the Jacobi coordinates in Fig. 1. $\mathbf{r}_\alpha$ is the relative coordinate between particles β and γ, and $\mathbf{k}_\alpha$ is its canonically conjugated momentum. $\mu_\alpha = \frac{m_\beta m_\gamma}{m_\beta + m_\gamma}$ is their reduced mass. Similarly, $\boldsymbol{\rho}_\alpha$ is the relative coordinate between the c.m. of the pair (β, γ) and particle α, and $\mathbf{q}_\alpha$ is its canonically conjugated relative momentum. M_α is given by Eq. (2.7), $M = \sum\limits_{\nu=1}^{3} m_\nu$ is total mass of the three-body system. There are actually three sets of Jacobi coordinates $\mathbf{r}_\nu, \boldsymbol{\rho}_\nu$, where $\nu = \alpha, \beta, \gamma$. We frequently need the relations between the coordinates, and respective momenta for a channel $\nu = \beta, \gamma$ and the corresponding $\alpha-$channel variables. They are given by the following relations

$$\begin{pmatrix} \boldsymbol{\rho}_\nu \\ \mathbf{r}_\nu \end{pmatrix} = \begin{pmatrix} -\frac{m_\alpha}{M - m_\nu} & \epsilon_{\nu\alpha} \frac{\mu_\nu}{M_\alpha} \\ -\epsilon_{\nu\alpha} & -\frac{m_\nu}{m_{\beta\gamma}} \end{pmatrix} \begin{pmatrix} \boldsymbol{\rho}_\alpha \\ \mathbf{r}_\alpha \end{pmatrix} \tag{3.1}$$

$$\begin{pmatrix} \mathbf{q}_\nu \\ \mathbf{k}_\nu \end{pmatrix} = \begin{pmatrix} -\frac{m_\nu}{m_{\beta\gamma}} & \epsilon_{\nu\alpha} \\ -\epsilon_{\nu\alpha} \frac{\mu_\alpha}{M_\nu} & -\frac{m_\alpha}{M - m_\nu} \end{pmatrix} \begin{pmatrix} \mathbf{q}_\alpha \\ \mathbf{k}_\alpha \end{pmatrix} \tag{3.2}$$

where $\nu = \beta, \gamma$ and the antisymmetric symbol $\epsilon_{\alpha\nu} = -\epsilon_{\nu\alpha}$, with $\epsilon_{\alpha\nu} = 1$ for (α, ν) being a cyclic permutation of $(1, 2, 3)$, and $\epsilon_{\alpha\alpha} = 0$. The motion of the three particles is described by the Schrödinger equation in the configuration space

$$\{E - T_{\mathbf{r}_\alpha} - T_{\boldsymbol{\rho}_\alpha} - V\} \Psi^{(+)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \tag{3.3}$$

where $V = \sum\limits_{\nu=1}^{3} V_\nu$, $V_\nu = V_\nu^C(\mathbf{r}_\nu) + V_\nu^N(\mathbf{r}_\nu)$. V_ν^C is the Coulomb potential which is given by $V_\alpha^C(\mathbf{r}_\alpha) = \frac{z_\beta z_\gamma}{r_\alpha}$. Similarly, V_ν^N is the nuclear potential between the particles of the $\nu-$ pair, where $\nu = \alpha, \beta, \gamma$. $T_{\mathbf{r}_\alpha} = -\frac{\triangle_{\mathbf{r}_\alpha}}{2\mu_\alpha}$, is the kinetic energy operator for the relative motion of particles β and γ, and $T_{\boldsymbol{\rho}_\alpha} = -\frac{\triangle_{\boldsymbol{\rho}_\alpha}}{2M_\alpha}$ is the kinetic energy operator for the relative motion of particle α and the center of mass of the pair (β, γ), respectively.

We are interested in the asymptotic solution of the Schrödinger equation (3.3) of the three-body scattering wave function of the first type (see Chapter II, Sec. B).

These wave functions correspond to the energy spectrum $(0, \infty)$ and evolve from the initial three-body incident wave describing the three incident particles in the continuum. The asymptotic behavior of the three-body scattering wave function of the first type is given by Eq. (2.17) in the asymptotic region Ω_α. It is not clear from this equation how $\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ is determined. Formally we can determine the incident wave as an asymptotic difference

$$\tilde{\Psi}^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \approx \Psi^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} - \sum_{\nu=\alpha,\,\beta,\,\gamma} \varphi_\nu(\mathbf{r}_\nu) \frac{\mathcal{M}^{(\nu)}_{3\to 2}}{\rho_\nu}\, e^{i\, q_\nu\, \rho_\nu - i\overline{\eta}_\nu \ln(2q_\nu\, \rho_\nu)} - \frac{\mathcal{M}_{3\to 3}}{R^{5/2}}\, e^{i\kappa R - i\Pi\, \ln(2\kappa\, R) + i\, W} \tag{3.4}$$

From this equation it is clear that the three-body incident wave is the part of the full wave function, which does not contain the outgoing two- and three-body waves. For better understanding of the three-body incident wave we consider first the two-body case.

B. Asymptotic two-body scattering wave function

We will be referring to two body Coulomb scattering throughout this work. Therefore we present here some important relations for two body scattering. Let us consider two charged particles with masses m_1 and m_2 and charges z_1, and z_2 interacting via the potential $V = \frac{z_1 z_2}{r} + V^N(r)$. Scattering of two particles is described by the Schrödinger equation

$$\{E - H\}\psi^{(+)}_{\mathbf{k}}(\mathbf{r}) = 0, \tag{3.5}$$

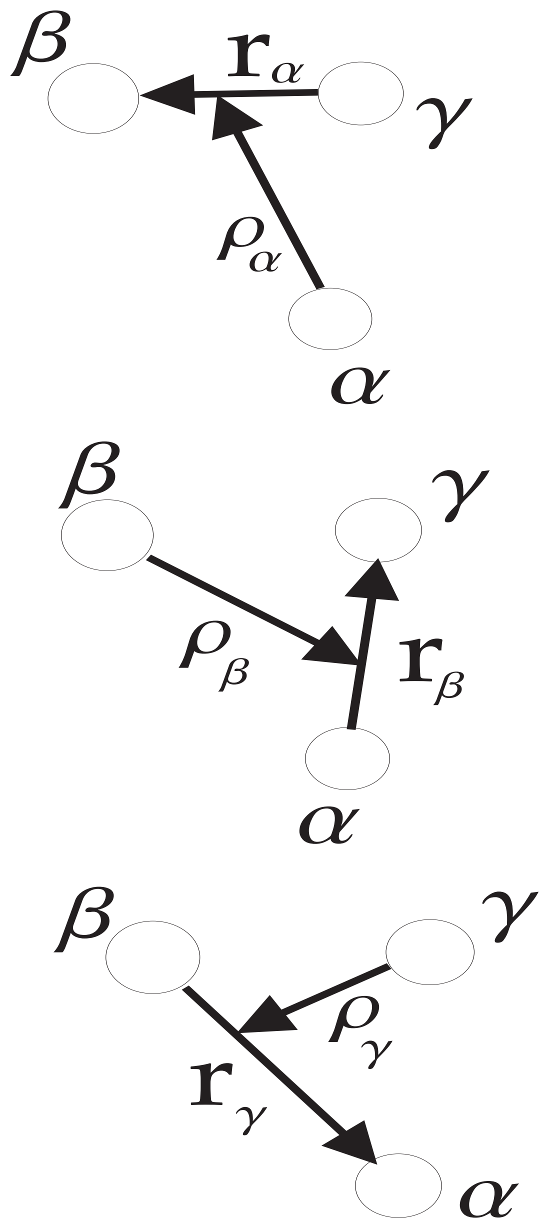

Fig. 1. Jacobi coordinate system.

where $\eta = \frac{z_1 z_2 \mu}{k}$ is Coulomb parameter, $E = \frac{k^2}{2\mu}$ is the relative kinetic energy of the interacting particles 1 and 2, $H = -\frac{\triangle_{\mathbf{r}}}{2\mu} + V$ is two body Hamiltonian, and $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is reduced mass of particles 1 and 2. For the pure Coulomb interaction case Eq. (3.5) can be solved analytically in parabolic coordinates, $\zeta = kr - \mathbf{k} \cdot \mathbf{r}$. Substituting

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = e^{i\mathbf{k}\cdot r} F(i\zeta), \tag{3.6}$$

into Eq. (3.5) gives the differential equation for the confluent hypergeometric function

$$[\frac{\triangle_{\mathbf{r}}}{2\mu} + \frac{i\mathbf{k} \cdot \nabla_{\mathbf{r}}}{\mu} - V]\, F(i\zeta) = 0. \tag{3.7}$$

which has the following solution

$$F(i\zeta) = N\, {}_1F_1(-i\eta, 1, i\zeta), \tag{3.8}$$

where $N = e^{-\pi\eta/2}\Gamma(1 + i\eta)$ is the normalization factor and ${}_1F_1(-i\eta, 1, i\zeta)$ is the hypergeometric function. The confluent hypergeometric function can be written as a sum of two Whittaker functions:

$$N\, F(-i\eta, 1, i\zeta) = \mathcal{F}^{(1)}(\zeta) + \mathcal{F}^{(2)}(\zeta). \tag{3.9}$$

Here,

$$\mathcal{F}^{(1)}(\zeta) = e^{\frac{\pi\eta}{2}} (i\zeta)^{-\frac{1}{2}} e^{i\frac{\zeta}{2}} W_{i\eta+\frac{1}{2},0}(i\zeta), \tag{3.10}$$

$$\mathcal{F}^{(2)}(\zeta) = -i\frac{\Gamma(1 + i\eta)}{\Gamma(-i\eta)} e^{\frac{\pi\eta}{2}} (i\zeta)^{-\frac{1}{2}} e^{i\frac{\zeta}{2}} W_{-i\eta-\frac{1}{2},0}(-i\zeta), \tag{3.11}$$

Taking into account the asymptotic behaviour of the Whittaker function at $\zeta \to \infty$

$$W_{\lambda,0}(i\zeta) = (i\zeta)^{\lambda} e^{-i\zeta/2} \left[1 - \frac{(\lambda - 1/2)^2}{i\zeta} + O(\frac{1}{i\zeta^2})\right], \tag{3.12}$$

we derive the asymptotic behavior of the Whittaker functions $\mathcal{F}^{(i)}(\zeta)$, $i = 1, 2$:

$$\mathcal{F}^{(1)}(i\zeta) \overset{\zeta\to\infty}{=} e^{i\eta \ln\zeta}\left[1 + O(\frac{1}{i\zeta})\right] \tag{3.13}$$

$$\mathcal{F}^{(2)}(i\zeta) \overset{\zeta\to\infty}{=} f^C \frac{e^{i\zeta}}{r} e^{-i\eta\ln 2kr}\left[1 + O(\frac{1}{i\zeta})\right], \tag{3.14}$$

where f^C is the on-the-energy-shell Coulomb scattering amplitude:

$$f^C = -\eta \frac{\Gamma(1+i\eta)}{\Gamma(1-i\eta)}(-i)^{-i\eta}e^{\pi\eta/2}\frac{e^{-i\eta\ln\sin^2\frac{\theta}{2}}}{2k\sin^2\frac{\theta}{2}}. \tag{3.15}$$

Taking into account Eqs. (3.6), (3.8), (3.9), (3.12) and (3.14) we get the asymptotic behavior of the Coulomb scattering wave function for a system of two particles in the coordinate space:

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) \overset{r\to\infty}{=} e^{i\,\mathbf{k}\cdot\mathbf{r}}e^{i\eta\ln\zeta}\,[1 + O(\frac{1}{i\zeta})] + f^C\frac{e^{ikr}}{r}e^{-i\eta\ln 2kr}\,[1 + O(\frac{1}{i\zeta})]. \tag{3.16}$$

Note that this asymptotic behavior is valid only for $|\zeta| \to \infty$. For $r \to \infty$ it is valid for all directions in the configuration space except for the so-called singular direction, for which $\hat{\mathbf{k}}\cdot\hat{\mathbf{r}} = 1$.

One can see a very interesting feature in the case of the two-body Coulomb scattering. The asymptotic Coulomb scattering wave function consists of two terms. The first one, $e^{i\mathbf{k}\cdot\mathbf{r}}e^{i\eta\ln\zeta}\,(1+O(\frac{1}{i\zeta})$ is the asymptotic form of $e^{i\mathbf{k}\cdot\mathbf{r}}\mathcal{F}^{(1)}(i\zeta)$ and represents the Coulomb distorted incident wave. The Coulomb distortion not only generates a logarithmic phase factor $\eta\,\ln\zeta$ as an additional phase factor to the plane wave phase factor $\mathbf{k}\cdot\mathbf{r}$, but it also generates an infinite series in powers of $1/\zeta$. This is in contrast to the two-body scattering problem for particles interacting via short-range potentials, where the incident wave is given just by the plane wave. The second term in Eq. (3.16) is the asymptotic form for $e^{i\mathbf{k}\cdot\mathbf{r}}\mathcal{F}^{(2)}(i\zeta)$ and generates the outgoing two-body spherical wave and also contains an asymptotic expansion in powers of $1/\zeta$.

C. Asymptotic three-body incident wave of three charged particles in continuum

After an explanation of the incident wave for the two-body case, it is easier to proceed to the incident wave for the three-body case. Our goal is to derive the asymptotic incident three-body wave function in the leading orders $O(1)$, $O(1/\rho_\nu)$, $O(1/\rho_\nu^2)$ in the asymptotic region Ω_ν, Eq. (2.2), where any two particles can be close to each other and far away from the third particle. Terms of order $O(1/\rho_\nu^2)$ are leading terms, which can be derived without explicit solution of the three-body Schrödinger equation . The next order term is the outgoing three-body scattered wave which is $O(1/R^{5/2})$. To find the amplitude of this term corresponding to the scattering process for 3 *particles* $\to$ 3 *particles*, one has to solve the three-body Schrödinger equation . As an example, we consider the asymptotic region Ω_α. Expressions for the asymptotic incident three-body wave functions in two other asymptotic regions Ω_β and Ω_ν can be derived by simple cyclic permutation of indexes α, β, γ. As we have mentioned earlier, the asymptotic incident three-body wave function is the part of the total three-body scattering wave function of the first type, which does not contain two- and three-body scattered waves. This wave function should smoothly transform into the asymptotic incident three-body wave function in the asymptotic region Ω_0. This smooth matching is the part of the boundary conditions that provides for a unique solution.

The leading asymptotic term of the three-body incident wave function in Ω_0 derived by Redmond [6, 7] is given by Eq. (2.10). It is the three-body Coulomb distorted plane wave. For practical applications Merkuriev [3], Garibotti and Miraglia [13] extended the asymptotic Redmond's term [6, 7] by substituting the confluent hypergeometric functions for the exponential Coulomb distortion factors. This extended wave function, often called the 3C wave function, is given by Eq. (2.13) and is well-behaved even in the singular directions ($\zeta_\nu < C$ for $r_\nu \to \infty$) where the Redmond's asymptotic term is not determined. If any of the particles is neutral, then the resulting asymptotic solution becomes the plane wave for the neutral particle and the exact two-body scattering wave function for the charged pair. However, neither Redmond's asymptotic term $\Psi^{(0)(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ nor the 3C wave function $\Psi^{(3C)(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ are asymptotic solutions of the Schrodinger equation in the asymptotic domains Ω_ν, $\nu = \alpha, \beta, \gamma$. Redmond's asymptotic term, by construction, satisfies the asymptotic Schrödinger equation up to terms $O(1/r_\alpha^2,\, 1/r_\beta^2,\, 1/r_\gamma^2)$. However, in the asymptotic region, Ω_ν, the distance between the particles of pair ν is limited: $r_\nu < C'$. Hence the terms $O(1/r_\nu)$ are not small and the potential V_ν^C in the Schrödinger equation has to be compensated exactly rather than asymptotically as happens when we use Redmond's asymptotic wave function in Ω_0. In the 3C wave function two very important effects are absent. Consider, for example, the asymptotic region Ω_α. In this region $r_\alpha << \rho_\alpha$. Hence the two-body relative motion of particles β and γ is distorted by the Coulomb field of the third particle α [16]. The second evident defect in the 3C function is the absence of the nuclear interaction between particles β and γ which can be close enough to each other in Ω_α. Nevertheless, the 3C wave function can be used as a starting point to derive the the leading asymptotic terms of the three-body incident wave in Ω_α [16, 17], because this asymptotic three-body incident wave should match Redmond's asymptotic term in Ω_0. We will demonstrate now how important the condition of the matching of the asymptotic wave functions is on the border of different asymptotic regions [16].

Let us consider the asymptotic Schrödinger equation in Ω_α. The asymptotic Hamiltonian in Ω_α can be written in leading order as

$$H_\alpha^{as} = \lim_{\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha \in \Omega_\alpha} H \,=\, T_{\mathbf{r}_\alpha} + T_{\boldsymbol{\rho}_\alpha} + V_\alpha + \upsilon_\alpha^C(\rho_\alpha). \tag{3.17}$$

Here

$$V_\beta(r_\beta) + V_\gamma(r_\gamma) \overset{\lim r_\alpha/\rho_\alpha \to 0}{\approx} \upsilon_\alpha^C(\rho_\alpha) + O(1/\rho_\alpha^2), \tag{3.18}$$

$$\upsilon_\alpha^C(\rho_\alpha) = \frac{Z_\alpha(Z_\beta + Z_\gamma)\, e^2}{\rho_\alpha}. \tag{3.19}$$

Here, $\upsilon_\alpha^C(\rho_\alpha)$ is the Coulomb potential between the charge Z_α and the total charge $(Z_\beta{+}Z_\gamma)$ of the system $\beta{+}\gamma$ concentrated in their center of mass. Then the asymptotic Schrödinger equation in $\Omega_\alpha :\ \rho_\alpha \to \infty,\ r_\alpha/\rho_\alpha \to 0$ in leading order reduces to

$$\{E - H_\alpha^{as}\}\Psi^{(as)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \tag{3.20}$$

where $E = \frac{k_\alpha^2}{2\mu'_\alpha} + \frac{q_\alpha^2}{2M_\alpha}$ is the total energy of the three-body system. Since $H_\alpha^{as} = \overline{H}_{\boldsymbol{\rho}_\alpha} + H_{\mathbf{r}_\alpha}$ is the sum of two sub-Hamiltonians

$$H_{\mathbf{r}_\alpha} = T_{\mathbf{r}_\alpha} + V_\alpha, \tag{3.21}$$

$$\overline{H}_{\boldsymbol{\rho}_\alpha} = T_{\boldsymbol{\rho}_\alpha} + \frac{Z_\alpha(Z_\beta + Z_\gamma)\, e^2}{\rho_\alpha}, \tag{3.22}$$

one of the possible solutions is a trivial factorized one

$$\overline{\Psi}^{(\alpha)(+)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\chi^{(+)}_{\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha). \tag{3.23}$$

Here, $\psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)$ is the scattering wave function of particles β and γ satisfying Schrödinger equation

$$\{\frac{k_\alpha^2}{2\mu_\alpha} - H_{\mathbf{r}_\alpha}\}\psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) = 0. \tag{3.24}$$

Correspondingly, $\chi^{(+)}_{\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ is the Coulomb scattering wave function describing the scattering state of particle α and the center of mass of the system $\beta + \gamma$ satisfying the Schrödinger equation

$$(\frac{q_\alpha^2}{2M_\alpha} - \overline{H}_{\boldsymbol{\rho}_\alpha})\chi^{(+)}_{\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha) = 0. \tag{3.25}$$

Since $\chi^{(+)}_{\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ satisfies the two-body Schrödinger equation with a pure Coulomb interaction we can write down its solution:

$$\chi^{(+)}_{\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha) = e^{i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\overline{N}_\alpha\, F(-i\overline{\eta}_\alpha,\, 1; \overline{\zeta}_\alpha), \tag{3.26}$$

where

$$\overline{\eta}_\alpha = \frac{Z_\alpha\,(Z_\beta + Z_\gamma)\, e^2\, M_\alpha}{q_\alpha}, \tag{3.27}$$

$$\overline{\zeta}_\alpha = q_\alpha\,\rho_\alpha - \mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha, \tag{3.28}$$

$$\overline{N}_\alpha = e^{-\pi\overline{\eta}_\alpha/2}\Gamma(1 + i\overline{\eta}_\alpha). \tag{3.29}$$

If the factorized solution (3.23) is a correct asymptotic solution in Ω_α, it should match Redmond's asymptotic term (2.10). To check it we just consider the asymptotic behavior of (3.23) in Ω_0, where $r_\alpha,\,\rho_\alpha \to \infty$. In leading order we get

$$\psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) \overset{r_\alpha\to\infty}{=} e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\, e^{i\eta_\alpha\,\ln\zeta_\alpha} + O(1/r_\alpha), \tag{3.30}$$

$$\chi^{(+)}_{\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha) \overset{\rho_\alpha\to\infty}{=} e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\, e^{i\overline{\eta}_\alpha\,\ln\overline{\zeta}_\alpha} + O(1/\rho_\alpha). \tag{3.31}$$

Then the factorized solution in leading order is

$$\begin{aligned}\overline{\Psi}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) &= \psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\,\chi^{(+)}_{\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\\ &\overset{r_\alpha,\,\rho_\alpha\to\infty}{=} e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\, e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\, e^{i\eta_\alpha\,\ln\zeta_\alpha}\, e^{i\overline{\eta}_\alpha\,\ln\overline{\zeta}_\alpha} + O(1/r_\alpha) + O(1/\rho_\alpha).\end{aligned} \tag{3.32}$$

We can see that the leading asymptotic term of the factorized solution, $\overline{\Psi}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ in Ω_0, has only two logarithmic phase factors in contrast to the three phase factors in Redmond's asymptotic term (2.10). Thus the factorized solution doesn't satisfy one of the important boundary conditions: it does not transform smoothly into the asymptotic solution in Ω_0. Hence, the factorized wave function, $\overline{\Psi}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, is not a solution of the asymptotic Schrödinger equation in Ω_α. This failure is entirely due to the long range of the Coulomb interactions. These Coulomb interactions cause

Coulomb distortions of the plane waves and these distortions are different in Redmond's asymptotic term in Ω_0 and in the factorized wave function. In Redmond's asymptotic incident wave three logarithmic phase factors appear, one phase factor for each pair, rather than the two phase factors in the factorized solution. It is a very important conclusion. In all the conventional approaches for breakup processes, including coupled channels codes like FRESCO, the three-body scattering wave function is approximated by the factorized one. From the consideration above, it is clear that if Coulomb interactions are important, such an approximation is not accurate. If the interactions are short-range, the factorized solution matches the asymptotic solution in Ω_0 and is justified in the asymptotic region Ω_α.

It was shown in [16, 17] that the actual asymptotic solution of the asymptotic Schrödinger equation $\Psi^{(as)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, which matches Redmond's asymptotic term in Ω_0, cannot be written in a factorized form and has a quite complicated behavior. In [16, 17] all the leading asymptotic terms up to $O(1/\rho_\alpha^2)$ of the asymptotic wave function $\Psi^{(as)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ have been derived in the asymptotic region Ω_α. In this work we will present a derivation of the expansion of the asymptotic wave function, $\Psi^{(as)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, up to terms $O(1/\rho_\alpha^3)$. The derived asymptotic expansion contains all the terms $O(1)$, $O(1/\rho_\alpha)$ and $O(1/\rho_\alpha^2)$. Since we are looking for the terms $O(1/\rho_\alpha^2)$, including approximation (3.18) is not enough. We need to keep the terms $O(1/\rho_\alpha^2)$ and we should keep the higher order terms up to $O(1/\rho_\alpha^3)$. Instead of the asymptotic expansion of the Coulomb potentials $V^C_\beta(\mathbf{r}_\beta)$ and $V^C_\gamma(\mathbf{r}_\gamma)$ in terms of $1/\rho_\alpha$, we will start our derivation from the exact three-body Schrödinger equation (3.3). The terms of $O(1/\rho_\alpha^3)$ will be dropped later. The asymptotic wave function in Ω_α should match the asymptotic wave function in Ω_0. The 3C wave function satisfies Eq. (3.3) up to terms $O(1/r_\alpha^2, 1/\rho_\alpha^2)$ and we can use it as the initial wave function. However, this wave function should be modified to satisfy the Schrödinger equation in Ω_α.

Note that usually in the literature it is assumed that Redmond's asymptotic term satisfies the Schrödinger equation in Ω_0 in leading order only. First we will show that the 3C wave function satisfies the Schrödinger equation in Ω_0 up terms of order $O(1/r_\nu^2)$. To this end we just substitute the 3C wave function (2.13) into the Schrödinger equation (3.3):

$$\begin{aligned}
&(E - T_{\mathbf{r}_\alpha} - T_{\boldsymbol{\rho}_\alpha} - V)[e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\,\varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta)\varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma)] \\
&= e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta)\varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma)[\frac{\triangle_{\mathbf{r}_\alpha}}{2\mu_\alpha} + \frac{i\mathbf{k}_\alpha\cdot\nabla_{\mathbf{r}_\alpha}}{\mu_\alpha} - V_\alpha \\
&+\frac{\triangle_{\boldsymbol{\rho}_\alpha}}{2M_\alpha} + \frac{i[\mathbf{q}_\alpha - i\sum\limits_{\nu=\beta,\gamma}\nabla_{\boldsymbol{\rho}_\alpha}\ln\varphi_{\mathbf{k}_\nu}]\cdot\nabla_{\boldsymbol{\rho}_\alpha}}{M_\alpha} \\
&+\frac{\nabla_{\mathbf{r}_\alpha}\varphi_{\mathbf{k}_\gamma}\cdot\nabla_{\mathbf{r}_\alpha}\varphi_{\mathbf{k}_\beta}}{\mu_\alpha\varphi_{\mathbf{k}_\beta}\varphi_{\mathbf{k}_\gamma}} + \frac{\nabla_{\boldsymbol{\rho}_\alpha}\varphi_{\mathbf{k}_\gamma}\cdot\nabla_{\boldsymbol{\rho}_\alpha}\varphi_{\mathbf{k}_\beta}}{M_\alpha\varphi_{\mathbf{k}_\beta}\varphi_{\mathbf{k}_\gamma}}]\varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha) \\
&+e^{i\mathbf{k}_\beta\cdot\mathbf{r}_\beta + i\mathbf{q}_\beta\cdot\boldsymbol{\rho}_\beta}\varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma)[\frac{\triangle_{\mathbf{r}_\beta}}{2\mu_\beta} + \frac{i\mathbf{k}_\beta\cdot\nabla_{\mathbf{r}_\beta}}{\mu_\beta} - V_\beta \\
&+\frac{\triangle_{\boldsymbol{\rho}_\beta}}{2M_\beta} + \frac{i[\mathbf{q}_\beta - i\sum\limits_{\tau=\alpha,\gamma}\nabla_{\boldsymbol{\rho}_\beta}\ln\varphi_{\mathbf{k}_\tau}]\cdot\nabla_{\boldsymbol{\rho}_\beta}}{M_\beta} \\
&+\frac{\nabla_{\mathbf{r}_\beta}\varphi_{\mathbf{k}_\gamma}\cdot\nabla_{\mathbf{r}_\beta}\varphi_{k_\alpha}}{\mu_\beta\varphi_{\mathbf{k}_\alpha}\varphi_{\mathbf{k}_\gamma}} + \frac{\nabla_{\boldsymbol{\rho}_\beta}\varphi_{\mathbf{k}_\gamma}\cdot\nabla_{\boldsymbol{\rho}_\beta}\varphi_{\mathbf{k}_\alpha}}{M_\beta\varphi_{\mathbf{k}_\alpha}\varphi_{\mathbf{k}_\gamma}}]\varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta) \\
&+e^{i\mathbf{k}_\gamma\cdot\mathbf{r}_\gamma + i\mathbf{q}_\gamma\cdot\boldsymbol{\rho}_\gamma}\varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta)[\frac{\triangle_{\mathbf{r}_\gamma}}{2\mu_\gamma} + \frac{i\mathbf{k}_\gamma\cdot\nabla_{\mathbf{r}_\gamma}}{\mu_\gamma} - V_\gamma \\
&+\frac{\triangle_{\boldsymbol{\rho}_\gamma}}{2M_\gamma} + \frac{i[\mathbf{q}_\gamma - i\sum\limits_{\omega=\alpha,\beta}\nabla_{\boldsymbol{\rho}_\gamma}\ln\varphi_{\mathbf{k}_\omega}]\cdot\nabla_{\boldsymbol{\rho}_\gamma}}{M_\gamma} \\
&+\frac{\nabla_{\mathbf{r}_\gamma}\varphi_{\mathbf{k}_\beta}\cdot\nabla_{\mathbf{r}_\gamma}\varphi_{k_\alpha}}{\mu_\beta\varphi_{\mathbf{k}_\alpha}\varphi_{\mathbf{k}_\beta}} + \frac{\nabla_{\boldsymbol{\rho}_\gamma}\varphi_{\mathbf{k}_\beta}\cdot\nabla_{\boldsymbol{\rho}_\gamma}\varphi_{\mathbf{k}_\alpha}}{M_\gamma\varphi_{\mathbf{k}_\alpha}\varphi_{\tilde{\mathbf{k}}_\beta}}]\varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma),
\end{aligned} \tag{3.33}$$

where $\varphi_{\mathbf{k}_\nu}(\mathbf{r}_\nu) = N\,F(-i\eta_\nu,\,1;i\zeta)$ and taking into account

$$[\frac{\triangle_{\mathbf{r}_\nu}}{2\mu_\nu} + \frac{i\mathbf{k}_\nu\cdot\nabla_{\mathbf{r}_\nu}}{\mu_\nu} - V_\nu]\varphi_{\mathbf{k}_\nu}(\mathbf{r}_\nu) = 0 \tag{3.34}$$

we derive

$$(E - T_{\mathbf{r}_\alpha} - T_{\boldsymbol{\rho}_\alpha} - V)[e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\,\varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\varphi_{\mathbf{k}_\beta}(\mathbf{r}_\beta)\varphi_{\mathbf{k}_\gamma}(\mathbf{r}_\gamma)] = O(1/r_\alpha^2, 1/r_\beta^2, 1/r_\gamma^2). \tag{3.35}$$

In the Ω_0 region the local momentum contributions dissappear, $\widetilde{\mathbf{k}}_\nu = \mathbf{k}_\nu$, as they are much smaller than $\mathbf{k}_\nu$. We did not use any approximation to get equation 3.35. Thus the 3C wave function indeed satisfies the Schrödinger equation in Ω_0 up to the terms $O(1/r_\alpha^2, 1/r_\beta^2, 1/r_\gamma^2)$ and hence the 3C wave function can be used as a starting wave function with proper modifications to look for an asymptotic solution in Ω_α.

$$\begin{aligned}\Psi^{(3C)(+)}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) &= e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\, e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\\ &\times [\mathcal{F}^{(1)}_\alpha(i\zeta_\alpha)\mathcal{F}^{(1)}_\beta(i\zeta_\beta)\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma) + \mathcal{F}^{(2)}_\alpha(i\zeta_\alpha)\mathcal{F}^{(1)}_\beta(i\zeta_\beta)\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)\\ &+\mathcal{F}^{(1)}_\alpha(i\zeta_\alpha)\mathcal{F}^{(2)}_\beta(i\zeta_\beta)\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma) + \mathcal{F}^{(1)}_\alpha(i\zeta_\alpha)\mathcal{F}^{(1)}_\beta(i\zeta_\beta)\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma)],\end{aligned} \tag{3.36}$$

where we kept only leading and the first order terms of the 3C function.

Let us rewrite Eq. (2.13) in a form which is suitable for consideration in the Ω_α asymptotic domain:

$$\begin{aligned}\Psi^{(3C)(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) &= e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\, e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\\ &\times [\mathcal{F}^{(1)}_\beta(i\zeta_\beta)\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)N_\alpha F_\alpha(i\zeta_\alpha) + \mathcal{F}^{(2)}_\beta(i\zeta_\beta)\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)N_\alpha F_\alpha(i\zeta_\alpha)\\ &+\mathcal{F}^{(1)}_\beta(i\zeta_\beta)\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma)N_\alpha F_\alpha(i\zeta_\alpha) + \mathcal{F}^{(2)}_\beta(i\zeta_\beta)\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma)N_\alpha F_\alpha(i\zeta_\alpha)].\end{aligned} \tag{3.37}$$

We took into account that

$$\varphi_{\mathbf{k}_\nu}(,\mathbf{r}_\nu) = N\,F(-i\eta_\nu,\,1;i\zeta) = \mathcal{F}^{(1)}(\zeta_\nu) + \mathcal{F}^{(2)}(\zeta_\nu). \tag{3.38}$$

Here, asymptotically, for $|\zeta_\nu| \to \infty$, the first term $\mathcal{F}^{(1)}(\zeta_\nu) \sim O(1)$ and the second term $\mathcal{F}^{(2)}(\zeta_\nu) \sim O(1/\zeta_\nu)$. Hence in the Ω_α $\;\mathcal{F}^{(1)}(\zeta_\nu)$ and $\mathcal{F}^{(2)}(\zeta_\nu)$, $\nu = \beta, \gamma$ can be treated asymptotically while $\varphi_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)$ should be considered explicitly, because Ω_α includes the region, where r_α is limited. Moreover, in the asymptotic region Ω_α the reltive motion of particles β and γ is distorted by the third particle α due to the long-range Coulomb interaction. It means that the wave function of the relative motion of particles β and γ in Ω_α will be different from the wave function $e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\,N_\alpha F_\alpha(i\zeta_\alpha)$ describing the relative motion of particles β and γ in the absence of the third particle. Since interacting particles β and γ can be close to each other, their nuclear interaction should also be taken into account. Following [17] we replace each $F_\alpha(i\zeta_\alpha)$ in Eq. (3.38) by the corresponding unknown function $\varphi_\alpha^{(nm)}(\mathbf{r}_\alpha)$, $n, m = 1, 2$:

$$\Psi^{(as)(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}\, e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}$$
$$\times[\mathcal{F}_\beta^{(1)}(i\zeta_\beta)\mathcal{F}_\gamma^{(1)}(i\zeta_\gamma)\varphi_\alpha^{(11)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) + \mathcal{F}_\beta^{(2)}(i\zeta_\beta)\mathcal{F}_\gamma^{(1)}(i\zeta_\gamma)\varphi_\alpha^{(21)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)$$
$$+\mathcal{F}_\beta^{(1)}(i\zeta_\beta)\mathcal{F}_\gamma^{(2)}(i\zeta_\gamma)\varphi_\alpha^{(12)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) + \mathcal{F}_\beta^{(2)}(i\zeta_\beta)\mathcal{F}_\gamma^{(2)}(i\zeta_\gamma)\varphi_\alpha^{(22)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)]. \qquad (3.39)$$

Derivation of $\varphi_\alpha^{(nm)}(\mathbf{r}_\alpha)$, $n, m = 1, 2$ is our final goal. Now we substitute Eq. (3.39) into the Schrödinger equation (3.3). When substitutting Eq. (3.39) into the Schrödinger equation we assume that each term of the sum (3.39) satisfies the Schrödinger equation . Moreover, as we will see, each function $\varphi_\alpha(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)$ depends on the preceding functions $\mathcal{F}_\beta^{(n)}(i\zeta_\beta)\mathcal{F}_\gamma^{(m)}(i\zeta_\gamma)$ where $n, m = 1, 2$, i.e. for each term in (3.39) the modification is different. We also take into account that

$$(\frac{1}{2\mu_\nu}\boldsymbol{\Delta}_{\mathbf{r}_\nu} + i\,\frac{1}{\mu_\nu}\,\mathbf{k}_\nu\cdot\boldsymbol{\nabla}_{\mathbf{r}_\nu} - V_\nu^C)\,\mathcal{F}_\nu^{(1,2)}(i\zeta_\nu) = 0. \qquad (3.40)$$

Substitution of the first term of Eq. (3.39) into the Schrödinger equation generates the equation for $\varphi_\alpha^{(11)}(\mathbf{r}_\alpha)$:

$$\mathcal{F}_\beta^{(1)}(i\zeta_\beta)\mathcal{F}_\gamma^{(1)}(i\zeta_\gamma)[\frac{1}{2\mu_\alpha}\boldsymbol{\Delta}_{\mathbf{r}_\alpha} + \frac{1}{2M_\alpha}\boldsymbol{\Delta}_{\boldsymbol{\rho}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}_\alpha\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha} + i\,\frac{1}{M_\alpha}\,\mathbf{q}_\alpha\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha} +$$
$$\frac{1}{\mu_\alpha}\sum_{\nu=\beta,\gamma}\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}_\nu^{(1)}(i\zeta_\nu)\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha} + \frac{1}{M_\alpha}\sum_{\nu=\beta,\gamma}\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}_\nu^{(1)}(i\zeta_\nu)\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha} - V_\alpha(\mathbf{r}_\alpha) +$$
$$\frac{1}{\mu_\alpha}\,\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}_\beta^{(1)}(i\zeta_\beta)\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}_\gamma^{(1)}(i\zeta_\gamma) + \frac{1}{M_\alpha}\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}_\beta^{(1)}(i\zeta_\beta)\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}_\gamma^{(1)}(i\zeta_\gamma)]$$
$$\times\varphi_\alpha^{(11)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = 0. \quad (3.41)$$

Since particles β and γ are allowed to be close in Ω_α their interaction potential is given by the sum of the Coulomb and nuclear potentials. Now we will simplify this equation by dropping all the terms $O(1/\rho_\alpha^3)$ and explicitly compensate all the terms $O(1)$, $O(1/\rho_\alpha)$, $O(1/\rho_\alpha^2)$. We consider only the nonsingular directions, i. e. $\hat{\mathbf{k}}_\nu\cdot\hat{\mathbf{r}}_\nu \neq 1,\ \nu = \beta, \gamma$. To analyze the fifth term in the brackets we use equations

$$\mathcal{F}_\nu^{(1)}(i\zeta_\nu) = \tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu)[1 - i\,\frac{\eta_\nu^2}{\zeta_\nu} + O(1/\zeta_\nu^2)], \quad (3.42)$$

$$\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu) = e^{i\,\eta_\nu\ln\zeta_\nu}, \quad (3.43)$$

$$\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}_\nu^{(1)}(i\zeta_\nu) = \boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu) - i\frac{m_\nu}{m_{\beta\gamma}}\frac{\eta_\nu^2}{k_\nu\,r_\nu^2}\,\frac{\hat{\mathbf{r}}_\nu - \hat{\mathbf{k}}_\nu}{(1 - \hat{\mathbf{k}}_\nu\cdot\hat{\mathbf{r}}_\nu)^2} + O(1/r_\nu^3), \quad (3.44)$$

$$\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_\nu) = \boldsymbol{\nabla}_{\mathbf{r}_\alpha}e^{\frac{m_\nu}{m_{\beta\gamma}}\epsilon_{\nu\,\alpha}\mathbf{r}_\alpha\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}}\ln\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\alpha})$$
$$= \epsilon_{\nu\,\alpha}\,\frac{m_\nu}{m_{\beta\gamma}}\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\,\alpha}) + \frac{m_\nu^2}{m_{\beta\,\gamma}^2}(\mathbf{r}_\alpha\cdot\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha})\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\,\alpha}), \quad (3.45)$$

$$\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}_\nu^{(1)}(i\zeta_{\nu\,\alpha}) = i\eta_\nu\,\epsilon_{\nu\alpha}\,\frac{1}{\rho_\alpha}\frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu}\hat{\boldsymbol{\rho}}_\alpha}{1 - \epsilon_{\alpha\nu}\hat{\mathbf{k}}_\nu\cdot\hat{\boldsymbol{\rho}}_\alpha} + O(\frac{1}{\rho_\alpha^2}), \quad (3.46)$$

$$\boldsymbol{\nabla}_{\mathbf{r}_\alpha}[-i\,\frac{\eta_\nu^2}{\zeta_\nu}] = i\,\eta_\nu^2\,\frac{m_\nu}{m_{\beta\,\gamma}}\,\frac{1}{k_\nu\,\rho_\alpha^2}\,\frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu}\hat{\boldsymbol{\rho}}_\alpha}{(1 - \epsilon_{\alpha\nu}\hat{\mathbf{k}}_\nu\cdot\hat{\boldsymbol{\rho}}_\alpha)^2} + O(\frac{1}{\rho_\alpha^3}). \quad (3.47)$$

To estimate the sixth and the ninth terms we use equations

$$\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}^{(1)}_\nu(i\zeta_\nu) = i\eta_\nu \frac{1}{r_\nu}\, \epsilon_{\nu\alpha}\, \frac{\hat{\mathbf{k}}_\nu - \hat{\mathbf{r}}_\nu}{1 - \hat{\mathbf{k}}_\nu \cdot \hat{\mathbf{r}}_\nu} + O(\frac{1}{r^2_\nu}) \tag{3.48}$$

$$= i\eta_\nu\, \epsilon_{\nu\alpha}\, \frac{1}{\rho_\alpha} \frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu}\hat{\boldsymbol{\rho}}_\alpha}{1 - \epsilon_{\alpha\nu}\hat{\mathbf{k}}_\nu \cdot \hat{\boldsymbol{\rho}}_\alpha} + O(\frac{1}{\rho^2_\alpha}). \tag{3.49}$$

To estimate the eighth term we use equation

$$\boldsymbol{\nabla}_{\mathbf{r}_\alpha} \ln \mathcal{F}^{(1)}_\nu(i\zeta_\nu) = i\eta_\nu \frac{m_\nu}{m_{\beta\gamma}}\, \frac{1}{r_\nu} \frac{\hat{\mathbf{k}}_\nu - \hat{\mathbf{r}}_\nu}{1 - \hat{\mathbf{k}}_\nu \cdot \hat{\mathbf{r}}_\nu}. \tag{3.50}$$

Note that in Ω_α radius r_α is limited *a priori* (more strictly, it is allowed to grow but slower than ρ_α). That is why we cannot use an asymptotic expansion in terms of $1/\zeta_\alpha$ in the asymptotic region Ω_α. Eqs (3.45), (3.47), (3.46) and (3.49) are valid only in Ω_α, while Eqs (3.44), (3.50) and (3.48) are valid both in Ω_0 and Ω_α.

Thus we reduced a three-body problem with Coulomb interactions to a two-body problem: we need to find a solution of Eq. (3.41), which describes the relative motion of particles β and γ in the presence of the third particle α, which is far away, but it still distorts the relative motion of particles β and γ due to the long-range Coulomb interaction. This distortion results in the dependence of $\varphi^{(11)}_\alpha(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha)$ on $\boldsymbol{\rho}_\alpha$. When ρ_α increases this distortion should be weakened. Hence, $\varphi^{(11)}_\alpha(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha)$ actually depends on $1/\rho_\alpha$ and

$$\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\, \varphi^{(11)}_\alpha(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha) \sim \frac{1}{\rho^2_\alpha}. \tag{3.51}$$

Because of that we may drop the second and sixth terms in Eq. (3.41) and rewrite it in the form

$$[\frac{1}{2\mu_\alpha}\mathbf{\Delta}_{\mathbf{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}_\alpha\cdot\mathbf{\nabla}_{\mathbf{r}_\alpha} + i\,\frac{1}{M_\alpha}\,\mathbf{q}_\alpha\cdot\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha} + \frac{1}{\mu_\alpha}\sum_{\nu=\beta,\gamma}\mathbf{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(1)}_\nu(i\zeta_\nu)\cdot\mathbf{\nabla}_{\mathbf{r}_\alpha}$$
$$-V_\alpha(\mathbf{r}_\alpha) + \frac{1}{\mu_\alpha}\,\mathbf{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(1)}_\beta(i\zeta_\beta)\cdot\mathbf{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)$$
$$+\frac{1}{M_\alpha}\,\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(1)}_\beta(i\zeta_\beta)\cdot\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)]\varphi^{(11)}_\alpha(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = 0. \qquad (3.52)$$

The last two terms are of $O(1/\rho_\alpha^2)$. Note that to satisfy this equation up to terms of $O(1/\rho_\alpha^3)$ all the terms of $O(1/\rho_\alpha^2)$ must be compensated. Taking into account Eqs (3.45) and (3.47) we can rewrite Eq. (3.52) as

$$[\frac{1}{2\mu_\alpha}\,\mathbf{\Delta}_{\mathbf{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}^{(11)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{\nabla}_{\mathbf{r}_\alpha} + i\,\frac{1}{M_\alpha}\,\mathbf{q}_\alpha\cdot\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}$$
$$+\frac{1}{\mu_\alpha}\sum_{\nu=\beta,\gamma}\frac{m_\nu^2}{m_{\beta\gamma}^2}(\mathbf{r}_\alpha\cdot\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha})\,(\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}\,\ln\tilde{\mathcal{F}}^{(1)}_\nu(i\zeta_{\nu\,\alpha})\cdot\mathbf{\nabla}_{\mathbf{r}_\alpha}) - V_\alpha(\mathbf{r}_\alpha)$$
$$+(\epsilon_{\beta\,\alpha}\,\epsilon_{\gamma\,\alpha}\,\frac{1}{m_{\beta\,\gamma}} + \frac{1}{M_\alpha})\,\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}\,\ln\mathcal{F}^{(1)}_\beta(i\zeta_{\beta\,\alpha})\cdot\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}\,\ln\mathcal{F}^{(1)}_\gamma(i\zeta_{\gamma\,\alpha})]$$
$$\times\varphi^{(11)}_\alpha(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = O(1/\rho_\alpha^3). \qquad (3.53)$$

We introduced here a new local momentum

$$\mathbf{k}^{(11)}_\alpha = \mathbf{k}_\alpha - i\sum_{\nu=\beta,\gamma}\frac{m_\nu}{m_{\beta\gamma}}\,[\,\epsilon_{\nu\,\alpha}\,\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}^{(1)}_\nu(i\zeta_{\nu\,\alpha}) + i\,\eta_\nu^2\,\frac{1}{k_\nu\,\rho_\alpha^2}\,\frac{\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu}\hat{\boldsymbol{\rho}}_\alpha}{(1-\epsilon_{\alpha\nu}\hat{\mathbf{k}}_\nu\cdot\hat{\boldsymbol{\rho}}_\alpha)^2}]. \qquad (3.54)$$

Note that variables $\mathbf{\nabla}_{\mathbf{r}_\alpha}$ and $\mathbf{\nabla}_{\boldsymbol{\rho}_\alpha}$ are mixed up only in the fourth term of Eq. (3.53). We are looking for a solution in the form

$$\varphi^{(11)}_\alpha(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = \varphi^{(11)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)\,(1 + \frac{\chi(\widehat{\boldsymbol{\rho}}_\alpha)}{\rho_\alpha}) + \frac{\varphi^{(11)}_{\alpha\,(1)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)}{\rho_\alpha^2}, \qquad (3.55)$$

where $\varphi^{(11)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)$ is a solution of

$$[\frac{1}{2\mu_\alpha}\mathbf{\Delta}_{\mathbf{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}^{(11)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{\nabla}_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha)]\varphi^{(11)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = 0. \qquad (3.56)$$

$\chi(\widehat{\boldsymbol{\rho}}_\alpha) \sim O(1)$ and is a solution of the first order differential equation

$$
\begin{aligned}
& i\,\frac{1}{M_\alpha}\,\mathbf{q}_\alpha\!\cdot\!\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\frac{\chi(\widehat{\boldsymbol{\rho}}_\alpha)}{\rho_\alpha} \\
& = -(\epsilon_{\beta\,\alpha}\,\epsilon_{\gamma\,\alpha}\,\frac{1}{m_{\beta\,\gamma}} + \frac{1}{M_\alpha})\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}^{(1)}_\beta(i\zeta_{\beta\,\alpha})\!\cdot\!\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}^{(1)}_\gamma(i\zeta_{\gamma\,\alpha}). \qquad (3.57)
\end{aligned}
$$

Finally $\varphi^{(11)}_{\alpha\,(1)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) \sim O(1)$ is a solution of the inhomogemeous equation

$$
\begin{aligned}
& [\frac{1}{2\mu_\alpha}\boldsymbol{\Delta}_{\mathbf{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}^{(11)}_\alpha\!\cdot\!\boldsymbol{\nabla}_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha)]\,\varphi^{(11)}_{\alpha\,(1)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = -i\,\frac{\rho^2_\alpha}{M_\alpha}\,\mathbf{q}_\alpha\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\,\varphi^{(11)}_{\alpha\,(0)}(\mathbf{r}_\alpha) \\
& -\frac{\rho^2_\alpha}{\mu_\alpha}\sum_{\nu=\beta,\gamma}\frac{m^2_\nu}{m^2_{\beta\,\gamma}}(\mathbf{r}_\alpha\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha})\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}^{(1)}_\nu(i\zeta_{\nu\,\alpha})\!\cdot\!\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\,\varphi^{(11)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha). \qquad (3.58)
\end{aligned}
$$

Note that all the equations (3.56), (3.57) and (3.58) are ”two-body” differential equations. On the left hand side they contain gradients and Laplacians over only one of the variables, $\mathbf{r}_\alpha$ or $\boldsymbol{\rho}_\alpha$. These equations can be solved numerically.

Now we consider the second term of Eq. (3.39). It satisfies the equation

$$
\begin{aligned}
& \mathcal{F}^{(2)}_\beta(i\zeta_\beta)\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)[\frac{1}{2\mu_\alpha}\boldsymbol{\Delta}_{\mathbf{r}_\alpha} + \frac{1}{2M_\alpha}\boldsymbol{\Delta}_{\boldsymbol{\rho}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}_\alpha\!\cdot\!\boldsymbol{\nabla}_{\mathbf{r}_\alpha} + i\,\frac{1}{M_\alpha}\,\mathbf{q}_\alpha\!\cdot\!\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha} + \\
& \frac{1}{\mu_\alpha}\,[\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta) + \boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)]\!\cdot\!\boldsymbol{\nabla}_{\mathbf{r}_\alpha} \\
& +\frac{1}{M_\alpha}\,[\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta) + \boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)]\!\cdot\!\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha} - V_\alpha(\mathbf{r}_\alpha) + \\
& \frac{1}{\mu_\alpha}\,\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta)\!\cdot\!\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma) + \frac{1}{M_\alpha}\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta)\!\cdot\!\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(1)}_\gamma(i\zeta_\gamma)] \\
& \times\varphi^{(21)}_\alpha(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = O(1/\rho^3_\alpha). \qquad (3.59)
\end{aligned}
$$

Here, in the nonsingular directions ($\hat{\mathbf{k}}_\nu\cdot\hat{\mathbf{r}}_\nu \neq 1,\ \nu \neq \alpha$)

$$
\mathcal{F}^{(2)}_\nu(i\zeta_\nu) \overset{\zeta_\nu\to\infty}{=} \eta_\nu\,\frac{\Gamma(1+i\,\eta_\nu)}{\Gamma(1-i\,\eta_\nu)}\,\frac{e^{-i\,\eta_\nu\,\ln\,\zeta_\nu}}{\zeta_\nu}\,e^{i\,\zeta_\nu}\,[1+O(\frac{1}{\zeta_\nu})]. \qquad (3.60)
$$

Also, in the nonsingular directions for $\nu \neq \alpha$

$$\nabla_{\mathbf{r}_\alpha} \ln \mathcal{F}_\nu^{(2)}(i\,\zeta_\nu) = i\,\nabla_{\mathbf{r}_\alpha}\zeta_\nu + O(1/r_\nu) = i\,\frac{m_\nu}{m_{\beta\gamma}}\,k_\nu(\hat{\mathbf{k}}_\nu - \hat{\mathbf{r}}_\nu) + O(1/r_\nu) \tag{3.61}$$

$$= i\,\frac{m_\nu}{m_{\beta\gamma}}\,k_\nu\,(\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu}\,\hat{\boldsymbol{\rho}}_\alpha) + O(1/\rho_\alpha) \tag{3.62}$$

and

$$\nabla_{\boldsymbol{\rho}_\alpha} \ln \mathcal{F}_\nu^{(2)}(i\zeta_\nu) = i\nabla_{\boldsymbol{\rho}_\alpha}\zeta_\nu + O(1/r_\nu) = i\epsilon_{\nu\alpha}(-k_\nu\hat{\mathbf{r}}_\nu + \mathbf{k}_\nu) + O(1/r_\nu) \tag{3.63}$$

$$= i\,k_\nu\,(\hat{\boldsymbol{\rho}}_\alpha - \epsilon_{\alpha\nu}\hat{\mathbf{k}}_\nu) + O(1/\rho_\alpha). \tag{3.64}$$

When deriving (3.59) we took into account that

$$(\frac{1}{2\mu_\nu}\boldsymbol{\Delta}_{\mathbf{r}_\nu} + i\,\frac{1}{\mu_\nu}\,\mathbf{k}_\nu\cdot\nabla_{\mathbf{r}_\nu} - V_\nu^C)\,\mathcal{F}_\nu^{(2)}(i\zeta_\nu) = 0. \tag{3.65}$$

To get an asymptotic equation from Eq. (3.59) which is valid up to $O(1/\rho_\alpha^3)$, all the coefficients of $O(1)$, $O(1/\rho_\alpha)$ and $O(1/\rho_\alpha^2)$ should be kept in the left-hand-side of the equation. Since in the nonsingular directions in Ω_α region, $\mathcal{F}_\beta^{(2)}(i\zeta_\beta) \sim O(1/\rho_\alpha)$ only coefficients of $O(1)$ and $O(1/\rho_\alpha)$ in the brackets of Eq. (3.59) should be left. Taking into account Eqs (3.45), (3.62) and (3.64) we get

$$\begin{aligned}
&[\frac{1}{2\mu_\alpha}\,\boldsymbol{\Delta}_{\mathbf{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha)\cdot\nabla_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha)\\
&+i\,\frac{1}{\mu_\alpha}\,\frac{m_\beta^2}{m_{\beta\gamma}^2}\,k_\beta\,\frac{1}{\rho_\alpha}\,(\mathbf{r}_\alpha - \hat{\boldsymbol{\rho}}_\alpha\,(\hat{\boldsymbol{\rho}}_\alpha\cdot\mathbf{r}_\alpha))\cdot\nabla_{\mathbf{r}_\alpha} + i\,\frac{1}{M_\alpha}\,\mathbf{q}_\alpha^{(21)}\cdot\nabla_{\boldsymbol{\rho}_\alpha}\\
&-i\,\epsilon_{\alpha\beta}\,\frac{1}{m_\alpha}\,k_\beta\,(\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta}\;\hat{\boldsymbol{\rho}}_\alpha)\cdot\nabla_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta_{\gamma\alpha})]\,\varphi_\alpha^{(21)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = O(1/\rho_\alpha^2).
\end{aligned} \tag{3.66}$$

Here $\nabla_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}_\gamma^{(1)}(i\zeta_{\gamma\alpha})$ is given by Eq. (3.46). We also introduced new local momenta

$$\mathbf{k}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha + \frac{m_\beta}{m_{\beta\gamma}}\,k_\beta\,(\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta}\;\hat{\boldsymbol{\rho}}_\alpha) + i\,(i\,\eta_\beta + 1)\,\frac{m_\beta}{m_{\beta\gamma}}\,\frac{1}{\rho_\alpha}\,\frac{\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\beta}\hat{\boldsymbol{\rho}}_\alpha}{1 - \epsilon_{\alpha\beta}\hat{\mathbf{k}}_\beta\cdot\hat{\boldsymbol{\rho}}_\alpha}, \tag{3.67}$$

and

$$\mathbf{q}_\alpha^{(21)}(\boldsymbol{\rho}_\alpha) = \mathbf{q}_\alpha + k_\beta\,(\hat{\boldsymbol{\rho}}_\alpha - \epsilon_{\alpha\beta}\,\hat{\mathbf{k}}_\beta). \tag{3.68}$$

We also took into account that for $\nu \neq \sigma \neq \tau,\ \nu \neq \tau,\ \epsilon_{\nu\tau},\ \ \epsilon_{\nu\sigma} = -1$, and

$$-\epsilon_{\alpha\gamma}\,\frac{1}{m_{\beta\gamma}}\,(\hat{\mathbf{k}}_{\beta} - \epsilon_{\alpha\beta}\ \hat{\boldsymbol{\rho}}_{\alpha}) + \frac{1}{M_{\alpha}}\,(\hat{\boldsymbol{\rho}}_{\alpha} - \epsilon_{\alpha\beta}\hat{\mathbf{k}}_{\beta}) = -\epsilon_{\alpha\beta}\,\frac{1}{m_{\alpha}}\,(\hat{\mathbf{k}}_{\beta} - \epsilon_{\alpha\beta}\ \hat{\boldsymbol{\rho}}_{\alpha}). \tag{3.69}$$

We are looking for a solution of Eq. (3.67) in the form

$$\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = \varphi_{\alpha\,(0)}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) + \frac{\varphi_{\alpha\,(1)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha})}{\rho_{\alpha}}, \tag{3.70}$$

where $\varphi_{\alpha\,(0)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha})$ satisfies

$$[\frac{1}{2\mu_{\alpha}}\boldsymbol{\Delta}_{\mathbf{r}_{\alpha}} + i\,\frac{1}{\mu_{\alpha}}\,\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})\cdot\boldsymbol{\nabla}_{\mathbf{r}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})]\,\varphi_{\alpha\,(0)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha}) = 0. \tag{3.71}$$

Finally $\varphi_{\alpha\,(1)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha}) \sim O(1)$ is a solution of equation

$$\begin{aligned}
&[\frac{1}{2\mu_{\alpha}}\,\boldsymbol{\Delta}_{\mathbf{r}_{\alpha}} + i\,\frac{1}{\mu_{\alpha}}\,\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})\cdot\nabla_{\mathbf{r}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})]\varphi_{\alpha\,(1)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha})\\
&= -[i\,\frac{1}{\mu_{\alpha}}\,\frac{m_{\beta}^{2}}{m_{\beta\gamma}^{2}}\,k_{\beta}\,(\mathbf{r}_{\alpha} - \hat{\boldsymbol{\rho}}_{\alpha}\,(\hat{\boldsymbol{\rho}}_{\alpha}\cdot\mathbf{r}_{\alpha}))\cdot\nabla_{\mathbf{r}_{\alpha}}]\varphi_{\alpha\,(0)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha})\\
&-i\,\frac{\rho_{\alpha}}{M_{\alpha}}\mathbf{q}_{\alpha}^{(21)}\cdot\nabla_{\rho_{\alpha}}\varphi_{\alpha\,(0)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha})\\
&+i\,\epsilon_{\alpha\beta}\,\frac{\rho_{\alpha}}{m_{\alpha}}\,k_{\beta}\,(\hat{\mathbf{k}}_{\beta} - \epsilon_{\alpha\beta}\ \hat{\boldsymbol{\rho}}_{\alpha})\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_{\alpha}}\ln\tilde{\mathcal{F}}_{\gamma}^{(1)}(i\zeta_{\gamma\,\alpha})\varphi_{\alpha\,(0)}^{(21)}(\mathbf{r}_{\alpha},\ \boldsymbol{\rho}_{\alpha}).
\end{aligned} \tag{3.72}$$

Since in Eq. (3.72) we keep only terms of order $O(1/\rho_{\alpha})$ local momentum $\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})$ can be replaced by

$$\mathbf{k}_{\alpha(0)}^{(21)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} + \frac{m_{\beta}}{m_{\beta\gamma}}\,k_{\beta}\,(\hat{\mathbf{k}}_{\beta} - \epsilon_{\alpha\beta}\ \hat{\boldsymbol{\rho}}_{\alpha}). \tag{3.73}$$

A formal solution of Eq. (3.72) is

$$\varphi^{(21)}_{\alpha\,(1)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = \varphi^{(21)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) + e^{-\mathbf{k}^{(21)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}\int \mathrm{d}\,\mathbf{r}'_\alpha\, G(\mathbf{r}_\alpha,\,\mathbf{r}'_\alpha)\, e^{\mathbf{k}^{(21)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}'_\alpha}$$
$$[-[i\,\frac{1}{\mu_\alpha}\,\frac{m^2_\beta}{m^2_{\beta\gamma}}\,k_\beta\,(\mathbf{r}'_\alpha - \hat{\boldsymbol{\rho}}_\alpha\,(\hat{\boldsymbol{\rho}}_\alpha\cdot\mathbf{r}'_\alpha))\cdot\nabla_{\mathbf{r}_\alpha}]\varphi^{(21)}_{\alpha\,(0)}(\mathbf{r}'_\alpha,\,\boldsymbol{\rho}_\alpha)$$
$$-i\,\frac{1}{M_\alpha}\,\mathbf{q}^{(21)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\,\varphi^{(21)}_{\alpha\,(0)}(\mathbf{r}'_\alpha,\,\boldsymbol{\rho}_\alpha)$$
$$-i\,\epsilon_{\alpha\,\beta}\,\frac{1}{m_\alpha}\,k_\beta\,(\hat{\mathbf{k}}_\beta - \epsilon_{\alpha\,\beta}\;\hat{\boldsymbol{\rho}}_\alpha)\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}^{(1)}_\gamma(i\zeta'_{\gamma\,\alpha})\,\varphi^{(21)}_{\alpha\,(0)}(\mathbf{r}'_\alpha,\,\boldsymbol{\rho}_\alpha)], \qquad (3.74)$$

Here $\varphi^{(21)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)$ is the solution of the homogeneous Eq. (3.71). $G(\mathbf{r}_\alpha,\,\mathbf{r}'_\alpha)$ is Green's function describing the relative motion of particles β and γ.

The third equation for $\varphi^{(12)}_\alpha(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)$ is obtained by substituting the third term in (3.39) to (3.3). Following the same steps, which we used to derive the second equation, or just interchanging $\beta \leftrightarrow \gamma$ in (3.59) we find $\varphi^{(12)}_\alpha(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)$ in the following form:

$$\varphi^{(12)}_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \varphi^{(12)}_{\alpha\,(0)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) + \frac{\varphi^{(12)}_{\alpha\,(1)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)}{\rho_\alpha}, \qquad (3.75)$$

where $\varphi^{(12)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha)$ is a solution of

$$[\frac{1}{2\mu_\alpha}\boldsymbol{\Delta}_{\mathbf{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}^{(12)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha)]\,\varphi^{(12)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = 0. \qquad (3.76)$$

We can derive a similar equation to Eq. (3.72) for $\varphi^{(12)}_{\alpha\,(1)}(\mathbf{r}_\alpha,\,\rho_\alpha)$ which has a formal solution

$$\varphi^{(12)}_{\alpha\,(1)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) = \varphi^{(12)}_{\alpha\,(0)}(\mathbf{r}_\alpha,\,\boldsymbol{\rho}_\alpha) + e^{-\mathbf{k}^{(12)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}\int \mathrm{d}\,\mathbf{r}'_\alpha\, G(\mathbf{r}_\alpha,\,\mathbf{r}'_\alpha)\, e^{\mathbf{k}^{(12)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}'_\alpha}$$
$$[-[i\,\frac{1}{\mu_\alpha}\,\frac{m^2_\gamma}{m^2_{\beta\gamma}}\,k_\gamma\,(\mathbf{r}'_\alpha - \hat{\boldsymbol{\rho}}_\alpha\,(\hat{\boldsymbol{\rho}}_\alpha\cdot\mathbf{r}'_\alpha))\cdot\nabla_{\mathbf{r}_\alpha}]\varphi^{(12)}_{\alpha\,(0)}(\mathbf{r}'_\alpha,\,\boldsymbol{\rho}_\alpha)$$
$$-i\,\frac{1}{M_\alpha}\,\mathbf{q}^{(12)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\,\varphi^{(12)}_{\alpha\,(0)}(\mathbf{r}'_\alpha,\,\boldsymbol{\rho}_\alpha)$$
$$-i\,\epsilon_{\alpha\,\gamma}\,\frac{1}{m_\alpha}\,k_\gamma\,(\hat{\mathbf{k}}_\gamma - \epsilon_{\alpha\,\gamma}\;\hat{\boldsymbol{\rho}}_\alpha)\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\tilde{\mathcal{F}}^{(1)}_\beta(i\zeta'_{\beta\,\alpha})\,\varphi^{(12)}_{\alpha\,(0)}(\mathbf{r}'_\alpha,\,\boldsymbol{\rho}_\alpha)]. \qquad (3.77)$$

The fourth equation can be derived after substituting the last term of Eq. (3.39) into Eq. (3.3) and it is automatically satisfied up to the terms of order $O(1/{\rho_\alpha}^3)$ in Ω_α because the product $\mathcal{F}^{(2)}_\beta(i\zeta_\beta)\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma) = O(1/{\rho_\alpha}^2)$. The fourth term in Eq. (3.39) leads to an equation for $\varphi^{(22)}_\alpha(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha)$:

$$\begin{aligned}\mathcal{F}^{(2)}_\beta(i\zeta_\beta)\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma)[\frac{1}{2\mu_\alpha}\boldsymbol{\Delta}_{\mathbf{r}_\alpha} + \frac{1}{2M_\alpha}\boldsymbol{\Delta}_{\rho_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}_\alpha\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha} + i\,\frac{1}{M_\alpha}\,\mathbf{q}_\alpha\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha} \\ +\frac{1}{\mu_\alpha}\,[\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta) + \boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma)]\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha} \\ +\frac{1}{M_\alpha}\,[\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta) + \boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma)]\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha} \\ -V_\alpha(\mathbf{r}_\alpha) + \frac{1}{\mu_\alpha}\,\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta)\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha}\ln\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma) \\ +\frac{1}{M_\alpha}\,\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(2)}_\beta(i\zeta_\beta)\cdot\boldsymbol{\nabla}_{\boldsymbol{\rho}_\alpha}\ln\mathcal{F}^{(2)}_\gamma(i\zeta_\gamma)] \times \varphi^{(22)}_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = O(1/\rho^3_\alpha)\end{aligned} \tag{3.78}$$

Using the same arguments we have used before, we may drop all the terms containing derivatives over $\boldsymbol{\rho}_\alpha$ when looking for a solution in leading order. Then the equation for $\varphi^{(22)}_\alpha$ reduces to

$$[\frac{1}{2\mu_\alpha}\boldsymbol{\Delta}_{\mathbf{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\mathbf{k}^{(22)}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\boldsymbol{\nabla}_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha)]\,\varphi^{(22)}_\alpha(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha) = 0, \tag{3.79}$$

with a local momentum

$$\mathbf{k}^{(22)}_\alpha(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha + \sum_{\nu=\beta,\gamma}\frac{m_\nu}{m_{\beta\gamma}}\,k_\nu\,(\hat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu}\,\hat{\boldsymbol{\rho}}_\alpha). \tag{3.80}$$

If V_α is a pure Coulomb potential, $V_\alpha = V^C_\alpha$, then Eqs (3.56), (3.71), (3.76), (3.79) have the following solution

$$\varphi^{(ij)}_\alpha(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha) = N^{(ij)}_\alpha(\,\boldsymbol{\rho}_\alpha)F(-i\eta^{(ij)}_\alpha(\,\boldsymbol{\rho}_\alpha), 1; i\zeta^{(ij)}(\,\boldsymbol{\rho}_\alpha)), \tag{3.81}$$

Here, $i = 1, 2$; $j = 1, 2$ and $N^{(ij)}_\alpha(\,\boldsymbol{\rho}_\alpha)$ is defined as

$$N^{(ij)}_\alpha(\,\boldsymbol{\rho}_\alpha) = e^{-\pi\eta^{(ij)}_\alpha(\,\boldsymbol{\rho}_\alpha)/2}\Gamma(1 + i\eta^{(ij)}_\alpha(\,\boldsymbol{\rho}_\alpha)), \tag{3.82}$$

where $\eta_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha) = \frac{z_\beta z_\gamma e^2 \mu_\alpha}{k_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha)}$, and $\zeta^{(ij)}(\boldsymbol{\rho}_\alpha) = k_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha) r_\alpha - \mathbf{k}_\alpha^{(ij)}(\boldsymbol{\rho}_\alpha) \cdot \mathbf{r}_\alpha$.

If V_α is not a pure Coulomb potential, then the differential equations above, which parametrically depend on $\boldsymbol{\rho}_\alpha$, should be solved numerically. Since all equations are of the two-body type, numerical methods are well developed and have been in use for a long time. They can be applied to solve the differential equations above as well. All the solutions found this way are valid in all directions of the asymptotic region Ω_α except for singular directions.

Thus, returning to Eq. (3.39) we can claim that, after derivation of all four wave functions $\varphi_{\alpha\,(1)}^{(ij)}(\mathbf{r}_\alpha,\, \rho_\alpha)$, i, j $= 1, 2$, we know the asymptotic solution of the three-body scattering wave function up to terms $O(1/\rho_\alpha^3)$. This asymptotic solution represents the incident three-body wave of the scattering wave function of the first type.

D. Generalized asymptotic scattering wave function valid in all regions Ω_ν, where $\nu = \alpha,\, \beta,\, \gamma$

Now we are in position to present a generalized asymptotic scattering wave function which satisfies the Schrödinger equation up to second order and which is valid in all the asymptotic regions:

$$\Psi_{\mathbf{k}_\alpha \mathbf{q}_\alpha}^{(\alpha\beta\gamma)(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \equiv e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} \varphi_{\widetilde{\mathbf{k}}_\alpha}(\mathbf{r}_\alpha) \varphi_{\widetilde{\mathbf{k}}_\beta}(\mathbf{r}_\beta) \varphi_{\widetilde{\mathbf{k}}_\gamma}(\mathbf{r}_\gamma). \tag{3.83}$$

After substituting (3.83) into (3.3) and dropping the higher order terms we get,

$$\{E - T_{\mathbf{r}_\alpha} - T_{\vec{\rho}_\alpha} - V\}[e^{i\mathbf{k}_\alpha\cdot\vec{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\varphi_{\widetilde{\mathbf{k}}_\alpha}(\mathbf{r}_\alpha)\varphi_{\widetilde{\mathbf{k}}_\beta}(\mathbf{r}_\beta)\varphi_{\widetilde{\mathbf{k}}_\gamma}(\mathbf{r}_\gamma)]$$

$$= e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\varphi_{\widetilde{\mathbf{k}}_\alpha}(\mathbf{r}_\alpha)\varphi_{\widetilde{\mathbf{k}}_\gamma}(\mathbf{r}_\gamma)[\frac{\triangle_{\mathbf{r}_\alpha}}{2\mu_\alpha} + \frac{i\widetilde{\mathbf{k}}_\alpha\cdot\nabla_{\mathbf{r}_\alpha}}{\mu_\alpha} - V_\alpha]\varphi_{\widetilde{\mathbf{k}}_\alpha}(\mathbf{r}_\alpha) \quad (3.84)$$

$$+ e^{i\mathbf{k}_\beta\cdot\mathbf{r}_\beta + i\mathbf{q}_\beta\cdot\boldsymbol{\rho}_\beta}\varphi_{\widetilde{\mathbf{k}}_\alpha}(\mathbf{r}_\alpha)\varphi_{\widetilde{\mathbf{k}}_\gamma}(\mathbf{r}_\gamma)[\frac{\triangle_{\mathbf{r}_\beta}}{2\mu_\beta} + \frac{i\widetilde{\mathbf{k}}_\beta\cdot\nabla_{\mathbf{r}_\beta}}{\mu_\beta} - V_\beta]\varphi_{\widetilde{\mathbf{k}}_\beta}(\mathbf{r}_\beta)$$

$$+ e^{i\mathbf{k}_\gamma\cdot\mathbf{r}_\gamma + i\mathbf{q}_\gamma\cdot\boldsymbol{\rho}_\gamma}\varphi_{\widetilde{\mathbf{k}}_\alpha}(\mathbf{r}_\alpha)\varphi_{\widetilde{\mathbf{k}}_\beta}(\mathbf{r}_\beta)[\frac{\triangle_{\mathbf{r}_\gamma}}{2\mu_\gamma} + \frac{i\widetilde{\mathbf{k}}_\gamma\cdot\nabla_{\mathbf{r}_\gamma}}{\mu_\gamma} - V_\gamma]\varphi_{\widetilde{\mathbf{k}}_\gamma}(\mathbf{r}_\gamma)$$

$$= \begin{cases} O(\frac{1}{r_\alpha^2}, \frac{1}{r_\beta^2}, \frac{1}{r_\gamma^2}),\ \mathbf{r}_\alpha, \mathbf{r}_\beta, \mathbf{r}_\gamma \in \Omega_0 \\ O(\frac{1}{r_\beta^2}, \frac{1}{r_\gamma^2}),\ \mathbf{r}_\beta, \mathbf{r}_\gamma \in \Omega_\alpha \\ O(\frac{1}{r_\alpha^2}, \frac{1}{r_\gamma^2}),\ \mathbf{r}_\alpha, \mathbf{r}_\gamma \in \Omega_\beta \\ O(\frac{1}{r_\alpha^2}, \frac{1}{r_\beta^2}),\ \mathbf{r}_\alpha, \mathbf{r}_\beta \in \Omega_\gamma \end{cases}, \quad (3.85)$$

where the local momentum is given by

$$\widetilde{\mathbf{k}}_\nu = \mathbf{k}_\nu - i\sum_{\tau=\alpha,\beta,\gamma}(1 - \delta_{\nu,\tau})\nabla_{\mathbf{r}_\nu}\ln\varphi_{\widetilde{\mathbf{k}}_\tau}. \quad (3.86)$$

In the asymptotic region Ω_0, each local momentum, $\widetilde{\mathbf{k}}_\nu$, can be replaced by the corresponding asymptotic momentum, $\mathbf{k}_\nu$. In the asymptotic region Ω_α, Eq. (3.85) reduces to the quasi-two-particle differential equation:

$$[\frac{\triangle_{\mathbf{r}_\alpha}}{2\mu_\alpha} + \frac{i\widetilde{\mathbf{k}}_\alpha\cdot\nabla_{\mathbf{r}_\alpha}}{\mu_\alpha} - V_\alpha]\varphi_{\widetilde{\mathbf{k}}_\alpha}(\mathbf{r}_\alpha) = O(\frac{1}{r_\beta}, \frac{1}{r_\gamma}). \quad (3.87)$$

The solution of this equation is evident and provides the Coulomb-nuclear scattering wave function with the local momentum $\widetilde{\mathbf{k}}_\alpha$. Similarly we can get the asymptotic solution in leading order in the other two asymptotic regions Ω_β and Ω_γ.

E. Conclusion

In this chapter we derived the three-body asymptotic incident wave, which satisfies the Schrödinger equation up to terms of order $1/\rho_\nu^3$ in the asymptotic region Ω_ν, $\nu = \alpha,\, \beta,\, \gamma$. This asymptotic incident wave gives the leading asymptotic terms of the three-body scattering wave function of the first type and is an extention of the asymptotic wave function derived in [16, 17]. It is worth mentioning that the asymptotic solution satisfying the Schrödinger equation in the asymptotic region Ω_ν up to the $O(1/\rho_\nu^2)$ can be found analytically [16, 17]. To find an asymptotic solution satisfying the Schrödinger equation in Ω_ν up to terms of $O(1/\rho_\nu^3)$ we need to solve two-body type differential equations numerically. The next order term in the asymptotic three-body scattering wave function represents the outgoing 3 *particles* $\rightarrow$ 3 *particles* scattered wave and can be found only by a numerical solution of the three-body Schrödinger equation or Faddeev equations.

The resulting asymptotic solution provides extended boundary conditions in all the asymptotic regions and can be used in the direct numerical solution of the Schrödinger equation or in practical calculations as a leading asymptotic term of the three-body scattering wave function.

CHAPTER IV

ASYMPTOTIC BEHAVIOR OF THE THREE-BODY SCATTERED WAVE FOR THREE CHARGED PARTICLES *

A. Introduction

In the previous chapter we derived the leading asymptotic terms of the three-body Coulomb scattering wave function of the first type. These terms actually represent the leading asymptotic terms of the three-body Coulomb distorted incident wave and are valid in all four asymptotic regions. As has been indicated in Chapters I and II, there is a second type of three-body Coulomb scattering wave functions which are evolved from the two-body incident wave. These wave functions are orthogonal to the scattering wave functions of the first type and correspond to the three branches of the energy spectrum. Each of these branches begins from the $-\epsilon_\nu$, $\nu = \alpha,\, \beta,\, \gamma$, where ϵ_ν is the ground-state binding energy of the pair ν. Knowledge of the asymptotic behavior of the scattering wave functions of the second type is extremely important for a solution of the three-body problem with the Coulomb interaction and correct formulation of the breakup reaction theory in the presence of the Coulomb interactions, especially taking into account the progress in high-performance computing. In particular, the most advanced computers allow for a direct numerical solution of the Schrödinger equation [18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31]. This method has emerged as a powerful technique to analyze scattering processes with three charged particles.

However, such methods require knowledge of the asymptotic behaviour of the scattered wave function corresponding to the proccess of 2 *particles* $\rightarrow$ 3 *particles* in all asymptotic regions of the configuration space. This is because the asymptotic wave functions are used directly as boundary conditions in solving the differential Schrödinger equation or Faddeev type equations, or for extracting the scattering amplitudes from integral expressions involving the full scattering wave function. Below the three-body breakup threshold when only two-cluster channels are open, there is no difficulty with the application of the aforementioned approaches in combination with some additional, but reasonable, approximation schemes. However, it should be emphasised that attempts to follow exact algorithms have thus far limited these approaches to essentially model problems [32, 33, 34, 35, 36, 37, 38]. To get a unique solution to the Schrödinger's equation above the breakup threshold, one must impose the boundary conditions in the regions where all three particles are "asymptotically free". The most studied system of this type is that of electron-hydrogen scattering. No success has been achieved in the analysis of nuclear breakup processes for charged particles. The methods mentioned above provide an accurate three-body scattering wave function in an "internal" region in coordinate space and the ionization amplitude is extracted by matching to ionization boundary conditions in the asymptotic region. In each method, the extraction process relies on *approximate* ionization boundary conditions. For example, in the close-coupled-channel (CCC) method [39, 40], the ionization flux is initially obtained by discretizing the target continuum. The ionization amplitude is then constructed by means of a renormalization of the square-integrable positive-energy target states with the true target continuum. Implicit in this approach is the representation of the three-body continuum states as a product of plane and Coulomb waves without electron-electron correlation. In the T-matrix [19], R-matrix [24], and exterior complex scaling (ECS) [26] methods, an integral representation of the ionization amplitude is used but again the three-body continuum states are approximated, this time by a product of two fixed-charge Coulomb waves for the two free electrons. This yields an ionization amplitude with a divergent phase as a function of matching radius, although the magnitude of the amplitude converges. Thus, due to the necessity to eventually calculate the flux at infinity, none of these methods can really avoid the asymptotic form of the scattered wave, rather they approximate it. Despite some success of these practical approaches in providing accurate electron-hydrogen ionization cross sections, a formal theory of breakup with charged particles remains incomplete. The formal theory given over thirty years ago [8, 41, 42] is still considered the state of the art. The first and the only attempt to solve the Schrödinger equation for electron-impact ionization of hydrogen by directly matching to exact ionization boundary conditions is limited to the S-wave model [43]. Though an asymptotic form of the scattered wave for electron-impact ionization of hydrogen for the case when all interparticle distances are large was obtained by Peterkop [44, 45, 46] four decades ago, it has not been successfully implemented in the approaches mentioned above.

One reason is that a direct numerical solution of the Schrödinger equation for the full hydrogen-ionization problem requires a partial-wave analysis of the asymptotic wave function and a suitable partial-wave decomposition of the Peterkop wave function does not exist. The problem with the partial-wave decomposition is that Peterkop's asymptotic wave function is invalid when the two electrons are close to each other. In the general case any extension of the Peterkop wave function will be invalid in the asymptotic regions Ω_ν, where two particles are close to each other and far away from the third particle. Thus, for full-scale numerical calculations a representation of the wave function describing breakup/ionization in all the asymptotic regions is necessary.

In addition, Peterkop used six-dimensional hyperspherical coordinates which effectively transform the Schrödinger equation describing the development of the system into the Hamilton-Jacobi type equation as the asymptotic motion of the particles becomes classical. For this reason, the Peterkop asymptotic wave suffers from an amplitude-phase ambiguity problem, since some part of the hyperspherical ionization amplitude can be moved to the phase factor and the resulting wavefunction is still a solution to the original Hamilton-Jacobi equation [8]. Accordingly, the remainder amplitude can equally well be called an ionization amplitude. Thus, generally speaking, the hyperspherical approach is not capable of uniquely identifying the ionization amplitude. This amplitude-phase ambiguity has caused problems in the formal theory of breakup at a very fundamental level.

Finally, a full knowledge of the asymptotic behavior of the scattered wave forms the basis for the Kohn variational approach to breakup scattering [47, 48, 49, 50, 51]. Due to the absence of the asymptotic wave function for breakup scattering of three charged particles, the validity of the variational approach to such processes was shown [6, 7] only in the region Ω_0 where distances between all particles are large. For the case of proton-deuteron breakup, for example, the validity of the variational principle is yet to be proven when all three particles in the final state are in the continuum but the neutron is close to one of the protons and the other proton is far away. Therefore, in order for the recent Kohn variational proton-deuteron scattering calculations [50, 51] to be extended to calculations of the deuteron breakup amplitude, an unambiguous asymptotic form of the total scattered wave is necessary. In this case it is expected that the proton, which is far away, distorts the relative motion of the other proton and neutron due to the long range Coulomb interaction between the protons. Thus the knowledge of the asymptotic behavior of the three-body scattered wave in all regions of the configuration space is crucial in calculations of atomic and nuclear breakup processes.

In Ref. [52] a relationship between the total wave function describing ionization in the electron-hydrogen system and the one representing scattering of three particles of the system in the continuum was established. On the basis of this relationship, forms for the scattered wave for breakup/ ionization valid in all asymptotic domains relevant to ionization were obtained and the amplitude-phase ambiguity of the Peterkop wave function was resolved [53]. This removed the above-mentioned problems in practical calculations and made the correct extraction of observables possible.

The aim of this chapter is to derive the asymptotic three-body scattered wave in the asymptotic regions Ω_ν, where two particles are close to each other and far away from the third particle for an arbitrary system of three charged particles. The asymptotic wave obtained here should match smoothly with the Peterkop asymptotic wave in the asymptotic region Ω_0 in the case of electron-hydrogen ionization. To derive the asymptotic three-body scattered wave we applied the Green's function formalism [54]. Introducing the spectral decomposition of the three-body Green's function we can connect the first and second type scattering wave functions. A similar technique is applied to obtain asymptotic forms of the three-body Coulomb Green's function. The latter are important in the formulation of the three-body problem [55, 56]. Asymptotic forms of the three-particle Green's function also play a central role, for instance, when calculating the optical potentials [16, 57, 58] and the non-perturbative calculations of the dynamical dipole polarization terms [59]. Spectral decomposition of the Green's function also is given in [3]. The Green's function formalism allows us to resolve the phase-amplitude ambiguity, which has been an unresolved problem in the Peterkop approach.

The Chapter is set out as follows. In Sec. B we give a relationship between the total wave function of a breakup process in two-cluster collisions taking place in an arbitrary three charged particles system and the wave function of the process of scattering of all three particles of the system in the continuum. Calculations of asymptotic forms of the scattered wave based on this relationship will be presented in Sec. C. Asymptotic forms of the three-body Green's function are given in Sec. D. Finally, in Sec. E we summarize the results of the present work and discuss their possible applications.

B. Derivation of the intergral representation of the scattering wave in a Coulomb three body system

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 Jacobian variables: $\boldsymbol{r}_\alpha$ 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 c.m. 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 $\beta, \gamma = 1, 2, 3$, and $\alpha \neq \beta \neq \gamma$.
For further reference we note that

$$\boldsymbol{r}_\nu = -\frac{m_\nu}{m_{\beta\gamma}}\boldsymbol{r}_\alpha - \epsilon_{\nu\alpha}\boldsymbol{\rho}_\alpha \ , \qquad \boldsymbol{\rho}_\nu = \epsilon_{\nu\alpha}\frac{\mu_\nu}{M_\alpha}\boldsymbol{r}_\alpha - \frac{m_\alpha}{M - m_\nu}\boldsymbol{\rho}_\alpha \tag{4.1}$$

and

$$\boldsymbol{k}_\nu = -\frac{m_\alpha}{M - m_\nu}\boldsymbol{k}_\alpha - \epsilon_{\nu\alpha}\frac{\mu_\alpha}{M_\nu}\boldsymbol{q}_\alpha \ , \qquad \boldsymbol{q}_\nu = \epsilon_{\nu\alpha}\boldsymbol{k}_\alpha - \frac{m_\nu}{m_{\beta\gamma}}\boldsymbol{q}_\alpha, \tag{4.2}$$

Consider a scattering of particle α with incident momentum $\boldsymbol{q}_i$ off a bound pair (β, γ) in the initial ground state $\phi_0(\boldsymbol{r}_\alpha)$ with a bound state energy $E_{0_\alpha} = -\epsilon_\alpha$. Assume that the energy of the projectile $q_i^2/2M_\alpha$ is enough to break up the target. The total three-body wave function describing this process satisfies the Schrödinger equation

$$(E - H)\Psi^{(+)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \tag{4.3}$$

where $H = -\Delta_{\boldsymbol{r}_\alpha}/2\mu_\alpha - \Delta_{\boldsymbol{\rho}_\alpha}/2M_\alpha + V_\alpha + V_\beta + V_\gamma$ is the three-body Hamiltonian and $E = E_{0_\alpha} + q_i^2/2M_\alpha = k_\alpha^2/2\mu_\alpha + q_\alpha^2/2M_\alpha$ is the total energy of the system.

$$V_\alpha = V_\alpha^C + V_\alpha^S, \qquad V_\alpha^C = \frac{z_\beta z_\gamma}{r_\alpha}, \tag{4.4}$$

V_α^C (V_α^S) is the Coulomb (short-range) interaction between particles β and γ. The wave function $\Psi^{(+)}$ consists of the incoming initial-channel wave $\Phi^{(i)}$ and outgoing scattered wave $\Phi^{(\mathrm{sc})(+)}$:

$$\Psi^{(+)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = \Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) + \Phi^{(\mathrm{sc})(+)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{4.5}$$

where $\Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha)$ is separable and is given by

$$\Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = \chi_{\boldsymbol{q}_i}(\boldsymbol{\rho}_\alpha)\phi_0(\boldsymbol{r}_\alpha) \tag{4.6}$$

With Eq. (4.5) the Schrödinger equation Eq. (4.3) can be rewritten as

$$(E - H)\Phi^{(\mathrm{sc})(+)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = \overline{V}_\alpha \Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{4.7}$$

where $\overline{V}_\alpha = V_\beta + V_\gamma$ is the interaction of the projectile particle with the target particles. Then applying the three-body Green's function $G^+ = (E - H + i0)^{-1}$ to both sides of Eq. (4.7) we get

$$\Phi^{(\mathrm{sc})(+)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = \int d\boldsymbol{r}'_\alpha d\boldsymbol{\rho}'_\alpha G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0)\overline{V}_\alpha \Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha). \tag{4.8}$$

Next we apply a spectral decomposition for the Green's function. To this end we consider another scattering process within the same three-body system but one where all three particles in the initial channel are in the continuum (the so called, $3 \to 3$ scattering as opposed to $2 \to 3$ breakup scattering in two-cluster collisions). We take the boundary condition for the wave function $\Psi^{(-)}$ describing this process in the form of a Coulomb-distorted three-body plane wave and incoming scattered wave. This wave function is also an eigenstate of the same Hamiltonian H, i.e.

$$(E - H)\Psi^{(-)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0. \tag{4.9}$$

Therefore, it is well suited for our purposes.

$$G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0) = \int \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3} \frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3} \frac{\Psi^{(-)}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha)\, \Psi^{(-)*}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0}$$
$$+ \sum_{\nu=\beta,\gamma} \int \frac{d\boldsymbol{q}'_{i,\nu}}{(2\pi)^3} \frac{\Psi^{(-)}_{\boldsymbol{q}'_{i,\nu}}(\boldsymbol{r}_\nu, \boldsymbol{\rho}_\nu)\Psi^{(-)*}_{\boldsymbol{q}'_{i,\nu}}(\boldsymbol{r}'_\nu, \boldsymbol{\rho}'_\nu)}{E - E_{0_\nu} - q'^2_{i,\nu}/2M_\nu + i0} + \cdots\,, \tag{4.10}$$

As will become clear below, the reason for choosing this form of the total wave function as the basis for the decomposition rather than $\Psi^{(+)}$, which consists of the Coulomb-distorted three-body plane wave and outgoing scattered wave, is twofold. First, $\Psi^{(+)}$ would eventually lead to the incoming scattered wave $\Phi^{(\mathrm{sc})(-)}$ instead of the outgoing $\Phi^{(\mathrm{sc})(+)}$ which is inconsistent with the scattering boundary condition Eq. (4.5). Second, we are not able to introduce the breakup amplitude in a standard form using $\Psi^{(+)}$.

Thus by using the spectral decomposition for the three-body Green's function $G^{(+)}$ in Eq. (4.8) in terms of the three-body scattering wave functions $\Psi^{(-)}$, we arrive at

$$\begin{aligned}\Phi^{(\mathrm{sc})+}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \;=\; & \int d\boldsymbol{r}'_\alpha d\boldsymbol{\rho}'_\alpha \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3} \frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3} \frac{\Psi^{(-)}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha)\, \Psi^{(-)*}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0} \overline{V}_\alpha \Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha) \\ & + \sum_{\nu=\beta,\gamma} \int d\boldsymbol{r}'_\alpha d\boldsymbol{\rho}'_\alpha \frac{d\boldsymbol{q}'_{i,\nu}}{(2\pi)^3} \frac{\Psi^{(-)}_{\boldsymbol{q}'_{i,\nu}}(\boldsymbol{r}_\nu, \boldsymbol{\rho}_\nu)\Psi^{(-)*}_{\boldsymbol{q}'_{i,\nu}}(\boldsymbol{r}'_\nu, \boldsymbol{\rho}'_\nu)}{E - E_{0_\nu} - q'^2_{i,\nu}/2M_\nu + i0} \\ & \times \overline{V}_\alpha \Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha) + \cdots\,. \end{aligned} \tag{4.11}$$

Here $\Psi^{(-)}_{\boldsymbol{q}_{i,\nu}}(\boldsymbol{r}_\nu, \boldsymbol{\rho}_\nu)$ is a wave function of a two cluster channel $\nu = \beta,\ \gamma$, where particles in the ν pair are bound in a ground state with energy E_{0_ν} and particle ν is travelling free with momentum $\boldsymbol{q}_{i,\nu}$. The dots indicate that all other contributions, such as excitations are not shown explicitly. These contributions represent all possible three-body bound states of the Hamiltonian H and the two-cluster-channels. The latter case will be discussed later on.

Defining an amplitude for the breakup $\alpha + (\beta, \gamma) \to \alpha + \beta + \gamma$ and

$$\mathcal{M}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha; \boldsymbol{q}_i} = \int d\boldsymbol{r}_\alpha d\boldsymbol{\rho}_\alpha \Psi^{(-)*}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \overline{V}_\alpha \Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{4.12}$$

and an amplitude for particle transfer

$$\mathcal{M}_{\boldsymbol{q}_{i,\nu}; \boldsymbol{q}_i} = \int d\boldsymbol{r}_\alpha d\boldsymbol{\rho}_\alpha \Psi^{(-)*}_{\boldsymbol{q}_{i,\nu}}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \overline{V}_\alpha \Phi^{(i)}_{\boldsymbol{q}_i}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{4.13}$$

we rewrite Eq. (4.11) in the form leaving only the scattered wave for the breakup

$$\Phi^{(\mathrm{sc})(+)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) = \int \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3} \frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3} \frac{\mathcal{M}_{\boldsymbol{k}'_\alpha, \boldsymbol{q}'_\alpha; \boldsymbol{q}_i} \Psi^{(-)}_{\boldsymbol{k}'_\alpha, \boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0} + \cdots . \tag{4.14}$$

We shall show in the Chapter V that Eq. (4.12) is the desired breakup amplitude. Eq. (4.14) establishes a relationship between the scattered part of the total wave functions of the second type, which describes any $2 \to 3$ breakup process in a three charged-particle system, and the scattering wave function of the first type, which describes the $3 \to 3$ process for scattering with all three particles of the system in the continuum, through the corresponding breakup amplitude. We introduce the following notations for asymptotic forms of $\Phi^{(\mathrm{sc})(+)}$ and $\Psi^{(-)}$ in $\Omega_\nu, \nu = 0, \alpha$:

$$\Phi^{(\mathrm{sc})(+)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \xrightarrow{\Omega_\nu} \Phi^{(sc,\nu)(+)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{4.15}$$

$$\Psi^{(-)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha) \xrightarrow{\Omega_\nu} \Psi^{(\nu)(-)}_{\boldsymbol{k}_\alpha, \boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha), \tag{4.16}$$

Since in the Ω_0 domain all components of $\Psi^{(-)}$ involving two-body and three-body bound states have an exponentially decreasing contribution, all the contribution to $\Phi^{(\mathrm{sc})(+)}$ comes from the continuum part of $\Psi^{(-)}$. Therefore, we get from Eq. (4.14) a fundamental asymptotic relationship

$$\Phi^{(sc,0)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = \int \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3}\frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3}\frac{\mathcal{M}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha;\boldsymbol{q}_i}\Psi^{(0)(-)}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0}. \tag{4.17}$$

Here, $\Psi^{(0)(-)}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)$ is the Redmond asymptotic wave function in Ω_0 given by Eq. (2.10). Let us turn now to the case when particles β and γ remain close to each other. All components of $\Psi^{(-)}$ involving three-particle bound states and two-cluster states with non-α partition decrease exponentially in the Ω_α domain as well. Thus one can write from Eq. (4.14) another asymptotic relationship

$$\Phi^{(sc,\alpha)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = \int \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3}\frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3}\frac{\mathcal{M}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha;\boldsymbol{q}_i}\Psi^{(\alpha)(-)}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0}. \tag{4.18}$$

Different approximate relationships resembling Eq. (4.18) have been in use, e.g., in the close-coupling formalism, for a long time. However, we emphasise that Eqs. (4.17) and (4.18) are exact.

C. Asymptotic forms of the scattered wave for the breakup channel

1. Asymptotic scattered wave in Ω_0 region

In this section we investigate the asymptotic behavior of the scattered wave $\Phi^{(\mathrm{sc})(+)}$ for a system of three arbitrary charged particles and calculate its leading-order terms in Ω_0 and Ω_α based on the relationships (4.17) and (4.18). Below we refer to asymptotic wave functions $\Phi^{(sc,\nu)(+)}$ and $\Psi^{(\nu)(-)}$, $\nu = 0, \alpha$, to denote the leading order terms of the relevant wave functions.

To this end we need leading-order asymptotic terms of $\Psi^{(-)}$. For Ω_0 in non-singular directions ($\hat{\boldsymbol{k}}_\nu \cdot \hat{\boldsymbol{r}}_\nu \neq -1,\ \nu = \alpha, \beta, \gamma$) this term is the Redmond asymptotic three-body Coulomb distorted plane wave given by Eq. (2.10). For Ω_α the leading asymptotic terms were obtained in [16]:

$$\Psi^{(\alpha)(-)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha + i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\varphi_{\widetilde{\boldsymbol{k}}_\alpha}(\boldsymbol{r}_\alpha)\prod_{\nu=\beta,\gamma} e^{-i\eta_\nu \ln\zeta(\boldsymbol{k}_\nu,\boldsymbol{r}_\nu)}. \tag{4.19}$$

The wave function $\varphi_{\widetilde{\boldsymbol{k}}_\alpha}(\boldsymbol{r}_\alpha)$ satisfies the equation

$$\left[\frac{1}{2\mu_\alpha}\Delta_{\boldsymbol{r}_\alpha} + i\,\frac{1}{\mu_\alpha}\,\widetilde{\boldsymbol{k}}_\alpha\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_\alpha} - V_\alpha\right]\varphi_{\widetilde{\boldsymbol{k}}_\alpha}(\boldsymbol{r}_\alpha) = 0 \tag{4.20}$$

with the incoming-wave boundary condition and describes the relative motion of particles β and γ, interacting via the potential given by the sum of the Coulomb and short-range potentials $V_\alpha = V_\alpha^C + V_\alpha^S$. If V_α is pure Coulomb potential, $V_\alpha = V_\alpha^C$, then $\varphi_{\widetilde{\boldsymbol{k}}_\alpha}(\boldsymbol{r}_\alpha)$ is given by

$$\varphi_{\widetilde{\boldsymbol{k}}_\alpha}(\boldsymbol{r}_\alpha) \;=\; \Gamma(1-i\widetilde{\eta}_\alpha)\exp(-\pi\widetilde{\eta}_\alpha/2)\,{}_1F_1(i\widetilde{\eta}_\alpha,1;-i\zeta(\widetilde{\boldsymbol{k}}_\alpha,\boldsymbol{r}_\alpha)), \tag{4.21}$$

$$\widetilde{\eta}_\alpha = \frac{z_\beta z_\gamma \mu_\alpha}{\widetilde{k}_\alpha}, \tag{4.22}$$

where ${}_1F_1$ is the confluent hypergeometric function. The relative local momentum $\widetilde{\boldsymbol{k}}_\alpha$ of particles β and γ in the Coulomb field of the third particle is given by

$$\widetilde{\boldsymbol{k}}_\alpha = \boldsymbol{k}_\alpha + \sum_{\nu=\beta,\gamma}\frac{m_\nu}{m_{\beta\gamma}}\eta_\nu\frac{\hat{\boldsymbol{k}}_\nu + \hat{\boldsymbol{r}}_\nu}{1+\hat{\boldsymbol{k}}_\nu\cdot\hat{\boldsymbol{r}}_\nu}\frac{1}{r_\nu}. \tag{4.23}$$

Thus, the relative motion of particles β and γ is correlated by particle α at infinity due to the long-range nature of the Coulomb interaction. The importance of this three-body effect was first demonstrated [52] in the case of electron-impact ionization. The effect provided a consistency in the underlying scattering theory, for instance, when two electrons are close to each other. When $\Omega_\alpha \to \Omega_0$ the function (4.19) smoothly transforms to the Redmond function as the local corrections in momentum $\widetilde{\boldsymbol{k}}_\alpha$ become negligible. All second-order terms of $\Psi^{(-)}$ in Ω_α have been found by [17]. However, as we are interested here in the main leading-order terms of the scattered wave, the wave function derived in Ref. [16] is sufficient for our purposes.

Let us proceed now to the asymptotic behavior of the scattered wave $\Phi^{(\mathrm{sc})(+)}$. The standard procedure, due to Peterkop [44, 45], is to write Eq. (4.3) in 6-dimensional hyperspherical coordinates. Then in Ω_0 the Schrödinger equation (4.3) transforms into a Hamilton-Jacobi type equation as the motion of the particles becomes classical. The Peterkop wave function was originally given for the case of two light particles in the Coulomb field of an infinitely heavy third particle. For further reference here we give a similar wave function for the case of three arbitrary Coulomb particles. Thus, following Peterkop's procedure, we get, in leading order,

$$\Phi^{(sc,0)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = A(\widehat{\omega})R^{-5/2}e^{i\kappa R - i\lambda_0 \ln(2\kappa R)}, \tag{4.24}$$

where

$$R = \left(\frac{\mu_\alpha}{m} r_\alpha^2 + \frac{M_\alpha}{m}\rho_\alpha^2\right)^{1/2} \tag{4.25}$$

is a hyperradius, m is an arbitrary mass constant introduced for convenience so that the hyperradius has units of length[2], which can be chosen as $m = \sqrt{\mu_\nu M_\nu}$, $\widehat{\omega} = (\widehat{\boldsymbol{r}}_\alpha, \widehat{\boldsymbol{\rho}}_\alpha, \phi_\alpha)$ is a 5-dimensional hyperangle, with

$$\phi_\alpha = \arctan\left[\left(\frac{\mu_\alpha}{M_\alpha}\right)^{1/2}\frac{r_\alpha}{\rho_\alpha}\right], \quad 0 \le \phi_\alpha \le \pi/2, \tag{4.26}$$

$\kappa = (2mE)^{1/2}$ and the Coulomb parameter λ_0 is given by

$$\lambda_0 = \sum_{\nu=\alpha,\beta,\gamma} \eta_\nu. \tag{4.27}$$

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

$A(\widehat{\omega})$ is the breakup amplitude. From Eq. (5.7) Note that hyperangles ϕ_ν, $\nu = \beta, \gamma$ are related to ϕ_α as

$$\sin\phi_\nu = \left[\frac{\mu_\nu}{M_\alpha}\cos^2\phi_\alpha + \frac{m_\nu^2}{m_{\beta\gamma}^2}\frac{\mu_\nu}{\mu_\alpha}\sin^2\phi_\alpha + \epsilon_{\nu\alpha}\frac{\mu_\nu m_\nu}{m_{\beta\gamma}\sqrt{\mu_\alpha M_\alpha}}\sin 2\phi_\alpha \widehat{r}_\alpha \cdot \widehat{\rho}_\alpha\right]^{1/2}. \quad (4.28)$$

Eq. (4.27) explicitly shows that the generalized Peterkop wave function given by Eq. (4.24) is not valid in the regions where $\phi_\nu \to 0$, i.e. when any two particles of the system are close to each other and far from the third one. The main drawback of the Peterkop asymptotic form, however, is that there exists an amplitude-phase ambiguity problem, i.e. some part of $A(\widehat{\omega})$ can be moved to the phase factor and the resulting wave function is still a solution to the original Hamilton-Jacobi equation [8]. Accordingly, the remainder $A'(\widehat{\omega})$ can equally well be called a breakup amplitude. Thus, generally speaking, the hyperspherical approach is not capable of uniquely identifying the breakup amplitude. Our approach will enable us to fix this problem, unambiguously, relating the 'hyperspherical' definition of the breakup amplitude to its standard quantum-mechanical one given by Eq. (4.12).

Let us now calculate the same wave function $\Phi^{(sc,0)(+)}$ using the relationship (4.17) and noting the leading-order asymptotic term given in Eq. (2.10)). Using the asymptotic forms makes it possible to evaluate Eq. (4.17). To this end we consider first the integral over $\boldsymbol{k}'_\alpha$:

$$I_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha, \boldsymbol{q}'_\alpha) = \int \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3}\frac{\mathcal{M}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha;\boldsymbol{q}_i} e^{i\boldsymbol{k}'_\alpha \boldsymbol{r}_\alpha} e^{-i\eta'_\alpha \ln\zeta(\boldsymbol{k}'_\alpha,\boldsymbol{r}_\alpha)}}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0} \times \prod_{\nu=\beta,\gamma} \exp\left[-i\eta'_\nu \ln\zeta(\boldsymbol{k}'_\nu, \boldsymbol{r}_\nu)\right], \quad (4.29)$$

where $\boldsymbol{k}'_\nu = -\mu_\nu/m_\gamma\, \boldsymbol{k}'_\alpha - \epsilon_{\nu\alpha}\mu_\alpha/M_\nu\, \boldsymbol{q}'_\alpha,\ \nu = \beta,\, \gamma.$

We take advantage of the fact that in the Ω_0 domain $r_\alpha \to \infty$ and use an asymptotic form of the plane wave

$$e^{i\boldsymbol{k}\boldsymbol{r}} \overset{r\to\infty}{\sim} \frac{2\pi}{ikr}\left[\delta(\widehat{\boldsymbol{k}}-\widehat{\boldsymbol{r}})e^{ikr}-\delta(\widehat{\boldsymbol{k}}+\widehat{\boldsymbol{r}})e^{-ikr}\right], \tag{4.30}$$

which can be obtained from the asymptotic form of the partial wave expansion of the plane wave (see, e.g., [60]). Then we get (in leading order)

$$I_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha,\boldsymbol{q}'_\alpha) = \frac{1}{(2\pi)^2}\frac{1}{ir_\alpha}\int_{-\infty}^{\infty} dk'_\alpha \frac{k'_\alpha \mathcal{M}_{k'_\alpha\widehat{\boldsymbol{r}}_\alpha,\boldsymbol{q}'_\alpha;\boldsymbol{q}_i} e^{ik'_\alpha r_\alpha} e^{-i\eta'_\alpha \ln\zeta(k'_\alpha\widehat{\boldsymbol{r}}_\alpha,\boldsymbol{r}_\alpha)}}{E-k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0} \times \prod_{\nu=\beta,\gamma}\exp\left[-i\eta'_\nu \ln\zeta(\boldsymbol{k}'_\nu,\boldsymbol{r}_\nu)\right], \tag{4.31}$$

where $\boldsymbol{k}'_\nu = -m_\alpha/(M-m_\nu)\; k'_\alpha\widehat{\boldsymbol{r}}_\alpha - \epsilon_{\nu\alpha}\mu_\alpha/M_\nu\; \boldsymbol{q}'_\alpha$.

The integrand has two simple poles. Apart from that it is an analytic function on the complex energy plane. Therefore, we can calculate this integral closing the integration contour, e.g. in the upper-half of the complex plane (a semi-circular complex contour of infinite radius does not contribute to the integral due to the $e^{ik'_\alpha r_\alpha}$ factor). Using the Cauchy theorem to take the residue at the pole singularity (ps) gives:

$$I_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha,\boldsymbol{q}'_\alpha) = -\frac{\mu_\alpha}{2\pi}\frac{e^{ik^{(\mathrm{ps})}_\alpha r_\alpha}}{r_\alpha}\mathcal{M}_{k^{(\mathrm{ps})}_\alpha\widehat{\boldsymbol{r}}_\alpha,\boldsymbol{q}'_\alpha;\boldsymbol{q}_i} e^{-i\eta^{(\mathrm{ps})}_\alpha \ln\zeta(k^{(\mathrm{ps})}_\alpha\widehat{\boldsymbol{r}}_\alpha,\boldsymbol{r}_\alpha)} \times \prod_{\nu=\beta,\gamma}\exp\left[-i\eta^{(\mathrm{ps})}_\nu \ln\zeta(\boldsymbol{k}^{(ps)}_\nu,\boldsymbol{r}_\nu)\right], \tag{4.32}$$

where $\boldsymbol{k}^{(ps)}_\nu = -m_\alpha/(M-m_\nu)\; k^{(\mathrm{ps})}_\alpha\widehat{\boldsymbol{r}}_\alpha - \epsilon_{\nu\alpha}\mu_\alpha/M_\nu\; \boldsymbol{q}'_\alpha$. This brings energy conservation into play and the magnitude of k'_α is now fixed at

$$k^{(\mathrm{ps})}_\alpha = \left(2\mu_\alpha E - \frac{\mu_\alpha}{M_\alpha}\, q'^2_\alpha\right)^{1/2}. \tag{4.33}$$

Thus, we have

$$\Phi^{(\mathrm{sc},0)+}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = \int \frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3} e^{i\boldsymbol{q}'_\alpha\boldsymbol{\rho}_\alpha} I_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha,\boldsymbol{q}'_\alpha)$$
$$= -\frac{\mu_\alpha}{(2\pi)^3}\frac{1}{ir_\alpha\rho_\alpha}\int_0^{(2M_\alpha E)^{1/2}} dq'_\alpha q'_\alpha e^{-i\eta_\alpha^{(\mathrm{ps})}\ln\zeta(k_\alpha^{(\mathrm{ps})}\widehat{\boldsymbol{r}}_\alpha,\boldsymbol{r}_\alpha)}$$
$$\times\Big\{e^{ik_\alpha^{(\mathrm{ps})}r_\alpha+iq'_\alpha\rho_\alpha}\mathcal{M}_{k_\alpha^{(\mathrm{ps})}\widehat{\boldsymbol{r}}_\alpha,q'_\alpha\widehat{\boldsymbol{\rho}}_\alpha;\boldsymbol{q}_i}\prod_{\nu=\beta,\gamma}\exp\left[-i\eta_\nu^{(\mathrm{ps}(+))}\ln\zeta(\boldsymbol{k}_\nu^{ps(+)},\boldsymbol{r}_\nu)\right]$$
$$- e^{ik_\alpha^{(\mathrm{ps})}r_\alpha-iq'_\alpha\rho_\alpha}\mathcal{M}_{k_\alpha^{(\mathrm{ps})}\widehat{\boldsymbol{r}}_\alpha,-q'_\alpha\widehat{\boldsymbol{\rho}}_\alpha;\boldsymbol{q}_i}\prod_{\nu=\beta,\gamma}\exp\left[-i\eta_\nu^{\mathrm{ps}(-)}\ln\zeta(\boldsymbol{k}_\nu^{ps(-)},\boldsymbol{r}_\nu)\right]\Big\}. \qquad (4.34)$$

Here for simplicity we define $\boldsymbol{k}_\nu^{ps(+)} = -m_\alpha/(M-m_\nu)\ k_\alpha^{(\mathrm{ps})}\widehat{\boldsymbol{r}}_\alpha - \epsilon_{\nu\alpha}\mu_\alpha/M_\nu\ q'_\alpha\widehat{\boldsymbol{\rho}}_\alpha$, and $\boldsymbol{k}_\nu^{ps(-)} = -m_\alpha/(M-m_\nu)\ k_\alpha^{(\mathrm{ps})}\widehat{\boldsymbol{r}}_\alpha + \epsilon_{\nu\alpha}\mu_\alpha/M_\nu\ q'_\alpha\widehat{\boldsymbol{\rho}}_\alpha$.

At this stage we have no information about the individual physical momenta $\boldsymbol{k}_\alpha$ and $\boldsymbol{q}_\alpha$ but their values will become apparent upon evaluating the integral using asymptotic techniques. In Ω_0, where r_α and ρ_α are asymptotically large, the integrand is extremely oscillatory. For this reason one should only expect significant contribution to the integral from the neighborhood of stationary-phase (sp) points if there are any. One can verify that the first term of the integrand in Eq. (4.34) has a single stationary-phase point at

$$q_\alpha^{(\mathrm{sp})} = \frac{M_\alpha}{m}\frac{\kappa}{R}\rho_\alpha \qquad (4.35)$$

while the second one does not have any. This is why a contribution to the integral from the second term in curly brackets is negligibly small. In Eq. (4.39) we used the fact that at the stationary-phase point Eq. (4.33) is written as

$$k_\alpha^{(\mathrm{sp})} = \frac{\mu_\alpha}{m}\frac{\kappa}{R}r_\alpha, \qquad (4.36)$$

and consequently

$$-\frac{\mu_\nu}{m_\gamma}\, k_\alpha^{(\mathrm{ps})}\widehat{\boldsymbol{r}}_\alpha - \epsilon_{\nu\alpha}\frac{\mu_\alpha}{M_\nu}\, q_\alpha^{(\mathrm{sp})}\widehat{\boldsymbol{\rho}}_\alpha = \frac{\mu_\nu}{m}\frac{\kappa}{R}\boldsymbol{r}_\nu, \qquad \nu = \beta, \gamma. \tag{4.37}$$

We also note that the physical momenta $\boldsymbol{k}_\alpha$ and $\boldsymbol{q}_\alpha$ are given by

$$\boldsymbol{k}_\alpha = \frac{\mu_\alpha}{m}\frac{\kappa}{R}\boldsymbol{r}_\alpha, \qquad \boldsymbol{q}_\alpha = \frac{M_\alpha}{m}\frac{\kappa}{R}\boldsymbol{\rho}_\alpha. \tag{4.38}$$

Evaluating the remaining integral by means of the stationary-phase method [61], we obtain

$$\begin{aligned}\Phi^{(\mathrm{sc},0)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) &= \frac{(2\pi i)^{1/2}}{(2\pi)^3}\mathcal{M}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha;\boldsymbol{q}_i}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}}e^{i\kappa R} \\ &\quad \times \prod_{\nu=\alpha,\beta,\gamma}\exp\left[-i\eta_\nu \ln\left(\frac{2\mu_\nu}{m}\frac{\kappa}{R}r_\nu^2\right)\right]. \end{aligned} \tag{4.39}$$

In terms of hyperangles ϕ_ν, $\nu = \alpha, \beta, \gamma$ we finally have

$$\begin{aligned}\Phi^{(\mathrm{sc},0)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) &= \frac{(2\pi i)^{1/2}}{(2\pi)^3}\mathcal{M}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha;\boldsymbol{q}_i} \\ &\times \frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}}e^{i\kappa R - i\lambda_0 \ln(2\kappa R) - i\sigma_0}, \end{aligned} \tag{4.40}$$

with the additional phase

$$\sigma_0 = 2\sum_{\nu=\alpha,\beta,\gamma}\eta_\nu \ln(\sin\phi_\nu). \tag{4.41}$$

Thus the asymptotic form of $\Phi^{(\mathrm{sc})(+)}$ in Ω_0 comes as a result of the fundamental relationship between the total wave functions describing two different scattering processes within the same three-body system. Most importantly, our derivation leads to an unambiguous amplitude-phase form, which allows us to uniquely express the 'hyperspherical' breakup amplitude $A(\widehat{\omega})$ in terms of the standard definition of the breakup amplitude $\mathcal{M}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha;\boldsymbol{q}_i}$ given by Eq. (4.12):

$$A(\widehat{\omega}) = \frac{(2\pi i)^{1/2}}{(2\pi)^3}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\kappa^{3/2}\mathcal{M}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha;\boldsymbol{q}_{n_\alpha}}e^{-i\sigma_0}. \tag{4.42}$$

2. Asymptotic scattered wave in the Ω_α region

Having completed the derivation of the asymptotic form of $\Phi^{(\mathrm{sc},0)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)$ in Ω_0, it remains to proceed to Ω_α and evaluate the integrals contained in (4.18). To start with we emphasize that the calculation of the second term of Eq. (4.14) is trivial for large ρ_α and leads to a well known scattered wave in two-cluster channels.

Consider now the Eq. (4.18). By definition here r_α is limited as compared to ρ_α. Therefore, it cannot, strictly speaking, be used as an asymptotic parameter alongside ρ_α. However, the other two pairs of Jacobian variables $(\boldsymbol{r}_\nu,\boldsymbol{\rho}_\nu)$, $\nu=\beta,\gamma$, constitute suitable pairs of asymptotically large parameters should we represent the integral in terms of relevant canonical conjugate momentum space variables $(\boldsymbol{k}_\nu,\boldsymbol{q}_\nu)$. Below we use the $(\boldsymbol{k}_\beta,\boldsymbol{q}_\beta)$ space. Then

$$\begin{aligned}\Phi^{(sc,\alpha)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) \;\sim\; & \int \frac{d\boldsymbol{k}'_\beta}{(2\pi)^3}\frac{d\boldsymbol{q}'_\beta}{(2\pi)^3}\frac{\mathcal{M}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha;\boldsymbol{q}_i}e^{i\boldsymbol{k}'_\beta\boldsymbol{r}_\beta+i\boldsymbol{q}'_\beta\boldsymbol{\rho}_\beta}\varphi_\alpha(\widetilde{\boldsymbol{k}}_\alpha,\boldsymbol{r}_\alpha)}{E-k'^2_\beta/2\mu_\beta-q'^2_\beta/2M_\beta+i0}\\ & \times\prod_{\nu=\beta,\gamma}e^{-i\eta_\nu\ln\zeta(\boldsymbol{k}_\nu,\boldsymbol{r}_\nu)}.\end{aligned} \tag{4.43}$$

In the equation above, $\boldsymbol{r}_\nu$, $\boldsymbol{\rho}_\nu$, $\boldsymbol{k}'_\nu$ and $\boldsymbol{q}'_\nu$, $\nu=\gamma,\alpha$, are kept as short-hand notation. As functions of β-space variables they are given by Eqs. (5.7) and (5.8). Taking into account that

$$\frac{\mu_\beta}{m}r^2_\beta+\frac{M_\beta}{m}\rho^2_\beta=\frac{\mu_\alpha}{m}r^2_\alpha+\frac{M_\alpha}{m}\rho^2_\alpha \qquad \text{and} \qquad \frac{m}{\mu_\beta}k^2_\beta+\frac{m}{M_\beta}q^2_\beta=\frac{m}{\mu_\alpha}k^2_\alpha+\frac{m}{M_\alpha}q^2_\alpha \tag{4.44}$$

we can calculate the above integral in analogy with the procedure we used in Ω_0. We therefore omit the details. Evaluating the integrals and transforming the answer back to the variables $\boldsymbol{r}_\alpha$ and $\boldsymbol{\rho}_\alpha$ we arrive at the final result

$$\begin{aligned}\Phi^{(sc,\alpha)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) &= \frac{(2\pi i)^{1/2}}{(2\pi)^3}\mathcal{M}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha;\boldsymbol{q}_i}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}} \\ &\times\varphi_\alpha\left(\overline{\boldsymbol{k}}_\alpha,\boldsymbol{r}_\alpha\right)e^{i\kappa R-i\lambda_\alpha\ln(2\kappa R)-i\sigma_\alpha}, \end{aligned} \tag{4.45}$$

where

$$\lambda_\alpha = \sum_{\nu=\beta,\gamma}\eta_\nu \tag{4.46}$$

and

$$\sigma_\alpha = 2\sum_{\nu=\beta,\gamma}\eta_\nu\ln(\sin\phi_\nu). \tag{4.47}$$

The local momentum entering in the scattered wave (4.45) takes the form

$$\overline{\boldsymbol{k}}_\alpha = \frac{\mu_\alpha}{m}\frac{\kappa}{R}\boldsymbol{r}_\alpha + \sum_{\nu=\beta,\gamma}\frac{\mu_\alpha}{m_\gamma}\frac{\eta_\nu}{\mu_\nu}\frac{R}{\kappa r_\nu^3}\boldsymbol{r}_\nu, \tag{4.48}$$

If we take into account that the second term in Eq. (4.48) becomes negligible as r_α becomes large, then

$$\varphi_\alpha\left(\overline{\boldsymbol{k}}_\alpha,\boldsymbol{r}_\alpha\right) \overset{r_\alpha\to\infty}{\sim} \exp\left[-i\eta_\alpha\ln\left(2\kappa R\sin^2\phi_\alpha\right)\right]. \tag{4.49}$$

This means that Eq. (4.45) smoothly transforms to Eq. (4.40) when $\Omega_\alpha \to \Omega_0$.

It is now also not difficult to verify that the final results for the scattered wave are independent of the complementary mass constant m which we introduced earlier.

Our final note concerns the asymptotic domains Ω_ν, where $\nu \neq \alpha$. In this case the result given by Eq. (4.45) remains unchanged, the only difference being that $\Phi^{(\nu)+}$, $\nu \neq \alpha$, denotes the asymptotic form of the total $2 \to 3$ wave function as there is no incident wave in the non-α channels.

3. Generalized three-body scattered wave valid in all the asymptotic regions

Having completed the derivation of the asymptotic form of $\Phi^{(\mathrm{sc},\nu)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha)$ in Ω_ν, where $\nu = 0, \alpha$ it remains to generalize the result. The leading asymptotic term of the three-body incident wave, valid in all the asymptotic regions, was obtained in [16] and in Chapter III:

$$\Psi^{(\alpha\beta\gamma)(-)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) = e^{i\boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha + i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} \prod_{\nu=\alpha,\beta,\gamma} \varphi^{(-)}_{\widetilde{\boldsymbol{k}}_\nu}(\boldsymbol{r}_\nu). \tag{4.50}$$

The wave function $\varphi^{(-)}_{\widetilde{\boldsymbol{k}}_\nu}(\boldsymbol{r}_\nu)$ satisfies the two-body equation similar to Eq. (4.20) with the local momentum:

$$\widetilde{\boldsymbol{k}}_\nu = \boldsymbol{k}_\nu + \sum_{\tau=\alpha,\beta,\gamma} \frac{m_\tau}{M - m_\tau}\eta_\tau \frac{\hat{\boldsymbol{k}}_\tau + \hat{\boldsymbol{r}}_\tau}{1 + \hat{\boldsymbol{k}}_\tau \cdot \hat{\boldsymbol{r}}_\tau} \frac{1-\delta_{\nu,\tau}}{r_\tau}. \tag{4.51}$$

The general expression for the asymptotic three-body scattered wave valid in all four asymptotic regions can be derived from Eq. (4.14). After integration we have

$$\begin{aligned}\Phi^{(\alpha\beta\gamma)(+)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\boldsymbol{r}_\alpha,\boldsymbol{\rho}_\alpha) \;\;=\;\; & \frac{(2\pi i)^{1/2}}{(2\pi)^3}\mathcal{M}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha;\boldsymbol{q}_i}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}} \\ & \times e^{i\kappa R + i\pi/4} \prod_{\nu=\alpha,\beta,\gamma} \varphi^{(-)}_{\overline{\boldsymbol{k}}_\nu}(\boldsymbol{r}_\nu).\end{aligned} \tag{4.52}$$

where the asymptotic local momentum $\overline{\boldsymbol{k}}_\alpha$ entering in the scattered wave Eq. (4.52) is found similarly to Eq. (4.48) from Eq. (4.51). If we take into account that the second term in Eq. (4.51) becomes negligible as r_ν becomes large, then

$$\varphi_{\overline{\boldsymbol{k}}_\nu}(\boldsymbol{r}_\nu) \quad \overset{r_\nu\to\infty}{\sim} \quad \exp\left[-i\eta_\nu \ln\left(2\kappa R \sin^2\phi_\nu\right)\right]. \tag{4.53}$$

This means Eq. (4.52) smoothly transforms to Eq. (4.40) when $r_\nu \to \infty$, where $\nu = \alpha, \beta, \gamma$.

D. Asymptotic forms of the Coulomb three-body Green's function

In this section the derivation of the asymptotic forms of the Green's function for a system of three charged particles is presented. Because the methods used earlier form the basis of the derivations, we will omit technical details of the calculations. The asymptotic forms of the three-body Green's function are important in the formulation of the three-body problem [55, 56], in calculating the optical potentials [16, 57, 58] and for non-perturbational calculations of dynamical dipole polarization terms [59].

Thus, using a similar technique we can get leading-order terms of the three-body Green's function in the asymptotic domains Ω_0 and Ω_α. When $(r_\alpha, \rho_\alpha) \in \Omega_0$, from the spectral decomposition, we can write

$$G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0) \overset{(r_\alpha,\rho_\alpha)\in\Omega_0}{\longrightarrow} \int \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3}\frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3} \times \frac{\Psi^{(0)(-)}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha)\Psi^{(-)*}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0}. \tag{4.54}$$

Calculating the integrals we get

$$G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0) \overset{(r_\alpha,\rho_\alpha)\in\Omega_0}{\longrightarrow} \frac{(2\pi i)^{1/2}}{(2\pi)^3}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}}\Psi^{(-)*}_{\frac{\mu_\alpha}{m}\frac{\kappa}{R}\boldsymbol{r}_\alpha, \frac{M_\alpha}{m}\frac{\kappa}{R}\boldsymbol{\rho}_\alpha}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha) \times e^{i\kappa R - i\lambda_0 \ln(2\kappa R) - i\sigma_0}. \tag{4.55}$$

More interesting is the case when both (r_α, ρ_α) and $(r'_\alpha, \rho'_\alpha) \in \Omega_0$. Then we have

$$G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0) \overset{\substack{(r_\alpha,\rho_\alpha)\in\Omega_0 \\ (r'_\alpha,\rho'_\alpha)\in\Omega_0}}{\longrightarrow} \frac{(2\pi i)^{1/2}}{(2\pi)^3}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}} \times e^{i\kappa R - i\kappa R'(\sin\phi_\alpha \sin\phi'_\alpha\, \widehat{\boldsymbol{r}}_\alpha \widehat{\boldsymbol{r}}'_\alpha + \cos\phi_\alpha\cos\phi'_\alpha\, \widehat{\boldsymbol{\rho}}_\alpha\widehat{\boldsymbol{\rho}}'_\alpha)} \times \exp\left[-\frac{i}{\kappa}\sum_{\nu=\alpha,\beta,\gamma}\left(\frac{m}{\mu_\nu}\right)^{1/2}\frac{\eta_\nu}{\sin\phi_\nu}\ln\frac{2r_\nu}{r'_\nu(1+\widehat{\boldsymbol{r}}_\nu\widehat{\boldsymbol{r}}'_\nu)}\right], \tag{4.56}$$

with the condition that $R' \leq R$, otherwise the boundary condition for $G^{(+)}$ is violated.

The $R' > R$ case defines $G^{(-)}$.

When $(r_\alpha, \rho_\alpha) \in \Omega_\alpha$, we can write

$$G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0) \overset{(r_\alpha,\rho_\alpha)\in\Omega_\alpha}{\longrightarrow} \int \frac{d\boldsymbol{k}'_\alpha}{(2\pi)^3}\frac{d\boldsymbol{q}'_\alpha}{(2\pi)^3} \times \frac{\Psi^{(\alpha)-}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha)\Psi^{(-)*}_{\boldsymbol{k}'_\alpha,\boldsymbol{q}'_\alpha}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0} + \ldots \tag{4.57}$$

Calculating the integrals we arrive at

$$G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0) \overset{(r_\alpha,\rho_\alpha)\in\Omega_\alpha}{\longrightarrow} \frac{(2\pi i)^{1/2}}{(2\pi)^3}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}}\Psi^{-*}_{\frac{\mu_\alpha}{m}\frac{\kappa}{R}\boldsymbol{r}_\alpha, \frac{M_\alpha}{m}\frac{\kappa}{R}\boldsymbol{\rho}_\alpha}(\boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha) \times \psi_\alpha\left(\overline{\boldsymbol{k}}_\alpha, \boldsymbol{r}_\alpha\right) e^{i\kappa R - i\lambda_\alpha \ln(2\kappa R) - i\sigma_\alpha} + \ldots \tag{4.58}$$

If both (r_α, ρ_α) and $(r'_\alpha, \rho'_\alpha) \in \Omega_\alpha$ we have

$$G^{(+)}(\boldsymbol{r}_\alpha, \boldsymbol{\rho}_\alpha; \boldsymbol{r}'_\alpha, \boldsymbol{\rho}'_\alpha; E + i0) \overset{\substack{(r_\alpha,\rho_\alpha)\in\Omega_\alpha \\ (r'_\alpha,\rho'_\alpha)\in\Omega_\alpha}}{\longrightarrow} \frac{(2\pi i)^{1/2}}{(2\pi)^3}\frac{(\mu_\alpha M_\alpha)^{3/2}}{m^2}\frac{\kappa^{3/2}}{R^{5/2}}$$
$$\times \varphi^*_{\overline{\boldsymbol{k}}'_\alpha}(\boldsymbol{r}'_\alpha)\varphi_{\overline{\boldsymbol{k}}_\alpha}(\boldsymbol{r}_\alpha)\, e^{i\kappa R - i\kappa R'(\sin\phi_\alpha \sin\phi'_\alpha\, \widehat{\boldsymbol{r}}_\alpha \widehat{\boldsymbol{r}}'_\alpha + \cos\phi_\alpha \cos\phi'_\alpha\, \widehat{\boldsymbol{\rho}}_\alpha \widehat{\boldsymbol{\rho}}'_\alpha)}$$
$$\times \exp\left[-\frac{i}{\kappa}\sum_{\nu=\beta,\gamma}\left(\frac{m}{\mu_\nu}\right)^{1/2}\frac{\eta_\nu}{\sin\phi_\nu}\ln\frac{2r_\nu}{r'_\nu(1+\widehat{\boldsymbol{r}}_\nu\widehat{\boldsymbol{r}}'_\nu)}\right] \tag{4.59}$$

From Eq. (4.59) one can get an asymptotic Green's function for the case when $(r_\alpha, \rho_\alpha) \in \Omega_0$ but $(r'_\alpha, \rho'_\alpha) \in \Omega_\alpha$. Clearly, in this case bound states do not contribute. The leading order asymptotic terms of the Green's function for three-particles interacting via short-range potentials were given by [62].

E. Conclusion

Summarizing, the asymptotic behavior of the scattered wave function describing breakup processes in a system of three arbitrary charged particles has been investigated. Leading-order terms of the scattered wave are given for asymptotic domains where all three particles are widely separated and when any two are close to each other but far from the third particle. The derivations are based on the relationship between the scattered part of the scattering wave functions of the second type, which describes a breakup process in a three charged-particle system and the wave function of the first type which describes the scattering with all three particles of the system in the continuum. The asymptotic three-body wave that is derived is free of the logarithmically diverging phase factors in the asymptotic regions where two particles are close to each other and far away from the third particle. Another important consequence of the derivation presented here is that the forms obtained in this work are free of the phase ambiguities that are a feature of the previously derived Peterkop asymptotic form. A similar technique is used to obtain asymptotic forms of the three-body Coulomb Green's function.

The derived wave functions are suitable for use in calculations of ionization in electron/positron-atom and ion-atom collisions, double-photo ionization of helium and similar breakup processes in nuclear physics. For instance, the breakup amplitude can be extracted by direct comparison of the numerically calculated wave function for sufficiently large hyperradius with its analytic asymptotic forms given in the present work.

CHAPTER V

COULOMB BREAKUP: FROM EXACT TO DWBA AMPLITUDES

A. Introduction

Breakup processes have become an important tool in modern nuclear physics providing valuable information for topics ranging from nuclear structure to nuclear astrophysics [63, 64, 65, 66]. However, the theory of breakup reactions lags behind experiments. A treatment of breakup processes is always complicated due to the presence of the three-body final-state. It is even more complicated if Coulomb interactions are not negligible, as happens when the Coulomb parameters are large. Evidently, this is the case when the breakup reaction occurs at energies close to the breakup threshold or when the charges of the interacting nuclei are high [67, 68].

Until now there has been only one exact three-body calculation of the elementary process $p + d \to p + p + n$ [69]. Although only two particles are charged in this process, the inclusion of the Coulomb interaction created significant difficulties and a special technique, the so-called screening procedure, has been applied. The correct formulation of the Faddeev integral equations in momentum space when all three particles are charged is still an open problem [4, 5]. Moreover, in the presence of the Coulomb interaction the exact post form of the breakup amplitude, which is seemingly more convenient than the prior form, has not been derived until recently [70]. The calculation of the exact breakup matrix element is very difficult. Therefore, in practice the amplitude is often taken in the distorted-wave Born approximation (DWBA) [71, 72, 73]. However, in all the formulations of the DWBA the long-range nature of the Coulomb interaction in the continuum has not been properly taken into account. Besides, in conventional approaches the final-state wave function is written in a factorized form as a product of the wave function of the relative motion of two fragments and the wave function of the relative motion of the c.m. of two fragments and the third particle. At the same time, it is known that such a factorized form does not possess the correct asymptotic behavior in any asymptotic region, whether two particles are close to each other and far away from the third particle or all three final-state particles are well separated (see [16, 17] and Chapter III). Since the final-state wave function in the conventional approach has the wrong asymptotic behavior, the conventional DWBA amplitude turns out not to be a first-order term in the Born series expansion for the transition operator. In other words, it is not straightforward that the distorted-wave Born series is convergent. This calls for a revision of the derivation of the DWBA breakup amplitude in the presence of the Coulomb interaction.

The aim of this work is to present correct expressions for the exact *prior* and *post* forms of the breakup amplitude in terms of the three-body wave functions which have correct asymptotic behavior when Coulomb interactions are taken into account. In contrast to the electron-impact ionization of hydrogen [70], here we consider nuclear breakup processes and transition from exact to DWBA amplitude. We demonstrate that the post form exact breakup amplitude can be derived from the exact prior amplitude in the form of a surface integral in the six-dimensional configuration hyperspace. At the hyperradius $R \to \infty$, the functions in the integrand can be replaced by their leading asymptotic terms. In particular, we need to use the asymptotic form of the three-body scattered wave in the intial state which has been found in Chapter IV. This surface integral representation sets the stage for "ab-initio" (direct) calculations of the Schrödinger equation in the configuration space with subsequent substitution into the surface integral to get the breakup amplitude. The derivation of the post form exact breakup amplitude for charged particles is one of the main goals of this work.

We demonstrate also that in the presence of Coulomb interactions the transition to the DWBA from the exact amplitudes is not a straightforward procedure. The transition operator which defines the breakup amplitude plays a central role in few-body formalism and it is customary to consider it carefully when doing approximations. In particular, it is well known that the long-range nature of the Coulomb interaction is the main reason why the integral Faddeev equations for charged particles have not yet been solved above the breakup threshold [3]. The expressions suggested in this work will be useful not only for DWBA calculations but also for the most advanced methods to calculate the breakup amplitudes, like the continuum-discretized coupled-channel method (CDCC) (see [67] and references therein), especially when analyzing reactions at energies near the breakup threshold. A similar method has been used very successfully in electron-atom scattering by Bray and Stelbovics (see [28, 39, 40]) and is known as the convergent close coupling (CCC) method.

The Chapter is set as following way. In section B a conventional approximation to treat the three-body final-state scattering wave function in breakup processes is discussed. In section C the exact prior and post form breakup amplitudes are derived and the flaws of the conventional approach are shown. In section D we derive the DWBA type amplitudes. Finally, section E concludes the Chapter.

B. Final-state three-body wave function in continuum

Let us consider the following breakup process

$$\alpha + (\beta\,\gamma) \rightarrow \alpha + \beta + \gamma. \tag{5.1}$$

where $(\beta\,\gamma)$ is the bound state of particles β and γ. The total wave function describing process (5.1) in initial state satisfies the Schrödinger equation

$$(E - H)\Psi^{(+)}_{\mathbf{q}_i}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \tag{5.2}$$

The total wave function describing process (5.1) in the final state satisfies the Schrödinger equation

$$(E - H)\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = 0, \tag{5.3}$$

where

$$E = \varepsilon_{n_\alpha} + q^2_{n_\alpha}/2M_\alpha = k^2_\alpha/2\mu_\alpha + q^2_\alpha/\ 2M_\alpha \tag{5.4}$$

is the total energy of the system, $H = T + V$ is the three-body Hamiltonian,

$$T = T_{\mathbf{r}_\alpha} + T_{\boldsymbol{\rho}_\alpha} = -(1/2\,\mu_\alpha)\,\boldsymbol{\Delta}_{\mathbf{r}_\alpha} - (1/2\,M_\alpha)\,\boldsymbol{\Delta}_{\boldsymbol{\rho}_\alpha} \tag{5.5}$$

is the kinetic energy operator,

$$V(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \sum_{\nu=\alpha,\beta,\gamma} V_\nu(r_\nu) \tag{5.6}$$

is the full interaction, with $V_\nu = V^C_\nu + V^N_\nu$, where V^C_ν (V^N_ν) is the Coulomb (nuclear) interaction potential between the particles in ν pair, where $\nu = \alpha, \beta, \gamma$. Also here $\mathbf{r}_\alpha$ is the radius-vector connecting particles β and γ and $\boldsymbol{\rho}_\alpha$ is the radius-vector connecting particle α and the c.m. of the system $(\beta\,\gamma)$, $\mathbf{q}_i$ is the relative momentum between the fragments in the initial channel, ε_{n_α} is the bound state energy of β and γ particles in the initial state n_α, $\mathbf{k}_\alpha$ is the relative momentum of particles β and γ in the final state, $\mathbf{q}_\alpha$ is the relative momentum of the c.m. of the $\beta + \gamma$ system and particle α, $\mu_\alpha = m_\beta\, m_\gamma/m_{\beta\,\gamma}$ and $M_\alpha = m_\alpha\, m_{\beta\,\gamma}/M$, $m_{\beta\,\gamma} = m_\beta + m_\gamma$, $M = m_\alpha + m_\beta + m_\gamma$, m_ν is the mass of particle ν.

There are the following relations between Jacobi coordinates and moments for three particles in the center of mass system:

$$\boldsymbol{r}_\nu = -\frac{m_\nu}{m_{\beta\gamma}}\boldsymbol{r}_\alpha - \epsilon_{\nu\alpha}\boldsymbol{\rho}_\alpha\ , \qquad \boldsymbol{\rho}_\nu = \epsilon_{\nu\alpha}\frac{\mu_\nu}{M_\alpha}\boldsymbol{r}_\alpha - \frac{m_\alpha}{M-m_\nu}\boldsymbol{\rho}_\alpha \tag{5.7}$$

and

$$\boldsymbol{k}_\nu = -\frac{m_\alpha}{M-m_\nu}\boldsymbol{k}_\alpha - \epsilon_{\nu\alpha}\frac{\mu_\alpha}{M_\nu}\boldsymbol{q}_\alpha\ , \qquad \boldsymbol{q}_\nu = \epsilon_{\nu\alpha}\boldsymbol{k}_\alpha - \frac{m_\nu}{m_{\beta\gamma}}\boldsymbol{q}_\alpha, \tag{5.8}$$

where $\nu = \beta, \gamma,\ \epsilon_{\nu\alpha} = -\epsilon_{\alpha\nu}$ is the antisymmetric symbol, with $\epsilon_{\nu\alpha} = 1$ for $(\nu\alpha)$ being a cyclic permutation of (1, 2, 3), and $\epsilon_{\alpha\alpha} = 0$. Although all these notations have been introduced in the previous chapters, we give them here for convenience of the readers.

First we demonstrate why the conventional derivation of the exact post form breakup amplitude is not valid in the presence of Coulomb interactions. In the conventional approach a formal solution to (5.3) for the exact wave function in the final state is given as:

$$\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \ \psi^{(-)}_\alpha(\mathbf{r}_\alpha)\chi^{(-)}_\alpha(\boldsymbol{\rho}_\alpha) + G^{(-)}\,\overline{V}_\alpha\ \psi^{(-)}_\alpha(\mathbf{r}_\alpha)\chi^{(-)}_\alpha(\boldsymbol{\rho}_\alpha), \tag{5.9}$$

where $\psi^{(-)}_\alpha(\mathbf{r}_\alpha)$ is the scattering wave function of β and γ particles interacting via potential V_α, $\chi^{(-)}_\alpha(\boldsymbol{\rho}_\alpha)$ is the scattering wave function describing the relative motion of the c.m. of the system $\beta+\gamma$ and particle α interacting via the potential U_α. The factorized wave function $\psi^{(-)}_\alpha\chi^{(-)}_\alpha$ has the following asymptotic form

$$\psi^{(-)}_\alpha\chi^{(-)}_\alpha = e^{i\boldsymbol{k}_\alpha\cdot\mathbf{r}_\alpha}\ e^{i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}N_\alpha F(-i\eta_\alpha, 1; i\zeta_\alpha)\overline{N}_\alpha F(-i\overline{\eta}_\alpha, 1; i\overline{\zeta}_\alpha), \tag{5.10}$$

where $\zeta_\alpha = (k_\alpha r_\alpha + \boldsymbol{k}_\alpha\cdot\boldsymbol{r}_\alpha)$, $\overline{\zeta}_\alpha = (q_\alpha\rho_\alpha + \boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha)$, and $\overline{\eta}_\alpha = Z_\alpha(Z_\beta+Z_\gamma)M_\alpha/q_\alpha$. Eq. (5.9) is fully justified in the case of short range interactions, when Coulomb effects can be disregarded and it can be used to derive the post-form breakup amplitude from the prior form. However, in the presence of Coulomb interactions the incident wave in Eq. (5.9) is not a three-body incident wave in any asymptotic domain. Consider, for example, the asymptotic region Ω_0, where all three particles are far away from each other. The incident wave is given by Redmond's Coulomb-distorted plane wave, Eq. (2.10), which contains three Coulomb phase factors corresponding to the three interacting pairs in a three-body system [6, 7]. The asymptotic form of the factorized wave function (5.9) in Ω_0 contains only two phase factors:

$$\psi_\alpha^{(-)}\chi_\alpha^{(-)} \to e^{i\,\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha} e^{i\,\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\, e^{-i\eta_\alpha \ln(k_\alpha r_\alpha + \mathbf{k}_\alpha\cdot\mathbf{r}_\alpha)} e^{-i\overline{\eta}_\alpha \ln(q_\alpha \rho_\alpha + \mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha)} \tag{5.11}$$

Similarly in the asymptotic region Ω_α the incident wave (5.10) does not coincide with the leading asymptotic term (see [16] and Chapter IV, Eq. (4.19)).

Generally speaking, one can write down different solutions of Eq. (5.2), but the correct one is the one which satisfies the proper boundary conditions. For example, Eq. (5.9) looks formally correct and the wrong incident wave is compensated by the integral term in Eq. (5.9), But it means that the second term asymptotically has the same order, $O(1)$, as the incident wave (5.10), i. e. the integral term does not decay as the outgoing scattered wave. It means that the operator $G^{(-)}\,\overline{V}_\alpha$ in the integral term in Eq. (5.9) is noncompact.

C. The prior and post forms of the breakup amplitude

1. The exact prior form of the breakup amplitude

In Chapters III and IV we have discussed two types of three-body scattering wave functions satisfying two different types of boundary conditions: the wave function of the first type which evolves from the three-body incident wave and the wave function of the second type, which evolves from the two-body incident wave. To find both functions one needs to solve the three-body Schrödinger equation . The breakup amplitude can be written in two forms. The first type of amplitude is expressed in terms of the three-body scattering wave function of the first type describing the final-state and the two-body channel wave function describing the intial state of the breakup process. Such an amplitude is called the exact prior form amplitude. The second form contains the exact initial three-body scattering wave function of the second type and the three-body channel wave function describing the final state. Such an amplitude is called the post-form amplitude. We start this part from the derivation of the prior form amplitude. To do it we use the three-body scattering wave function of the second type and using the Green's function formalism, as we did in the previous chapter, we express the second type of the scattering wave function in terms of the first type and the prior breakup amplitude. A formal solution of Eq. (5.2) satisfying the initial two-body incident-wave and the outgoing scattered-wave boundary condition (second type of wave function) is

$$\Psi^{(+)}_{\mathbf{q}_i}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \varphi_{n_\alpha}(\mathbf{r}_\alpha)\chi^{(+)}_{\mathbf{q}_i}(\boldsymbol{\rho}_\alpha) + G^{(+)}\overline{V}_\alpha\,\varphi_{n_\alpha}(\mathbf{r}_\alpha)\chi^{(+)}_{\mathbf{q}_i}(\boldsymbol{\rho}_\alpha). \tag{5.12}$$

Here $\varphi_{n_\alpha}(\boldsymbol{r}_\alpha)$ is the wave function of the n_α-th bound state of the $(\beta\,\gamma)$ system, $\chi^{(+)}_{\mathbf{q}_i}(\boldsymbol{\rho}_\alpha)$ is the distorted wave describing the relative motion of particles $(\beta\,\gamma)$ and α in the initial state. The latter satisfies the equation

$$\big((1/2\,M_\alpha)\,\boldsymbol{\Delta}_{\boldsymbol{\rho}_\alpha} - U_\alpha(\boldsymbol{\rho}_\alpha) + q^2_{n_\alpha}/2M_\alpha\big)\,\chi^{(+)}_{\mathbf{q}_{n_\alpha}}(\boldsymbol{\rho}_\alpha) = 0, \tag{5.13}$$

where $\mathbf{q}_i$ is the relative momentum in the initial two-fragment channel, $U_\alpha(\boldsymbol{\rho}_\alpha)$ is the "channel" potential, which describes the interaction of particle α with the c.m. of the bound subsystem $(\beta\,\gamma)$ and is written as

$$U_\alpha(\boldsymbol{\rho}_\alpha) = V_\beta(\boldsymbol{\rho}_\alpha) + V_\gamma(\boldsymbol{\rho}_\alpha). \tag{5.14}$$

Also in Eq. (5.12)

$$G^{(+)}(z) = (z - T - V)^{-1} \tag{5.15}$$

is the total three-body Green's resolvent, $z = E + i0$,

$$\overline{V}_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = V - V_\alpha - U_\alpha = V_\beta + V_\gamma - U_\alpha. \tag{5.16}$$

First we show how to derive the exact *prior*-form breakup amplitude from Eq. (5.12). We use the spectral decomposition of the Green's function [3] and Eq. (4.10) from Chapter IV:

$$G^{(+)}(\mathbf{r}'_\alpha, \boldsymbol{\rho}'_\alpha; \mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \int \frac{d\,\mathbf{k}'_\alpha}{(2\pi)^3} \frac{d\,\mathbf{q}'_\alpha}{(2\pi)^3} \frac{\Psi^{(-)}_{\mathbf{k}'_\alpha, \mathbf{q}'_\alpha}(\mathbf{r}'_\alpha,\, \boldsymbol{\rho}'_\alpha) \Psi^{(-)*}_{\mathbf{k}'_\alpha, \mathbf{q}'_\alpha}(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0} + ..., \tag{5.17}$$

where $\Psi^{(-)}_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}(\mathbf{r}_\alpha,\, \boldsymbol{\rho}_\alpha)$ is the exact three-body scattering wave function of the first type describing the scattering of three particles α, β and γ in the continuum in the final state with the three-body Coulomb distorted incident plane wave. The dots indicate the contribution from all the (both three- and two-body) bound states of the system. Then from Eq. (5.12) we have

$$\begin{aligned} \Psi^{(+)}_{\mathbf{q}_i}(\,\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) &= \varphi_{n_\alpha}(\mathbf{r}_\alpha)\, \chi^{(+)}_{\mathbf{q}_i}(\boldsymbol{\rho}_\alpha) \\ &+ \int \frac{d\mathbf{k}'_\alpha}{(2\pi)^3} \frac{d\mathbf{q}'_\alpha}{(2\pi)^3} \frac{\Psi^{(-)}_{\mathbf{k}'_\alpha, \mathbf{q}'_\alpha}(\,\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)}{E - k'^2_\alpha/2\mu_\alpha - q'^2_\alpha/2M_\alpha + i0} \mathcal{M}^{prior}_{\mathbf{k}'_\alpha, \mathbf{q}'_\alpha; \mathbf{q}_i} + ... \end{aligned} \tag{5.18}$$

We now show that the amplitude

$$\mathcal{M}^{prior}_{\mathbf{k}_\alpha, \mathbf{q}_\alpha; \mathbf{q}_i} = \left\langle \Psi^{(-)}_{\mathbf{k}_\alpha, \mathbf{q}_\alpha} \left| \overline{V}_\alpha \right| \varphi_{n_\alpha} \chi^{(+)}_{\mathbf{q}_i} \right\rangle, \tag{5.19}$$

with the on-shell momenta $\mathbf{k}_\alpha$ and $\mathbf{q}_\alpha$, is the exact *prior*-form breakup amplitude [53]. To prove it one should calculate the integral in Eq. (5.18) in all the asymptotic regions of the six-dimensional configuration space $(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$.

In asymptotic regions, $\Psi^{(-)}_{\mathbf{k}_\alpha, \mathbf{q}_\alpha}$ can be replaced by its corresponding leading asymptotic terms. We substitute in Eq. (5.18) the generalized asymptotic wave function (3.83) for $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$, because Eq. (3.83) gives the leading asymptotic term of $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ in all the asymptotic regions. The integral in Eq. (5.18) is taken out using an asymptotic form of the plane wave, the residue in the pole of the integrand and the stationary phase method (see Chapter IV). The leading order term will be generated by the first term of Eq. (3.39) or $\widetilde{\Psi}^{(\alpha\beta\gamma)(-)}_{\boldsymbol{k}_\alpha,\boldsymbol{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ producing the asymptotically three-body outgoing wave:

$$\begin{aligned}\int \frac{d\mathbf{k}'_\alpha}{(2\pi)^3}\frac{d\mathbf{q}'_\alpha}{(2\pi)^3}\frac{\Psi^{(-)}_{\mathbf{k}'_\alpha,\mathbf{q}'_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)}{E-k'^2_\alpha/2\mu_\alpha-q'^2_\alpha/2M_\alpha+i0}\mathcal{M}^{prior}_{\mathbf{k}'_\alpha,\mathbf{q}'_\alpha;\mathbf{q}_i} \\ \overset{\Omega}{\longrightarrow}\frac{1}{(2\pi)^{5/2}}\mathcal{M}^{prior}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i}\frac{(\mu_\alpha M_\alpha)^{\frac{3}{2}}}{m^2}\frac{\kappa^{\frac{3}{2}}}{R^{5/2}}e^{i\kappa R+i\pi/4} \\ \times\prod_{\nu=\alpha,\beta,\gamma}\varphi^{(-)}_{\tilde{\mathbf{k}}_\nu}(\mathbf{r}_\nu)=\Phi_i^{(sc)(+)},\end{aligned}\tag{5.20}$$

where Ω is any of the asymptotic regions Ω_0 or Ω_ν (for definitions of the asymptotic regions see Chapter I) and $\kappa=\sqrt{2mE}$. Thus the coefficient in the outgoing three-body wave (5.20) is nothing but the breakup amplitude (5.19) taken at momenta aligned along the corresponding radial directions: $\mathbf{q}_\alpha = M_\alpha\,\kappa/(m\,R)\,\boldsymbol{\rho}_\alpha$ and $\mathbf{k}_\alpha = \mu_\alpha\,\kappa/(m\,R)\,\mathbf{r}_\alpha$. Here m is the nucleon mass and the hyperradius is given by

$$R=\left((\mu_\alpha/m)\,r_\alpha^2+(M_\alpha/m)\,\rho_\alpha^2\right)^{1/2}.\tag{5.21}$$

Eq. (5.20), which proves that Eq. (5.19) is indeed the exact prior form breakup amplitude in the presence of the Coulomb interactions, is the first main result of this chapter. Although Eq. (5.19) gives an exact breakup amplitude it is not very popular because the three-body wave function $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ is available only asymptotically. Since the integration over r_α is protected by the bound-state wave function $\varphi_{n_\alpha}(\mathbf{r}_\alpha)$, at specific kinematic conditions $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ can be approximated by its leading asymptotic term $\Psi^{(\alpha)(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ in the asymptotic region Ω_α, where $r_\alpha/\rho_\alpha\to 0,\ \rho_\alpha\to\infty$ which has been found in Chapter III, Eq. (3.39).

2. The conventional post form of the breakup amplitude

First we will derive a conventional post form of the breakup amplitude from the exact one (5.19). Substituting a formal solution (5.9) into Eq. (5.19) gives a conventional post form of the breakup amplitude:

$$\begin{aligned} \mathcal{M}^{conv,post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} &= \left\langle \psi^{(-)}_\alpha \chi^{(-)}_\alpha \right| \overline{V}_\alpha + \overline{V}_\alpha \, G^{(+)} \, \overline{V}_\alpha \left| \varphi_{n_\alpha} \, \chi^{(+)}_{\mathbf{q}_i} \right\rangle \\ &= \left\langle \psi^{(-)}_\alpha \chi^{(-)}_\alpha \left| \overline{V}_\alpha \right| \Psi^{(+)}_{\mathbf{q}_i} \right\rangle . \end{aligned} \tag{5.22}$$

We call Eq. (5.22) the conventional post form amplitude because the channel wave function in the final-state (bra state) is given by the factorized form. To derive Eq. (5.22) from the exact prior form we used seemingly trivial manipulations. Since in the presence of Coulomb interactions the operator $\overline{V}_\alpha \, G^{(+)} \, \overline{V}_\alpha$ is noncompact, it is not evident that Eq. (5.22) coincides with the original prior form of the breakup amplitude (5.19). To verify this we transform the volume integral in Eq. (5.22) into a surface integral encircling the hypersphere in the six-dimensional space. Allowing for

$$(E - T) \, \Psi^{(+)}_{\mathbf{q}_i} = V \, \Psi^{(+)}_{\mathbf{q}_i}, \tag{5.23}$$

and

$$(E - T) \, \psi^{(-)}_\alpha \chi^{(-)}_\alpha = (V_\alpha + U_\alpha) \, \psi^{(-)}_\alpha \chi^{(-)}_\alpha, \tag{5.24}$$

we can rewrite Eq. (5.22) in the form

$$\mathcal{M}^{conv,post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} = \left\langle \psi^{(-)}_\alpha \chi^{(-)}_\alpha \left| \overleftarrow{T} - \overrightarrow{T} \right| \Psi^{(+)}_{\mathbf{q}_i} \right\rangle , \tag{5.25}$$

where the operator $\overleftarrow{T}$ ($\overrightarrow{T}$) acts on the function to the left (right). Using Green's theorem we transform $\mathcal{M}^{conv,post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i}$ into a surface integral

$$\mathcal{M}^{conv,post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} = \frac{1}{2}\frac{m^2}{(\mu_\alpha M_\alpha)^{3/2}} \lim_{R\to\infty} R^5 \int \mathrm{d}\,\hat{\mathbf{r}}_\alpha \mathrm{d}\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} \mathrm{d}\phi_\alpha \sin^2(\phi_\alpha)\cos^2(\phi_\alpha) \times \left[\psi_\alpha^{(-)*}\chi_\alpha^{(-)*}\frac{\partial}{\partial R}\Psi^{(+)}_{\mathbf{q}_i} - \Psi^{(+)}_{\mathbf{q}_i}\frac{\partial}{\partial R}(\psi_\alpha^{(-)*}\chi_\alpha^{(-)*})\right]. \tag{5.26}$$

Here,

$$\phi_\alpha = \arctan\left[(\mu_\alpha/M_\alpha)^{1/2}\, r_\alpha/\rho_\alpha\right], \qquad 0 \le \phi_\alpha \le \pi/2. \tag{5.27}$$

In order to calculate this integral we take into account the asymptotic behavior of $\Psi^{(+)}_{\mathbf{q}_i}$ (see Eqs.(4.39), and (4.45) in Chapter IV) :

$$\Psi^{(+)}_{\mathbf{q}_i} = \varphi_{n_\alpha}\,\chi^{(+)}_{\mathbf{q}_i} + \Phi_i^{(sc)(+)} + ... \tag{5.28}$$

The dots assume that the two-body rearrangement terms are included. First we show that when substituting Eq. (5.28) into (5.26) the integral containing $\varphi_{n_\alpha}\,\chi^{(+)}_{\mathbf{q}_i}$ dissapears. Then the integral containing $\overleftarrow{T}_{\boldsymbol{\rho}_\alpha} - \overrightarrow{T}_{\boldsymbol{\rho}_\alpha}$ vanishes because of the orthogonality of the $(\beta\,\gamma)$ bound state wave function $\varphi_{n_\alpha}(\mathbf{r}_\alpha)$ and scattering state wave function $\psi_\alpha^{(-)}(\mathbf{r}_\alpha)$. The integral containing $\overleftarrow{T}_{\mathbf{r}_\alpha} - \overrightarrow{T}_{\mathbf{r}_\alpha}$ also vanishes: the volume integral over $\mathbf{r}_\alpha$ can be transformed to the surface integral with infinitely large radii. Since the bound state wave function exponentially fades away, the surface integral vanishes for $r_\alpha \to \infty$. Similarly the integrals containing the terms in Eq. (5.28) shown by dots also vanish. The only nonzero integral is generated by the three-body scattered wave $\Phi_i^{(sc)(+)}$ whose explicit form has been derived is given by Eq. (5.20). Taking into account the factorized asymptotic wave function (5.11) for the final state $\psi_\alpha^{(-)}\chi_\alpha^{(-)}$

and the asymptotic scattered wave (5.20) Eq. (5.26) takes the form:

$$\mathcal{M}^{conv,post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} = \frac{m^2}{(\mu_\alpha\, M_\alpha)^{3/2}} \frac{i}{2} \lim_{R\to\infty} R^5$$
$$\times \int \mathrm{d}\hat{\mathbf{r}_\alpha} \mathrm{d}\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} \mathrm{d}\phi_\alpha\, \sin^2(\phi_\alpha)\, \cos^2(\phi_\alpha)\, e^{-i\boldsymbol{k}_\alpha\cdot\,\mathbf{r}_\alpha} e^{-i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} \Phi(\hat{\mathbf{r}}_\alpha, \hat{\boldsymbol{\rho}}_\alpha)$$
$$\times \left[\kappa + \boldsymbol{k}_\alpha \cdot \hat{\mathbf{r}_\alpha} \sqrt{m/\mu_\alpha}\, \sin(\phi_\alpha) + \boldsymbol{q}_\alpha \cdot \hat{\boldsymbol{\rho}_\alpha} \sqrt{m/M_\alpha} \cos(\phi_\alpha)\right], \qquad (5.29)$$

where for simplicity we have defined $\Phi_i^{(sc,0)(+)} \widetilde{\psi}_\alpha^{(-)*} \widetilde{\chi}_\alpha^{(-)*} \equiv \Phi(\hat{\mathbf{r}}_\alpha, \hat{\boldsymbol{\rho}}_\alpha)$. The integrations over $\hat{\boldsymbol{\rho}}_\alpha$ and $\hat{\mathbf{r}}_\alpha$ are straightforward after using the asymptotic equation for the plane wave as $r_\alpha,\ \rho_\alpha \to \infty$:

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \frac{2\pi}{ikr}[\delta(\hat{\mathbf{k}} - \hat{\mathbf{r}})e^{ikr} - \delta(\hat{\mathbf{k}} + \hat{\mathbf{r}})e^{-ikr}]. \qquad (5.30)$$

Then we have

$$\mathcal{M}^{conv,post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} = \frac{m^2}{(\mu_\alpha M_\alpha)^{3/2}} \frac{i}{2} \lim_{R\to\infty} R^5 \qquad (5.31)$$
$$\times \int_0^{\frac{\pi}{2}} \mathrm{d}\phi_\alpha \sin^2(\phi_\alpha) \cos^2(\phi_\alpha) \frac{2\pi}{ik_\alpha r_\alpha} \frac{2\pi}{iq_\alpha \rho_\alpha}$$
$$\times \left\{ e^{ik_\alpha r_\alpha + iq_\alpha\rho_\alpha} \Phi(-\hat{\mathbf{k}}_\alpha, -\hat{\mathbf{q}}_\alpha) \left[\kappa - k_\alpha \sqrt{m/\mu_\alpha} \sin(\phi_\alpha) - q_\alpha \sqrt{m/M_\alpha} \cos(\phi_\alpha)\right]\right.$$
$$-e^{ik_\alpha r_\alpha - iq_\alpha\rho_\alpha} \Phi(-\hat{\mathbf{k}}_\alpha, \hat{\mathbf{q}}_\alpha) \left[\kappa - k_\alpha \sqrt{m/\mu_\alpha} \sin(\phi_\alpha) + q_\alpha \sqrt{m/M_\alpha} \cos(\phi_\alpha)\right]$$
$$-e^{-ik_\alpha r_\alpha + iq_\alpha\rho_\alpha} \Phi(\hat{\mathbf{k}}_\alpha, -\hat{\mathbf{q}}_\alpha) \left[\kappa + k_\alpha \sqrt{m/\mu_\alpha} \sin(\phi_\alpha) - q_\alpha \sqrt{m/M_\alpha} \cos(\phi_\alpha)\right]$$
$$\left.-e^{-ik_\alpha r_\alpha - iq_\alpha\rho_\alpha} \Phi(\hat{\mathbf{k}}_\alpha, \hat{\mathbf{q}}_\alpha) \left[\kappa + k_\alpha \sqrt{m/\mu_\alpha} \sin(\phi_\alpha) + q_\alpha \sqrt{m/M_\alpha} \cos(\phi_\alpha)\right]\right\}.$$

This integral is highly oscillatory and only the last term will survive. The remaining integral over ϕ_α can be taken using the stationary point method giving the stationary point

$$k_\alpha \sqrt{m/\mu_\alpha}\, \cos(\phi_\alpha) = q_\alpha \sqrt{m/M_\alpha}\, \sin(\phi_\alpha). \qquad (5.32)$$

Thus we have

$$\begin{aligned}
\mathcal{M}^{conv,prior}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} &= \frac{i}{2}\frac{m^2}{(\mu_\alpha M_\alpha)^{3/2}} \lim_{R\to\infty} R^5 \int_0^{\pi/2} \mathrm{d}\alpha \sin(\phi_\alpha)\cos(\phi_\alpha) \\
&\times \frac{2\pi}{ik_\alpha R\sqrt{m/\mu_\alpha}}\frac{2\pi}{iq_\alpha R\sqrt{m/M_\alpha}} e^{-i(k_\alpha\sqrt{m/\mu_\alpha}\sin(\phi_\alpha)+q_\alpha\sqrt{m/M_\alpha}\cos(\phi_\alpha))R} \\
&\times \Phi(\hat{\mathbf{k}}_\alpha,\hat{\mathbf{q}}_\alpha)\left[\kappa + k_\alpha\sqrt{m/\mu_{bc}}\sin(\phi_\alpha) + q_\alpha\sqrt{m/\mu_{aA}}\cos(\phi_\alpha)\right] \\
&= \frac{m^2}{(\mu_\alpha M_\alpha)^{3/2}} e^{-i\pi/2}\frac{(2\pi)^{5/2}}{i\kappa^{3/2}} \lim_{R\to\infty} e^{-i\kappa R} R^{5/2}\Phi(\hat{\mathbf{k}}_\alpha,\hat{\mathbf{q}}_\alpha). \qquad (5.33)
\end{aligned}$$

Using $\Phi_i^{(sc,0)(+)}$ and the asymptotic behaviour of $\widetilde{\psi}_\alpha^{(-)*}\widetilde{\chi}_\alpha^{(-)*}$ for $r_\alpha \to \infty$, and $\rho_\alpha \to \infty$, that is in the Ω_0 region, the resulting integral boils down to

$$\mathcal{M}^{conv,post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} = \mathcal{M}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} \lim_{R\to\infty} e^{i\,N(R)}, \qquad (5.34)$$

where $N(R)$ is

$$\begin{aligned}
N(R) &= \overline{\eta}_\alpha \ln(2q_\alpha\,\rho_\alpha) - \eta_\beta \ln(2k_\beta\,r_\beta) - \eta_\gamma \ln(2k_\gamma\,r_\gamma) \\
&= (\overline{\eta}_\alpha - \eta_\beta - \eta_\gamma)\ln(2\,\kappa\,R) + \eta_\alpha \ln(\cos^2\phi_\alpha) \\
&- \eta_\beta \ln(\sin^2\phi_\beta) - \eta_\gamma \ln(\sin^2\phi_\gamma). \qquad (5.35)
\end{aligned}$$

Here we have defined hyperspheric angles in other channels similar to (5.27)

$$\phi_\beta = \arctan\left[(\mu_\beta/M_\beta)^{1/2}\ r_\beta/\rho_\beta\right] = \arctan\left[(M_\beta/\mu_\beta)^{1/2}\ k_\beta/q_\beta\right], \qquad 0 \le \phi_\beta \le \pi/2, \qquad (5.36)$$

$$\phi_\gamma = \arctan\left[(\mu_\gamma/M_\gamma)^{1/2}\ r_\gamma/\rho_\gamma\right] = \arctan\left[(M_\gamma/\mu_\gamma)^{1/2}\ k_\gamma/q_\gamma\right], \qquad 0 \le \phi_\gamma \le \pi/2. \qquad (5.37)$$

The phase factor $N(R)$ logarithmically diverges as $R \to \infty$. Thus making seemingly identical transformations we arrive at the post form which does not coincide with the starting prior form. This is the price we have to pay for using a factorized wave function with the wrong asymptotic behavior as the first term in the right-hand-side of Eq. (5.9). Since the conventional post amplitude differs from the exact one by the phase factor, one can still use Eq. (5.22) to calculate the breakup cross section. This is somewhat similar to the case known in atomic physics [54]. Eq. (5.34) is the second main result of this chapter.

3. The exact post form of the breakup amplitude

Now we discuss the derivation of the exact post form breakup amplitude in the presence of the Coulomb interaction. We demonstrate for the first time how to derive an exact expression for the post form of the breakup amplitude for particles of arbitrary masses and charges. Let us consider the exact three-body wave function $\Psi^{(+)}_{\mathbf{q}_i}$ satisfying the Schrödinger equation (5.2). Using Eq. (5.12) we can write it as

$$\Psi^{(+)}_{\mathbf{q}_i} = \varphi_{n_\alpha} \chi^{(+)}_{\mathbf{q}_i} + \Psi^{(sc)(+)}. \tag{5.38}$$

The second term describes all the outgoing waves including the three-body scattered wave $\Phi^{(sc)(+)}$ describing the channel $\alpha + \beta + \gamma$ in the continuum. Substituting it into Eq. (5.2) gives

$$(E - H)\Psi^{(sc)(+)} = \overline{V}_\alpha \, \varphi_{n_\alpha} \, \chi^{(+)}_{\mathbf{q}_i}. \tag{5.39}$$

Taking into account these equations, we transform the prior form of the breakup amplitude (5.19) as follows

$$\begin{aligned}
\mathcal{M}^{prior}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} &= \left\langle \Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| E - \overrightarrow{H} \right| \Psi^{(sc)(+)} \right\rangle && (5.40)\\
&= \left\langle \Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| \overleftarrow{H} - \overrightarrow{H} \right| \Psi^{(sc)(+)} \right\rangle && (5.41)\\
&= \left\langle \Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| \overleftarrow{T} - \overrightarrow{T} \right| \Psi^{(sc)(+)} \right\rangle && (5.42)\\
&= \left\langle \widetilde{\Psi}^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| \overleftarrow{T} - \overrightarrow{T} \right| \Psi^{(sc)(+)} \right\rangle && (5.43)\\
&= \left\langle \widetilde{\Psi}^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| \overleftarrow{T} - \overrightarrow{T} \right| \Psi^{(+)}_{\mathbf{q}_i} \right\rangle = \mathcal{M}^{post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i}. && (5.44)
\end{aligned}$$

As we learned before seemingly evident manipulations in the presence of the Coulomb interaction may not be valid. First we explain all the transformations for the transition from Eq. (5.40) to Eq. (5.44). The transition from Eq. (5.40) to Eq. (5.41) and the consequent transition to Eq. (5.42) are evident taking into account that $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ satisfies Eq. (5.2). To prove that two other matrix elements obtained from Eq. (5.42) are equivalent, we should transform the volume integral to the surface integral encircling an infinitely large hypersphere in the six-dimensional configuration space. Transformation of the matrix element (5.42) into the surface integral gives

$$\left\langle \Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| \overleftarrow{T} - \overrightarrow{T} \right| \Psi^{(sc)(+)} \right\rangle = \frac{1}{2}\,\frac{m^2}{(\mu_\alpha\, M_\alpha)^{3/2}}\, \lim_{R\to\infty} R^5 \int \mathrm{d}\hat{\mathbf{r}}_\alpha \mathrm{d}\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} \mathrm{d}\phi_\alpha \sin^2(\phi_\alpha)\, \cos^2(\phi_\alpha) \times \left[\Psi^{(-)*}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \frac{\partial}{\partial R} \Psi^{(sc)(+)} - \Psi^{(sc)(+)} \frac{\partial}{\partial R} \Psi^{(-)*}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \right]. \tag{5.45}$$

Replacing $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ in Eq. (5.45) by its leading asymptotic term Eq. (3.39)from Chapter III, we can see that only the contribution from the first term $\tilde{\Psi}^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ will survive, leading to

$$\begin{aligned} \mathcal{M}^{prior}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} &= \frac{1}{2}\,\frac{m^2}{(\mu_\alpha\, M_\alpha)^{3/2}}\, \lim_{R\to\infty} R^5 \int \mathrm{d}\hat{\mathbf{r}}_\alpha \mathrm{d}\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} \mathrm{d}\phi_\alpha \sin^2(\phi_\alpha)\, \cos^2(\phi_\alpha) \\ &\times \left[\widetilde{\Psi}^{(-)*}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \frac{\partial}{\partial R} \Psi^{(sc)(+)} - \Psi^{(sc)(+)} \frac{\partial}{\partial R} \widetilde{\Psi}^{(-)*}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \right] = \mathcal{M}^{post}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i}. \end{aligned} \tag{5.46}$$

Eq. (5.46) justifies Eq. (5.43). Substituting here the asymptotic form of $\Psi^{(sc)(+)}$, Eq. (5.20), and Eq. (3.39) we arrive at the identity $\mathcal{M}^{prior}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} \equiv \mathcal{M}^{prior}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i}$ confirming once more that all the transformations are correct. Similary as was done for the conventional integral Eq. (5.26), we can integrate Eq. (5.46) which exactly equals the breakup amplitude without any oscillatory phase because after integration the three distortion factors of $\tilde{\Psi}^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ will be cancelled by the three factors of $\Psi^{(sc)(+)}$. Now in

Eq. (5.46) $\Psi^{(sc)(+)}$ can be replaced by the exact wave function $\Psi^{(+)}_{\mathbf{q}_i}$, because

$$\begin{aligned}&\left\langle \widetilde{\Psi}^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| \overleftarrow{T} - \overrightarrow{T} \right| \varphi_{n_\alpha}(\mathbf{r}_\alpha)\, \chi^{(+)}_{\mathbf{q}_{n_\alpha}}(\boldsymbol{\rho}_\alpha) \right\rangle \\ &= \frac{1}{2}\, \frac{m^2}{(\mu_\alpha\, M_\alpha)^{3/2}} \lim_{R\to\infty} R^5 \int \mathrm{d}\hat{\mathbf{r}}_\alpha \mathrm{d}\hat{\boldsymbol{\rho}}_\alpha \int_0^{\pi/2} \mathrm{d}\phi_\alpha \sin^2(\phi_\alpha)\, \cos^2(\phi_\alpha) \\ &\times \left[\widetilde{\Psi}^{(-)*}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \frac{\partial}{\partial R} \left(\varphi_{n_\alpha}(\mathbf{r}_\alpha) \chi^{(+)}_{\mathbf{q}_i}(\boldsymbol{\rho}_\alpha) \right) - \varphi_{n_\alpha}(\mathbf{r}_\alpha) \chi^{(+)}_{\mathbf{q}_i}(\boldsymbol{\rho}_\alpha)\, \frac{\partial}{\partial R} \widetilde{\Psi}^{(-)*}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \right] = 0,\end{aligned} \tag{5.47}$$

which follows from the discussion of the integral in Eq. (5.26). The replacement of $\Psi^{(sc)(+)}$ by $\Psi^{(+)}_{\mathbf{q}_i}$ justifies Eq. (5.44). Thus we derived the exact post form amplitude from the prior form. As we see, it can be written as a volume integral with kinetic energy operators or a surface integral encircling an infinitely large hypersphere in the six-dimensional configuration space. Eq. (5.46) is the third main result of this chapter. We emphasise that the post form reduces to the conventional form (5.22) when the interactions are short-range. From the results here we can see that only the prior form of the breakup amplitude can be written as the volume integral with the transition operators expressed in terms of the interaction potentials. However, the prior form contains the exact three-body scattering wave function of the first type, which is known only asymptotically.

D. The DWBA amplitude for Coulomb breakup

1. Conventional DWBA amplitude for breakup processes with charged particles

Since the exact three-body wave function of the first type $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ and of the second type $\Psi^{(+)}_{\mathbf{q}_i}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ are not available in practical calculations of breakup processes, the distorted-wave-Born-approximation (DWBA) is being used. A conventional DWBA amplitude can be obtained by omitting the second term on the r.h.s. of Eq. (5.9) or equivalently the second term in the transition operator in Eq. (5.22). Then the exact prior-form amplitude reduces to the conventional DWBA one:

$$\mathcal{M}^{DW\,conv}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} = \left\langle \psi^{(-)}_\alpha \chi^{(-)}_\alpha \left| \overline{V}_\alpha \right| \varphi_{n_\alpha}\, \chi^{(+)}_{\mathbf{q}_i} \right\rangle . \tag{5.48}$$

However, as we have indicated before, the second term in the transiton operator in Eq. (5.22) cannot be neglected. It is a very important point which needs special attention. In the few-body approach with charged particles, the operators $\overline{V}^{(C)}_\alpha\, G^{(+)}$ and $\overline{V}^{(C)}_\alpha\, G^{(+)}\, \overline{V}^{(C)}_\alpha$, where $\overline{V}^{(C)}_\alpha$ is the long-range part of the potential defined in Eq. (5.16), play a crucial role. The operator $\overline{V}^{(C)}_\alpha$ can be written as

$$\overline{V}^{(C)}_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \frac{Z_\beta\, Z_\alpha}{|\boldsymbol{\rho}_\alpha + \lambda_\beta\, \mathbf{r}_\alpha|} + \frac{Z_\gamma\, Z_\alpha}{|\boldsymbol{\rho}_\alpha - \lambda_\gamma\, \mathbf{r}_\alpha|} - \frac{(Z_\beta + Z_\gamma)\, Z_\alpha}{|\boldsymbol{\rho}_\alpha|}, \tag{5.49}$$

where $\lambda_\beta = m_\gamma / m_{\beta\gamma}$, $\lambda_\gamma = m_\beta / m_{\beta\gamma}$. In the asymptotic region Ω_α, where $r_\alpha << \rho_\alpha$, one can use the asymptotic expansion

$$\overline{V}^{(C)}_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = O\left(r_\alpha/\rho^2_\alpha\right) + O\left(r^2_\alpha/\rho^3_\alpha\right) + ... \tag{5.50}$$

Thus in the asymptotic region, Ω_α, the effective Coulomb potential, $\overline{V}^{(C)}_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, decreases faster than the pure Coulomb potential and does not generate any problems. However, the situation is totally different in the asymptotic domain, Ω_0, where all three particles are well separated. In this region r_α and ρ_α are comparable and $\overline{V}^{(C)}_\alpha(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ behaves as the sum of three Coulomb potentials, which do not compensate each other [1]. In this case when the operator $\overline{V}^{(C)}_\alpha\, G^{(+)}$ appears under the integral containing the integration in the Ω_0 region and the energy is above the breakup threshold, the asymptotic decrease of the Green's function and the Coulomb potential $\overline{V}^{(C)}_\alpha$ is not fast enough to provide convergence of the integral. In few-body physics this case has been analyzed in momentum space by Veselova [74, 75]. If we write the integral in a momentum representation, the singularity of the operator $\overline{V}^{(C)}_\alpha\, G^{(+)}$ becomes noncompact due to the coincidence of the forward singularity of $\overline{V}^{(C)}_\alpha$ and the pole singularity of $G^{(+)}$. It also means that the perturbation expansion of the total Green's function over the channel Green's functions does not converge. It is easy to see that in the presence of the Coulomb interaction the matrix element in Eq. (5.22) generated by the transition operator $\overline{V}_{\alpha}(\mathbf{r}'_{\alpha}, \boldsymbol{\rho}'_{\alpha})\, G^{(+)}(\mathbf{r}'_{\alpha}, \boldsymbol{\rho}'_{\alpha}; \mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})\, \overline{V}_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ is not small compared to the DWBA matrix element defined in Eq. (5.48). Due to the presence of the bound state wave function $\varphi_{n_{\alpha}}$ in the ket state, the integration over $\mathbf{r}_{\alpha}$ is protected while the integration over $\boldsymbol{\rho}_{\alpha}$ is not. In contrast the integration over $\mathbf{r}'_{\alpha}$ and $\boldsymbol{\rho}'_{\alpha}$ on the left-hand-side extends to infinity. It means that we need to know the asymptotic behavior of the operator $\overline{V}_{\alpha}(\mathbf{r}'_{\alpha}, \boldsymbol{\rho}'_{\alpha})\, G^{(+)}(\mathbf{r}'_{\alpha}, \boldsymbol{\rho}'_{\alpha}; \mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})\, \overline{V}_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ in the asymptotic regions $(r_{\alpha}, \rho_{\alpha}) \in \Omega_{\alpha}$ and $(r'_{\alpha},\, \rho'_{\alpha}) \in \Omega_0$. The asymptotic form of the three-body Green function in these asymptotic regions is $\sim \exp(i\,\kappa\, R)/R^{5/2}$ [53]. Besides, in Ω_0, $r'_{\alpha} \sim \rho'_{\alpha}$ and $\overline{V}^{(C)}_{\alpha}(\mathbf{r}'_{\alpha}, \boldsymbol{\rho}'_{\alpha}) \sim 1/R$. Hence the integral in the six-dimensional space over $X' = (\mathbf{r}'_{\alpha}, \boldsymbol{\rho}'_{\alpha})$ does not converge. From the mathematical point of view, the operator $\overline{V}_{\alpha}\, G^{(+)}\, \overline{V}_{\alpha}$ is not compact. Hence the matrix element (5.48) taken from the first term of the operator $\overline{V}_{\alpha} + \overline{V}_{\alpha}\, G^{(+)}\, \overline{V}_{\alpha}$ is not the first-order perturbation term of the exact amplitude for breakup reactions with charged particles. This is the fourth main result of this chapter.

2. From the exact prior form to the DWBA amplitude

One of the evident flaws of the conventional DWBA amplitude is the missing post-decay Coulomb acceleration [76] contribution. This higher order effect is generated by the final-state Coulomb interaction between fragments β and γ and the target-nucleus α. Classically fragments β and γ moving in the Coulomb field of the third particle α will be accelerated differently if their charge/mass ratio is different. Classically and quantum mechanically it is a genuine three-body effect. However, if one uses the factorized wave function in the final-state the post-decay Coulomb acceleration effect disappears [76]. A better approximation for the final-state wave function, is to replace $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ by its extended asymptotic form $\Psi^{(\alpha)(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$, obtained in Chapter III, Eq. (3.39). Now a question arises: can we really write down the DWBA amplitude for breakup reactions for charged particles? The idea of DWBA is to replace the three-body wave function in the exact matrix by the "channel" wave function given by the product of the two-body wave functions so that the DWBA matrix element becomes the first order perturbation term in powers of the transition operator. DWBA works quite well for transfer reactions where the initial and final state channel wave functions are well defined. However, this is not the case for breakup processes. Since the post form of the amplitude is written in terms of kinetic energy operators, replacement of $\Psi^{(+)}_{\mathbf{q}_i}$ in Eq. (5.44) by the first term on the right-hand-side of Eq. (5.28) gives a matrix element equal to zero. This is evident after transformation of the volume matrix element in Eq. (5.44) to the surface one. Thus, derivation of the breakup amplitude can be derived only from the prior form given by Eq. (5.19). However, it is impossible to determine the final-state channel wave function which describes all three particles in the continuum and which is a solution of the Schrödinger equation in all the asymptotic regions. It means that there is no three-body incident wave with the correct asymptotic boundary conditions in all the asymptotic regions which can replace the exact final-state wave function $\Psi^{(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ to get the first order perturbation matrix element. Under specific kinematic conditions one of the four asymptotic regions ($\Omega_\nu,\ \nu = \alpha,\, \beta,\, \gamma,\, 0$) can give a dominant contribution to the reaction amplitude. For example, if the main contribution to the prior breakup matrix element comes from the region $\Omega_\alpha : r_\alpha << \rho_\alpha$ the exact prior matrix element can be approximated by [76]

$$\mathcal{M}^{DW}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha;\mathbf{q}_i} = \left\langle \Psi^{(\alpha)(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} \left| \overline{V}_\alpha \right| \varphi_{n_\alpha}\, \chi^{(+)}_{\mathbf{q}_i} \right\rangle . \tag{5.51}$$

$\Psi^{(\alpha)(-)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ is given by Eq. (53) of Ref. [17]. The amplitude (5.51) can be considered as the generalized DWBA amplitude for peripheral breakup processes in Ω_α. If kinematic conditions are such that the dominant contribution in the final-state comes from the interaction, for example, between particles α and γ, then the final-state three-body scattering wave function in Eq. (5.19) can be replaced by the leading asymptotic term in the asymptotic region Ω_β. This asymptotic function Eq. (3.39) has been derived in Chapter III. Note that to derive the leading asymptotic term in Ω_β proper interchange of indexes should be done in this equation.

E. Conclusion

Summarizing, a time-independent theory of the breakup processes in the presence of Coulomb interactions has been presented in this chapter. The exact prior form breakup amplitude has been derived using the spectral decomposition of the three-body Green's function. We also demonstrated the flaws of the conventional approach based on using of the incident three-body wave in the factorized form. The important result of this chapter is that the post form breakup amplitude derived from the prior form is given by a volume integral containing the exact final state three-body scattering wave function and the initial two-body channel wave function with the transition operator being expressed in terms of kinetic energy operators. We show that both the prior and post forms of the breakup amplitude can be written in terms of surface integrals in the six-dimensional hyperspace. The resulting expression for the asymptotic scattered three-body wave, Eq. (5.20), and the breakup amplitude (5.46) in terms of the surface integral in the six dimensional hyperspace can be used as a basis for the determination of the breakup amplitude from "ab-initio" calculations of the Schrödinger equation in configuration space. By matching the computer output with the boundary conditions Eq. (5.20), one can determine directly the breakup amplitude. However, such a procedure calls for very accurate calculations, because the calculations of the Schrödinger equation should start from the internal region and expand to asymptotically large distances. In such numerical calculations errors will be accumulated. Another approach is to interpolate the computer output for the outgoing three-body wave and to substitute it into the surface integral (5.46) which can give more accurate results than the first method.

We also discussed a flaw of the conventional DWBA and showed that, due to the presence of noncompact operators, the conventional procedure for writing a general expression for the DWBA amplitude may lead to a wrong result. For peripheral collisions in the asymptotic region, where two fragments are close to each other and far away from the spectator gives the dominant contribution, we suggest a generalized prior DWBA amplitude. This amplitude containing the asymptotic three-body Coulomb scattering wave function has been derived in Chapter IV.

CHAPTER VI

NONRADIATIVE TRIPLE COLLISIONS $^7Be(ep,e)^8B$ AND $^7Be(pp,p)^8B$ IN STELLAR ENVIRONMENTS

A. Introduction

In this chapter, the impact of stellar matter on reaction rates is considered under conditions existing in different stellar environments from the Sun's core to the X-ray burst's surface. Our purpose is to investigate the reaction rates of triple collisions, where a third particle is a spectator, and to compare them with reaction rates of the corresponding binary processes. In this work we estimate the reaction rates of ^{7}Be$(ep,e)^8$B and ^{7}Be$(pp,p)^8$B triple collisions leading to the nonradiative formation of ^{8}B. In general triple collisions have small probability, therefore these triple reactions are not included in stellar model calculations. But only direct calculations can show how small they are and the conditions when they might be important. It is well known that binary and sequential reactions like the triple α process are dominant in stellar conditions. Binary collisions have higher probability than triple collisions if both processes are not restricted by some quantum rules. That is why most reactions taking place in the stellar interior are predominantly binary. But conservation laws and selection rules can suppress some binary nuclear reactions, or high temperatures and densities may increase triple reaction rates. Therefore some reasonable calculations should be done to come to a final conclusion. Recently reaction rates were estimated in solar conditions for several triple reactions with an electron spectator [77],[78],[79]. The triple nonradiative reaction rates obtained for solar conditions are approximately 10^4 times smaller than the corresponding binary ones. In this work we estimate the impact of stellar matter on reaction rates under conditions existing in a stellar core, a hydrogen burning envelope in a binary system (nova) or in an X-ray Superburst. There is a static impact, which is also known as screening, and a dynamic impact of matter on a binary reaction in a stellar core. Here we consider the dynamic impact of matter on a binary reaction. Our purpose is to investigate the reaction rates of triple collisions where a third particle is a spectator and to compare them with reaction rates of the corresponding binary processes. Binary radiative capture in the presence of a spectator particle can proceed in two different ways. The first process is the so-called nonradiative capture, when an emitted photon in a binary process is absorbed by a third particle-spectator. The second process is radiative capture, when a photon is emitted in triple collisions. The radiative triple collisions are more difficult to analyze than the nonradiative ones. In this work we present calculations of reaction rates for nonradiative triple collisions. A quantum mechanical description of triple collisions dictates a knowledge of the three-body Coulomb scattering wave function in the initial state. It is the three-body scattering wave function of the first type (see Chapter III) since it evolves from the three-body incident wave. Due to the strong Coulomb barrier at stellar energies, the proton spectators interact with nuclei involved in the binary radiative process through the Coulomb interaction. Also the the Coulomb barrier keeps a spectator proton far away from the colliding nuclei. Hence, we can use the leading asymptotic terms of the three-body Coulomb scattering wave function in the asymptotic region to describe the initial state where two particles are close to each other and far away from the third. This wave function was found in Chapter III. The calculation of the triple reaction rates may be considered as a practical application of the three-body asymptotic Coulomb scattering wave function of the first type. The presence of the proton spectator changes the relative momentum of the colliding nuclei involved in the capture process, which may affect the cross section of the binary process. It is a genuine three-body effect [16, 17].

The same asymptotic wave function can be used to calculate the triple nonradiative process for electron spectators. In this case the Coulomb interaction between electron spectators and colliding nuclei is attractive, so the electron can be quite close to the interacting nuclei. However, the average distance between elctrons in a stellar plasma is significantly larger then the radius of the binary process. That is why the use of the three-body Coulomb asymptotic scattering wave function in the asymptotic region is justified. We use this three-body scattering wave function to estimate the reaction rates of nonradiative triple collisions and compare it with binary reaction rates.

We do calculations for the $^7Be(p,\gamma)^8\mathrm{B}$ capture reaction in the presence of a spectator electron or proton which absorbs the emitted photon. In particular, we estimate the reaction rates for the $^7Be(ep,e)^8\mathrm{B}$ and $^7Be(pp,p)^8\mathrm{B}$ triple collisions. These triple reactions are not included in solar model calculations since they are supposed to be very small. It is understandable because the ratio of the triple to binary reaction rates is $V_R\, n_\alpha$, where V_R is the reaction volume and n_α is the spectator particle number density. The effective volume of the nonradiative capture processes can be quite large and the ratio depends on the spectator particle number density. Only direct calculations can reveal the relative contribution of the triple collisions in different astrophysical environments.

The reaction rates of the binary $^7Be(p,\gamma)^8\mathrm{B}$ radiative process are calculated within the framework of the R-matrix approach [80, 81, 82, 83, 84] in the temperature range from 1.4×10^7K to 10^9K. As this reaction is extremely peripheral [85, 86], the overlap function $\langle ^7\mathrm{Be}|^8\mathrm{B}\rangle$ of the bound-state wave functions is approximated by its asymptotics with the amplitude given by the asymptotic normalization constant (ANC) for the virtual synthesis of $^7\mathrm{Be}+p\rightarrow {}^8\mathrm{B}$ [87], [88],[89], [90]. A general expression for the triple reaction rate has been derived in [91]. We will estimate the reaction rates of $^7Be(ep,e)^8$B and $^7Be(pp,p)^8$B in the range from $1.4 \times 10^7\,K$, corresponding to solar core conditions, to $10^9 K$ corresponding to the hydrogen burning envelope in novae and X-ray burts. Calculations of nucleosynthesis in novae cover temperature ranges from $0.145 \times 10^9\,K$ to $0.418 \times 10^9\,K$ and densities from 10 $g\,cm^{-3}$ to 10^5 $g\,cm^{-3}$ [92]. As a result of successive X-ray bursts, ^{12}C nuclei are accumulated in superbursts with densities significantly higher than in normal X-ray bursts. As was pointed out in [93], X-ray superbursts from accreting neutron stars, following X-ray bursts, present a unique opportunity to probe nuclear processes at superhigh densities and temperatures. Note that type I X-ray bursts are thermonuclear flashes of accumulated hydrogen and helium on an accreting neutron star. Superbursts are a new class of type I bursts which were discovered recently [94], [95], [96], [97]. In a superburst the density reaches $\rho \approx 10^9\,g\,cm^{-3}$ and the temperature $T > 10^9\,K$. At densities and temperatures existing in the superburst the reaction rates of triple collisions can be comparable with the reaction rates of the corresponding binary collisions.

This chapter is organized as follows. In Sec. B we address general definitions and important relations for a binary process. In Sec. C we present reaction rate for triple nonradiative collisions and we discuss the approximations we made in calculation of matrix elements and reaction rates for the $^7Be(ep,e)^8$B and $^7Be(pp,p)^8$B nonradiative collisions. Finally the results are presented and discussed in Sec. D.

B. Binary reaction rate

Here we recall some of the important relations and definitions concerning a binary process $\beta + \gamma \rightarrow \beta' + \gamma'$ [98, 99]. The reaction rate is one of the important nuclear astrophysical inputs to calculate element synthesis in stars. An understanding of the most critical stellar features, such as time scale, energy production, and nucleosynthesis of elements, depends directly on the magnitude of the reaction rate per particle pair for a number of reactions. Depending on the magnitude of the reaction rates different stellar models are constructed. These models can lead to different predicted fates for a particular star. Stellar matter in its core consists of hot plasma where mainly binary reactions take place.

Let us consider a stellar plasma with $n_{\beta(\gamma)}$ particles per unit volume of type $\beta(\gamma)$ with relative velocities v. The reaction rate per unit volume between particles of type β and γ is

$$r_{\beta\gamma} = \frac{n_\beta n_\gamma}{1+\delta_{\beta\gamma}} \left\langle \sigma v \right\rangle_{\beta\gamma}, \tag{6.1}$$

where $\left\langle \sigma v \right\rangle_{\beta\gamma}$ is the velocity averaged product of cross section and relative velocity, or average reaction rate per particle pair. The factor $(1+\delta_{\beta\gamma})^{-1}$ is introduced to take into account possible cases when particles β and γ are identical to avoid double counting, where $\delta_{\beta\gamma} = \begin{cases} 1, & \text{If } \beta = \gamma \\ 0, & \text{If } \beta \neq \gamma \end{cases}$. Normal stellar matter is considered to be a nondegenerate gas in thermodynamic equilibrium with particles (except possibly electrons) at nonrelativistic velocities which can be described by a Maxwell-Boltzmann velocity distribution. Therefore the velocity averaged reaction rate per particle pair is

$$\langle \sigma v \rangle = \left(\frac{8}{\pi\mu}\right)^{1/2} \int\limits_0^\infty \sigma(E) e^{-\frac{E}{k_B T}} E dE, \tag{6.2}$$

where $E = \mu v^2/2$ is the nonrelativistic relative kinetic energy of the β and γ nuclei. This equation characterizes the reaction rate per particle pair at a given stellar temperature. As a star evolves, its temperature changes, and, hence, the reaction rate $\langle \sigma v \rangle$ must be evaluated for each temperature of interest. The mean life of the β

nucleus is related to the reaction rate per particle pair as

$$\tau_\beta = \frac{1}{n_\gamma \left\langle \sigma \upsilon \right\rangle_{\beta\gamma}}. \tag{6.3}$$

In most cases mass densities of stellar matter and abundances of nuclei are tabulated rather than the number densities of the corresponding nuclei. Therefore, it is necessary to have a relation between them. Number particle densities are related to the total mass density ρ by

$$n_\beta = N_A \rho \frac{X_\beta}{A_\beta} = N_A \rho Y_\beta, \tag{6.4}$$

where X_β is the mass abundance of nucleus β with atomic number A_β, Y_β is the mole fraction, and N_A is Avogadro's number. If the reaction rate for the inverse process $\beta' + \gamma' \to \beta + \gamma$ is $r_{\beta'\gamma'}$ then the net energy production per unit mass is

$$\epsilon = (r_{\beta\gamma} - r_{\beta'\gamma'}) \frac{Q}{\rho} - \epsilon_\nu, \tag{6.5}$$

where ϵ_ν is the energy taken away by neutrino ν which leaves the star without further interactions.

All nuclear particles have positive charges that repell each other, and the Coulomb interaction prevents them from penetrating into the nuclear interior. Because of the exponential behavior of the probability for tunneling through the Coulomb interaction barrier, the astrophysical S factor is used in nuclear astrophysics instead of the reaction cross section:

$$S(E) = \sigma(E) E e^{2\pi\eta}. \tag{6.6}$$

Here the astrophysical factor $S(E)$ contains all of the nuclear effects. For nonresonant reactions $S(E)$ is a smoothly varying function of energy. Because of that, the astrophysical factor $S(E)$ is much more convenient for comparing different astrophysical processes at astrophysically relevant energies than cross sections.

We can write down the reaction rate per particle pair $\langle\sigma v\rangle$ in terms of the astrophysical S factor:

$$\langle\sigma v\rangle = \left(\frac{8}{\pi\mu}\right)^{1/2} \frac{1}{(kT)^{3/2}} \int\limits_0^\infty S(E) e^{-\frac{E}{k_B T} - (\frac{E_G}{E})^{1/2}} dE, \tag{6.7}$$

where the quantity E_G is called the Gamow energy and is given by

$$E_G = 2\mu(\pi e^2 z_1 z_2/h)^2. \tag{6.8}$$

For nonresonant reactions the energy dependence of the integrand in Eq. (6.7) is governed primarily by the exponential term $e^{-\frac{E}{k_B T} - \sqrt{\frac{E_G}{E}}}$. The penetration through the Coulomb barrier, determined by the Gamow factor $e^{-\sqrt{\frac{E_G}{E}}}$, becomes very small at low energies. The other exponential term, $e^{-\frac{E}{kT}}$, which vanishes at high energies, is a Maxwell-Boltzmann distribution factor. The integrand in Eq. (6.7) has a peak near the energy E_0, which is called a Gamow peak. Although the Maxwell-Boltzmann distribution has a maximum at the energy $E = kT$, the Gamow factor shifts the effective peak to the energy E_0. For a given stellar temperature T, nuclear reactions take place in a relatively narrow energy window around the effective burning energy E_0. If for relatively low energies the $S(E)$ factor is nearly constant over the energy window around the effective energy E_0, that is $S(E) \approx S(E_0)$, then Eq (6.7) can be approximated by

$$\langle\sigma v\rangle = \left(\frac{8}{\pi\mu}\right)^{1/2} \frac{1}{(kT)^{3/2}} S(E_0) \int\limits_0^\infty e^{-\frac{E}{k_B T} - (\frac{E_G}{E})^{1/2}} dE. \tag{6.9}$$

But one should be careful in using this approximation at higher temperatures.

1. Reaction rate of the binary radiative capture reaction $^{7}Be(p,\gamma)^{8}$B

Let us consider the $^{7}Be(p,\gamma)^{8}$B direct radiative capture reaction at stellar conditions. While $^{7}Be(p,\gamma)^{8}B$ reaction is the weakest of the three branches of the $pp-$chain, it is nevertheless important because the $\langle E_\nu\rangle = 7.3MeV$ neutrino produced in the positron decay of ^{8}B, $^{8}B \rightarrow\ ^{8}Be^{*}+e^{+}+\nu$, provides most of the neutrinos detected in many solar neutrino experiments [98, 100]. The solar neutrinos emerge from nuclear reactions which start from hydrogen burning or the so called $pp-$chain in stellar plasma.

According to the standard solar model ^{7}Be nuclei are produced from collisions of ^{3}He and ^{4}He nuclei formed during hydrogen burning through the radiative capture reaction $^{3}He+^{4}He \rightarrow^{7} Be+\gamma$. Then ^{7}Be is destroyed by electron capture which leads to the formation of ^{7}Li and by the proton capture reaction $^{7}Be(p,\gamma)^{8}B$ in $pp-$chain III, which leads to the formation of ^{8}B. The fate of ^{7}Be in the $pp-$chain is of special interest since the measurements of neutrino flux from the Sun lead to a paradoxical conclusion which means the production of ^{7}Be must be strongly suppressed. This paradox, though, was resolved by neutrino oscillation. The energy level scheme for this reaction is given in Fig. 2. The initial state of ^{7}Be$+p$ is defined by their relative momentum $\mathbf{k}_\alpha$, total spin J_i and its z-projection M_i. In the LS angular momentum coupling scheme, the initial scattering wave function describing the relative motion of a ^{7}Be and proton in the continuum is given by

$$\begin{aligned}\psi_{J_i\,M_i\,I_i} &= \sum_{l_i=0}^{\infty} i^{l_i} \sum_{m_i\nu_i}\sum_{M_aM_A} \langle l_i m_i I_i \nu_i | J_i M_i\rangle \langle J_a M_a J_A M_A | I_i \nu_i\rangle \\ &\quad \times \chi_{J_aM_a}\chi_{J_AM_A} Y_{l_i0}(\widehat{r}_\alpha)\sqrt{4\pi(2l_i+1)}\psi_{\lambda l_i}, \qquad (6.10)\end{aligned}$$

where $\psi_{\lambda l_i}$ is the radial scattering wave function, $\langle j_1\, m_{j_1}\, j_2\, m_{j_2} |\, j\, m_j\rangle$is a Clebsch-Gordon coefficient, $l_i\,(m_i)$ is the relative angular orbital momentum (projection) of

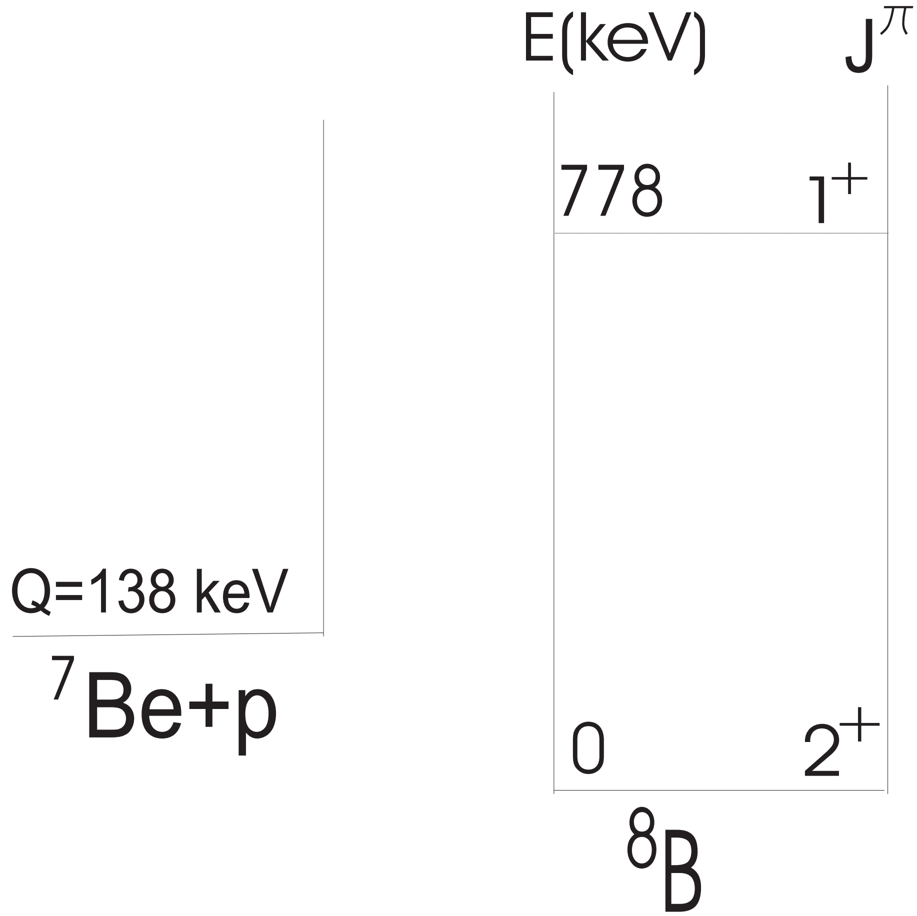

Fig. 2. Low lying energy levels of ^8B. The $^7Be(p,\gamma)^8B$ reaction proceeds at energies below the 640 keV resonance via a direct capture mechanism.

^{7}Be and proton in the initial state, $I_i\,(\nu_i)$ is the channel spin (projection), $J_j\;(M_j)$ is the spin (projection) of particle j, $\chi_{J_j,\,M_j}$ is the spin function of nucleus $j=\beta,\,\gamma$. The final state is described by the overlap function of the bound state wave functions of ^{8}B and ^{7}Be. This overlap function can be written as

$$I_{J_f\,M_f\,I_i} \;=\; i^{l_f}\sum_{m_f\nu_f}\sum_{M'_\gamma M'_\beta}\langle l_f m_f I_i\nu_f|J_f M_f\rangle \tag{6.11}$$

$$\times\left\langle J_\gamma M'_\gamma\,J_\beta M'_\beta|I_f\nu_f\right\rangle\chi_{J_\gamma M'_\gamma}\chi_{J_\beta M'_\beta}Y_{l_f m_f}(\widehat{r}_\alpha)\,I_{I_i\,l_f}. \tag{6.12}$$

Here, $l_f\;(m_f)$ is the relative orbital angular momentum (projection) of ^{7}Be and proton in the ground state of ^{8}B, $J_f\;(M_f)$ is the spin (projection) of ^{8}B, $I_{I_i\,l_f}$ is the radial overlap function. For peripheral radiative capture processes the radial overlap function can be approximated by its asymptotic form:

$$I_{I_i\,l_f}=C_{I_i l_f}\frac{W_{l_f}(r_\alpha)}{r_\alpha}, \tag{6.13}$$

where $C_{I_i\,l_f}$ is the asymptotic normalization coefficient (ANC) for the virtual synthesis of $^7\mathrm{Be}+p\rightarrow{}^8$B and W_{l_f} is the Whittaker function.

In the $R-$matrix method the expression for the S factor for the dipole radiative capture of $^7\mathrm{Be}+p\rightarrow{}^8$B is given by [83]

$$\begin{aligned} S(E) \;=\; & \frac{32\pi}{3}\frac{e^2}{4E}\frac{\hbar^2}{2\mu_\alpha}\frac{(2l_i+1)(2J_f+1)}{(2J_\beta+1)(2J_\gamma+1)(2l_f+1)} \\ & \times k_\gamma^3 P_{l_i}(r_0)^3\mu_\alpha^2\Big(\frac{z_\gamma}{m_\gamma}-\frac{z_\beta}{m_\beta}\Big)^2(\langle l_i 0\,1 0|l_f 0\rangle)^2 \\ & \times\left|F_{l_i}(r_0)G_{l_i}(r_0)W_{l_f}(r_0)J'_1(l_i,l_f)\right|^2 e^{2\pi\eta_\alpha}\sum_{I_i}C^2_{I_i\,l_f}. \end{aligned} \tag{6.14}$$

Here, k_γ is the momentum of the emitted photon, m_β and $z_\beta\,e$ is the mass and charge of ^{7}Be, m_γ and $z_\gamma\,e$ is the mass and charge of the proton, η_α is the Coulomb parameter in the initial channel, $P_{l_i}(r_0)$ is the barrier penetrability, F_{l_i} and G_{l_i} are the regular and singular Coulomb scattering solutions, r_0 is the channel radius and

$$J_1'(l_i, l_f) = \frac{1}{r_0^2} \int_{r_0}^{\infty} dr_\alpha r_\alpha \frac{W_{l_f}(r_\alpha)}{W_{l_f}(r_0)} \left[\frac{F_{l_i}(r_\alpha)}{F_{l_i}(r_0)} - \frac{G_{l_i}(r_\alpha)}{G_{l_i}(r_0)} \right]. \tag{6.15}$$

Finally recalling Eq.(6.7) we have for the binary reaction rate

$$\langle R_2 \rangle = n_p n_{^7\mathrm{Be}} \langle \sigma v \rangle = \sqrt{\frac{8}{\pi \mu_\alpha}} \frac{n_p n_{^7\mathrm{Be}}}{(kT)^{3/2}} \int_0^{\infty} dE\ S(E) e^{-\frac{E}{kT} - (\frac{E_G}{E})^{1/2}}, \tag{6.16}$$

where $n_{^7\mathrm{Be}}$, and n_p are particle densities of ^{7}Be nuclei and protons in stellar matter. At low temperatures using the aproximate equation Eq.(6.9) we can write the binary reaction rates as

$$\langle R_2 \rangle \approx n_p n_{^7\mathrm{Be}} \sqrt{\frac{8}{\pi \mu_\alpha}} \frac{S(E_0)}{(kT)^{3/2}} \int dE e^{-\frac{E}{kT} - (\frac{E_G}{E})^{1/2}}. \tag{6.17}$$

This approximation facilitates numerical calculations giving fairly good results. At high temperatures one has to use Eq.(6.16). Otherwise the approximate equation Eq.(6.17) underestimates the binary reaction rates by an order of magnitude. We have calculated the reaction rates for the binary ^{7}Be$(p, \gamma)^8$B direct radiative process using the R-matrix approach [80],[81],[82] at temperatures of $1.4 \times 10^7 K \leq T \leq 10^9 K$. Results for these reaction rates are presented in Table I.

C. Triple reaction rate

Let us consider the $\alpha + \beta + \gamma \to \alpha + (\beta\gamma)$ nonradiative reaction. Here $(\beta\gamma)$ is the bound state of particles β and γ. We assume that β and γ are close to each other but far away from the third particle α, i. e. our system is in the asymptotic region Ω_α. We suppose collisions occur in a stellar matter containing, respectively, n_α, n_β, and n_γ particles of each type per unit volume. The initial asymptotic state is defined by relative momentum $\mathbf{k}_\alpha$, total spin J_i and third component M_i of the particles β and

γ, and by the momentum $\mathbf{q}_\alpha$ of the spectator particle α with respect to the c.m. of the particles β and γ.

The final asymptotic state consists of the bound state of β and γ particles with spin J_f and projection M_f, and relative momentum $\mathbf{q}'_\alpha$ of the bound state $(\beta\gamma)$ and α. We neglect the spin of the spectator particle because it interacts with them only via the Coulomb force. All particles are assumed to be distinguishable. The multiparticle reaction rate in general form has been derived in [91]. Here we modify this multiparticle reaction rate to the three particle reaction rate in Jacobi coordinate representation. The corresponding triple reaction rate in the Jacobi coordinate system is given by

$$dR_3(\mathbf{k}_\alpha, \mathbf{q}_\alpha \to \mathbf{q}'_\alpha) = (2\pi)^7 d\mathbf{k}_\alpha d\mathbf{q}_\alpha d\mathbf{q}'_\alpha \delta(E_f - E_i)\frac{c}{\hbar c}\left|\mathcal{M}_{if}\right|^2 N_{k_\alpha} N_{q_\alpha} n_\alpha n_\beta n_\gamma, \quad (6.18)$$

where $\mathcal{M}_{if}$ is the transition amplitude for the nonradiative triple process. This equation gives the differential reaction rates for transitions $\alpha + \beta + \gamma \to \alpha + (\beta\gamma)$ per unit volume. In normal stellar matter the stellar gas is nondegenerate and the nuclei move nonrelativistically. The gas is in thermodynamic equilibrium, and the momenta of the nuclei $\mathbf{k}_\alpha$, and $\mathbf{q}_\alpha$ are distributed at temperature T according to the Maxwell-Boltzmann momentum distribution:

$$N_{k_\alpha}(T) = (2\pi\mu_\alpha kT)^{-\frac{3}{2}} \exp(-\frac{k_\alpha^2}{2\mu_\alpha kT}); \quad (6.19)$$

$$N_{q_\alpha}(T) = (2\pi M_\alpha kT)^{-\frac{3}{2}} \exp(-\frac{q_\alpha^2}{2M_\alpha kT}). \quad (6.20)$$

Here k is the Boltzmann constant, N_{k_α}, and N_{q_α} are normalized to unity, μ_ν, and M_ν are reduced masses, which are defined in the previous chapters. We need to average the reaction rate (6.18) over all the initial quantum numbers J_i, M_i, sum over all the final-state quantum numbers M_f and integrate over $\mathbf{k}_\alpha$, $\mathbf{q}_\alpha$, and $\mathbf{q}'_\alpha$. The resulting reaction rate of the triple collision depends only on the temperature of the stellar matter:

$$\langle R_3(T)\rangle = \sum_{J_i,M_i,M_f} \frac{1}{(2J_i+1)} \int dR_3(\mathbf{k}_\alpha, \mathbf{q}_\alpha \to \mathbf{q}'_\alpha). \tag{6.21}$$

Let α to be the spectator-particle (electron or proton), β and γ denote ^{7}Be and proton, correspondingly. By cancelling all particle densities in Eq.(6.21) we arrive at average reaction rate per particle triplet

$$\langle \Sigma(T)\rangle = \frac{\langle R_3(T)\rangle}{n_\alpha n_\beta n_\gamma}. \tag{6.22}$$

Just like the binary reaction rate we can calculate the triple reaction rate per unit volume multiplying Eq. 6.22 by $n_\alpha n_\beta n_\gamma$ at particular temperatures. To estimate the reaction rates of the ^{7}Be$(ep,e)^8$B and ^{7}Be$(pp,p)^8$B processes we assume that the ^{8}B nucleus can be considered as a bound state of a ^{7}Be cluster and a proton. Even at higher temperatures (up to $\sim 10^9 K$) we still can disregard the contributions from excited states of ^{8}B. Our final goal is the ratio of the reaction rates of triple and binary collisions which is given by

$$\frac{\langle R_3(T)\rangle}{\langle R_2(T)\rangle} = \frac{\langle \Sigma(T)\rangle\, N_A^2}{\langle \sigma v(T)\rangle\, N_A} \frac{n_s}{N_A}, \tag{6.23}$$

where N_A is Avagadro's number, n_s is the number spectator-particle density and $\langle R_2(T)\rangle$ is the binary reaction rate for the radiative capture ^{7}Be$(p,\gamma)^8$B given by Eq. (6.16). We consider various approximations for the triple reaction rate (6.21) below.

1. Matrix element of the triple collision and initial and final state wave functions

Let us consider the matrix element $\mathcal{M}_{if}$ in Eq.(6.18) in detail:

$$\mathcal{M}_{if} = \int\int \frac{d\mathbf{r}_\alpha}{(2\pi)^{3/2}} \frac{d\boldsymbol{\rho}_\alpha}{(2\pi)^3} \Psi_f^{(-)*} \overline{V}_\alpha \, \Psi^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}, \tag{6.24}$$

where the transition operator is given by $\overline{V}_\alpha = V_\beta + V_\gamma - U$, and $V_\nu = V_\nu^C + V_\nu^N$, $\nu = \beta, \gamma$. $U = U^C + U^N$ is the optical potential between α and the (β, γ) bound state in the exit channel and U^N, U^C are its nuclear and Coulomb parts, respectively. U^C is given by

$$U^C = \frac{(z_\beta + z_\gamma)\, z_\alpha\, e^2}{\rho_\alpha}. \tag{6.25}$$

The following are pure Coulomb interactions in β and γ pairs

$$V_\beta^C = \frac{z_\beta z_\alpha\, e^2}{|\boldsymbol{\rho}_\alpha + \lambda_\beta \mathbf{r}_\alpha|} \tag{6.26}$$

$$V_\gamma^C = \frac{z_\gamma z_\alpha e^2}{|\boldsymbol{\rho}_\alpha - \lambda_\gamma \mathbf{r}_\alpha|}, \tag{6.27}$$

where $\lambda_\beta = \mu_\alpha/m_\beta$ and $\lambda_\gamma = \mu_\alpha/m_\gamma$. Initially all three particles are in the three body continuum. Hence, the initial scattering wave function $\Psi^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha}$ is the three-body scattering wave function of the first type (Chapter III). This function is not available, but we need to know it in the asymptotic region Ω_α, where the spectator α is far away from the colliding particles β and γ. The leading asymptotic terms of this wave function were found in Chapter III. We can consider Eq. (3.83) as a starting point. In the asymptotic region Ω_α we can replace the local momenta $\widetilde{\mathbf{k}}_\nu$, $\nu = \beta$, γ in Eq. (3.83) by their asymptotic parts $\mathbf{k}_\nu$, $\nu = \beta$, γ, because in Ω_α $r_\alpha/\rho_\alpha \to 0$. Then we arrive to the generalized wave function in the asypmtotic region Ω_α:

$$\Psi^{(+)}_{\mathbf{k}_\alpha,\mathbf{q}_\alpha} = e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} N_\alpha(\boldsymbol{\rho}_\alpha) F(-i\eta_\alpha(\rho_\alpha), 1, i\xi_\alpha(\boldsymbol{\rho}_\alpha)) \prod_{\nu=\beta,\gamma} N_\nu F(-i\eta_\nu, 1, \xi_\nu), \tag{6.28}$$

where $\eta_\alpha(\boldsymbol{\rho}_\alpha) = \frac{z_\beta\, z_\gamma\, e^2 \mu_\alpha}{\widetilde{\mathbf{k}}_\alpha}$ is the Coulomb parameter, $N_\alpha(\boldsymbol{\rho}_\alpha) = e^{-\frac{\pi\eta_\alpha(\rho_\alpha)}{2}}\Gamma(1+i\eta_\alpha(\boldsymbol{\rho}_\alpha))$ is the normalization factor, and $\xi_\alpha(\boldsymbol{\rho}_\alpha) = \widetilde{k}_\alpha r_\alpha - \widetilde{\mathbf{k}}_\alpha \cdot \mathbf{r}_\alpha$ is the parabolic coordinate. The factor $N_\alpha(\boldsymbol{\rho}_\alpha)\, F(-i\eta_\alpha(\rho_\alpha), 1, i\xi_\alpha(\boldsymbol{\rho}_\alpha))$ takes into account the scattering of particles β and γ. The dependence on $\boldsymbol{\rho}_\alpha$ reflects the distortion of the relative motion of particles β and γ caused by the presence of the spectator particle. The local momentum in the α channel is

$$\widetilde{\mathbf{k}}_\alpha = \mathbf{k}_\alpha + \delta\mathbf{k}_\alpha \tag{6.29}$$

$$= \mathbf{k}_\alpha + \sum_{\nu=\beta,\gamma} \frac{m_\nu}{m_{\beta\gamma}} \frac{\eta_\nu}{\rho_\alpha} \frac{\widehat{\mathbf{k}}_\nu - \epsilon_{\alpha\nu}\widehat{\boldsymbol{\rho}}_\alpha}{1 - \epsilon_{\alpha\nu}\widehat{\mathbf{k}}_\nu \cdot \widehat{\boldsymbol{\rho}}_\alpha}. \tag{6.30}$$

Momenta $\mathbf{k}_\nu$ for $\nu = \beta, \gamma$ of the ν pairs can be expressed in terms of the α channel momenta as

$$\mathbf{k}_\nu = -\epsilon_{\nu\alpha} \frac{\mu_\alpha}{M_\nu} \mathbf{q}_\alpha - \frac{m_\alpha}{M - m_\nu} \mathbf{k}_\alpha. \tag{6.31}$$

In Eq. (6.28) we disregarded the nuclear interaction between β and γ in the initial state because the ^{7}Be$(p,\gamma)^8$B reaction is extremely peripheral. The last two factors $N_\beta\, F(-i\eta_\beta, 1, \xi_\beta)$ and $N_\gamma\, F(-i\eta_\gamma, 1, \xi_\gamma)$ take into account $\gamma + \alpha$ and $\beta + \alpha$ scatterings, caused by the long range Coulomb interaction. The wave function (6.28) will be used in this work to describe the initial three-body scattering state in triple stellar collisions. As usual the final bound-state wave function is normalized as:

$$\Big\langle \Phi_{J_f M'_f\, I'_f}(\mathbf{r}_\alpha) | \Phi_{J_f M_f\, I_f}(\mathbf{r}_\alpha) \Big\rangle = \delta_{J_f J'_f} \delta_{M_f M'_f}. \tag{6.32}$$

Now let us consider the ^{7}Be$(p,\gamma)^8$B radiative capture reaction in the presence of an electron or proton spectator. First we analyze common features for both cases then in the next sections we treat them seperately. The final state is the two-body continuum state of ^{8}B and the spectator particle described by the scattering wave function

$$\Psi^{(-)}_{\mathbf{q}'_\alpha}(\boldsymbol{\rho}_\alpha) = e^{i\mathbf{q}'_\alpha\cdot\boldsymbol{\rho}_\alpha} N F(i\eta, 1, -i\xi). \tag{6.33}$$

Here, the parabolic coordinate and momentum in the final state are given by the equations $\xi = q'_\alpha\rho_\alpha + \mathbf{q}'_\alpha \cdot \boldsymbol{\rho}_\alpha$, and $q'_\alpha = \sqrt{2\mu(\varepsilon_b + \frac{k_\alpha^2}{2\mu_\alpha} + \frac{q_\alpha^2}{2M_\alpha})}$, respectively. Since our aim is to estimate nonradiative reaction rates for ^{7}Be$(ep, e)^8$B, and ^{7}Be$(pp, p)^8$B, we can proceed with further simplifications. For charged particles with small energies, a window around the most efficient energy is enough to estimate the reaction rate. Contributions from energies smaller and larger then the effective energy are cut by the penetration factor and by Maxwell distributions, respectively. Even when the spectator particle is an electron which is attracted toward the positively charged pair (^{7}Be$, p$), we still can restrict the calculations to electron energies around the Maxwell peak energy which will dominate the reaction rate. Because $m_e/m_\alpha << 1$, where m_e is the electron mass amd $m_\alpha = m_{^7\mathrm{Be}}$ is the ^{7}Be mass, the Coulomb parameters for $\nu = \beta, \gamma$ pairs characterizing the Coulomb interactions of the electron with the ^{7}Be nucleus and the proton will be very small at energies around the Maxwell peak: $\eta_\nu \ll 1$.

The reaction rates for the ^{7}Be$(pp, p)^8$B process is more difficult to calculate but we still can use approximations similar to those used for the electron-spectator case. In contrast to the electron case, the proton spectator has the Coulomb barrier. In this case the Gamow peak energy of both protons dominates when calculating the reaction rates. At energies around the Gamow peak we can replace the local momentum $\widetilde{\mathbf{k}}_\alpha$ by the local momentum $\mathbf{k}_\alpha$ because $\frac{|\delta\mathbf{k}_\alpha|}{k_\alpha^G} \ll 1$. Here k_α^G is the relative momentum of β and γ at the Gamow peak for the ^{7}Be$(p, \gamma)^8$B reaction. We distinguish protons assuming one is closer to ^{7}Be and the second one is the spectator, which is far away from the colliding ^{7}Be and proton, i.e. $r_\alpha \ll \rho_\alpha$. This approximation will help us to integrate the matrix element using the stationary phase method.

Taking into account $|\mathbf{k}_\alpha| \gg |\delta\mathbf{k}_\alpha|$ and using the Taylor's expansion in Eq. (6.28) we get

$$N_\alpha(\boldsymbol{\rho}_\alpha)F(-i\eta_\alpha(\boldsymbol{\rho}_\alpha),1,i\xi_\alpha(\boldsymbol{\rho}_\alpha)) \approx N_\alpha F(-i\eta_\alpha,1,i\xi_\alpha)$$
$$\times[1+i\frac{\eta_\alpha}{k_\alpha}(\frac{\pi}{2}-i\psi(1+i\eta_\alpha))\frac{\delta\mathbf{k}_\alpha\cdot\widehat{\mathbf{k}}_\alpha}{\rho_\alpha}], \tag{6.34}$$

where $\psi(1+i\eta_\alpha)$ is the derivative of the Γ-function. If we disregard the $O(1/\rho_\alpha)$ term in Eq. (6.34), then Eq. (6.28) transforms to the 3C asymptotic three-body wave function in the Ω_0 region. This wave function has been found in Chapter III. As particles which we are considering have spins, we have to couple their spins with the orbital angular momenta. This is done by carrying out a partial wave expansion of the scattering wave function and coupling it to the spin. The spins of the ^{7}Be and proton are $\frac{3^-}{2}$, and $\frac{1}{2}$, respectively. We couple these into a channel spin. The ground state of ^{8}B is 2^+ and the relative orbital angular momentum of the ^{7}Be and proton is $l_f = 1$. The dipole transition in the binary capture ^{7}Be$(p,\,\gamma)^8$B is dominated by the $l_i = 0 \to l_f = 1$ transition. Therefore, in the partial wave expansion of the initial scattering wave function we may retain only the term with $l_i = 0$ for the part describing the relative motion of particles β and γ. The partial wave expansion of the wave function $e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}N_\alpha F(-i\eta_\alpha,1,i\xi_\alpha)$ describing the relative motion of $^7\mathrm{Be}+p$ is given by

$$e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha}N_\alpha F(-i\eta_\alpha,1,i\xi_\alpha) = \sum_{l_i=0}^{\infty}\sqrt{4\pi(2l_i+1)}\,i^{l_i}e^{i\delta_{l_i}}\frac{F_{l_i}(\eta_\alpha,k_\alpha r_\alpha)}{k_\alpha r_\alpha}Y_{l_i0}(\widehat{r}_\alpha). \tag{6.35}$$

Using this partial wave expansion we can couple the partial waves with the channel spin. Recalling Eqs.(6.10) and (6.13) we have for the initial three-body scattering state

$$\Phi_i^{(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) \approx \Phi_{\lambda J_i M_i}^{I_i} e^{i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \prod_{\nu=\beta,\gamma} N_\nu F(-i\eta_\nu, 1, \xi_\nu), \tag{6.36}$$

and for the final state $^8\mathrm{B} + p$, where $^8\mathrm{B} = (^7\mathrm{Be}\, p)$

$$\Psi_f(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \Phi_{\lambda J_f M_f}^{I_f}(\mathbf{r}_\alpha) \Psi_{q'_\alpha}^{(-)}(\boldsymbol{\rho}_\alpha) \tag{6.37}$$

We disregard the spin of the spectator particle because it is far away and, hence, interacts with the colliding ^{7}Be and proton only via the Coulomb force which does not depend on spin.

2. Triple reaction rate for the nonradiative $^7\mathrm{Be}(e^- p, e^-)^8\mathrm{B}$ reaction

Due to the high density of the stellar plasma, the ^{7}Be, proton and electron form a three-body initial state, which can lead to the following nonradiative reaction, $^7\mathrm{Be}(e^- p, e^-)^8\mathrm{B}$. We consider the asymptotic region, where the ^{7}Be and proton are close to each other but far away from the electron spectator. The average kinetic energy of the particles in the plasma is the same for nuclei and electrons. Since $\frac{m_e}{m_p} << 1$ the electron velocity is three orders of magnitude higher than that of a proton or ^{7}Be. We have the following mass relations: $\frac{\mu_\alpha}{M_\beta} \approx \frac{\mu_\alpha}{M_\gamma} \approx 1$ and $\frac{\mu_\beta}{m_\gamma} \approx \frac{\mu_\gamma}{m_\beta} \approx 0$. Then for the electron-spectator case Eq. (6.31) leads to $\mathbf{k}_\beta \approx \mathbf{q}_\alpha$ and $\mathbf{k}_\gamma \approx -\mathbf{q}_\alpha$. It means that the motion of the electron relative to the $(^7\mathrm{Be}, p)$ center of mass is totally uncoupled from the relative motion of the ^{7}Be and proton. Therefore, as has been done in [78], we can use the adiabatic approximation. In this approximation while the proton approaches ^{7}Be very slowly the electron flies "nearby" picking up energy and leaving the heavy particles in a bound state. Contrary to the proton-proton case the electron is attracted to the positively charged nuclei. Because there is no

Coulomb barrier factor for the electrons, the main contribution to the reaction rate comes from the electrons with energies nearly equal to the Maxwell-Boltzmann peak energy. Due to the small electron mass the Coulomb parameters for electron-nuclei Coulomb interactions are η, η_β, $\eta_\gamma \ll 1$. Therefore we can use this approximation

$$N_\beta N_\gamma F(-i\eta, 1, i\xi)\, F(-i\eta_\beta, 1, \xi_\beta) F(-i\eta_\gamma, 1, \xi_\gamma) \approx 1 \tag{6.38}$$

in the integrand of the integral in the matrix element Eq.(6.24), i. e. the motion of the electron relative to the center of mass of the heavy nuclei is described by a plane wave. The approximations above facilitate integration over $\boldsymbol{\rho}_\alpha$ in the matrix element. Since we replaced the electron motion by the plane wave the integral involving the channel potential U^C disappears and we define

$$\overline{V}_\alpha^C = V_\beta^C + V_\gamma^C, \tag{6.39}$$

where $\overline{V}_\alpha^C$ is the Coulomb potential describing the interaction of the electron with the ^{7}Be and proton and V_ν^C, $\nu = \beta, \gamma$ is given by Eqs.(6.26) and (6.27). The matrix element (6.24) for the electron spectator case takes the following form:

$$\mathcal{M}_{if} = \sum_{m_f} C_{l_f m_f J_i M_i}^{J_f M_f} \int d\mathbf{r}_\alpha Y_{l_f m_f}^*(\widehat{r}_\alpha) \phi_{l_f}^*(r_\alpha) \psi_0(r_\alpha) \int d\boldsymbol{\rho}_\alpha \overline{V}_\alpha^C\, e^{i(\mathbf{q}_\alpha - \mathbf{q}'_\alpha)\cdot\boldsymbol{\rho}_\alpha}. \tag{6.40}$$

Integration over $\boldsymbol{\rho}_\alpha$ is straightforward:

$$\int d\boldsymbol{\rho}_\alpha \overline{V}_\alpha e^{i\vec{p}\cdot\boldsymbol{\rho}_\alpha} = -\frac{4\pi\, e}{p^2}[z_\beta\, e\, e^{-i\lambda_\beta \vec{p}\cdot\mathbf{r}_\alpha} + z_\gamma\, e\, e^{i\lambda_\gamma \vec{p}\cdot\mathbf{r}_\alpha}], \tag{6.41}$$

where $\mathbf{p} = \mathbf{q}'_\alpha - \mathbf{q}_\alpha$ is the momentum transferred to the electron. Using the partial wave expansion of the plane waves in Eq.(6.41) in the integral of Eq. (6.40) we perform the angular integrations leaving only the integration over r_α:

$$\mathcal{M}_{if} = -\frac{4\pi\, i\, e}{p^2}\sqrt{4\pi(2l_f+1)}C^{J_f M_f}_{l_f 0 J_i M_i} \times \int r_\alpha^2 dr_\alpha \psi_0(r_\alpha)\phi^*_{\lambda l_f}(r_\alpha)[z_\gamma\, e\, j_{l_f}(\lambda_\gamma p r_\alpha) - z_\beta\, e\, j_{l_f}(\lambda_\beta p r_\alpha)], \quad (6.42)$$

where $j_{l_f}(\lambda_\nu p r_\alpha)$ is a Riccati-Bessel function. By averaging over the initial M_i and summing over final M_f spin orientations we obtain

$$\frac{1}{(2J_i+1)}\sum_{M_i,M_f}|\mathcal{M}_{if}|^2 = \frac{1}{(2J_i+1)}\frac{5(4\pi)^3}{p^4 k_\alpha^2}[e\, C_{I_f l_f}]^2 \times[\int_0^\infty \mathrm{d}r_\alpha F_0(\eta_\alpha, k_\alpha r_\alpha)W^*_{l_f}(2\kappa r_\alpha)(z_\gamma\, e\, j_{l_f}(\lambda_\gamma p r_\alpha) - z_\beta\, e\, j_{l_f}(\lambda_\beta p r_\alpha))]^2. \quad (6.43)$$

Finally, the reaction rate given by Eq.(6.21) for the ^{7}Be$(e^- p, e^-)^8$B nonradiative triple reaction takes the following form

$$\langle\Sigma(T)\rangle_e = \frac{320\pi e_\alpha^2}{(k_B T)^2}\sum_{J_i}\frac{C^2_{I_i l_f}}{2J_i+1}\sqrt{\frac{M_\alpha}{\mu_\alpha^3}}\int_0^\infty \mathrm{d}k_\alpha \int_0^\infty \mathrm{d}p e^{-\frac{M_\alpha(\frac{k_\alpha^2}{2\mu_\alpha}-\varepsilon-\frac{p^2}{2M_\alpha})^2}{2k_B T p^2}} e^{-\frac{k_\alpha^2}{2\mu k_B T}} \times\frac{(\int_0^\infty \mathrm{d}r_\alpha F_0(\eta_\alpha, k_\alpha r_\alpha)W^*_{l_f}(2\kappa r_\alpha)\{e_\gamma j_l(\lambda_\gamma p r_\alpha) - e_\beta j_l(\lambda_\beta p r_\alpha)\})^2}{p^3} \quad (6.44)$$

The electron density in stellar matter dominated by hydrogen can be found from

$$n_e \approx \frac{\rho}{M_H}\frac{(1+X_H)}{2}, \quad (6.45)$$

where M_H, and X_H are the hydrogen mass and atomic weight abundances, respectively. We use the reaction rate equation (6.44) to estimate the triple reaction rate per particle triplet for the ^{7}Be$(pe, e)^8$B nonradiative reaction. The results are shown in Table I.

3. Triple reaction rate for the nonradiative ^{7}Be$(pp,p)^8$B reaction

It is well known that hydrogen is the most abundant element in the Sun and in the Universe. Therefore the most important and dominant reactions in the stellar core, in a supernova hydrogen envelope or in any stellar object which has not used up its hydrogen fuel, are reactions involving hydrogen nuclei. Contrary to the ^{7}Be$(pe,e)^8$B reaction, the ^{7}Be$(pp,p)^8$B triple collision involves interacting particles that are positively charged. This leads to a strong Coulomb barrier. Therefore the reaction rate will have a strong temperature dependence, especially at low temperatures. As mentioned earlier, the initial state for this reaction consists of a ^{7}Be, a nearby proton and a far away proton which takes away the excessive energy emitted in the binary process. The far away proton must penetrate the Coulomb barrier of other two nuclei in order to pick up a virtual photon but it will still be far away from the colliding ^{7}Be and proton. This configuration allows us to distinguish the two protons from each other and disregard the antisymmetrization of their wave functions when estimating the nonradiative reaction rate. There are two identical protons, therefore, triple reaction rate Eq 6.18 is divided by two. Since the radiative capture is an extremely peripheral process, the transition operator in the matrix element (6.24) is approximated by its Coulomb parts:

$$\overline{V}_\alpha = V_\beta^C + V_\gamma^C - U^C, \tag{6.46}$$

where V_β^C, V_γ^C, U^C are given by Eqs. (6.25), (6.26), (6.27). Since we have $r_\alpha \ll \rho_\alpha$ in the Ω_α region we can further simplify the calculation by using a multipole expansion [76] of $\overline{V}_\alpha$:

$$\overline{V}_\alpha = z_\alpha e^2 \sum_{LM} \frac{4\pi}{2L+1} \mu_\alpha^L ((-1)^L \frac{z_\beta}{m_\beta^L} + \frac{z_\gamma}{m_\gamma^L}) \frac{r_\alpha^L}{\rho_\alpha^{L+1}} Y_{LM}^*(\widehat{\mathbf{r}}_\alpha) Y_{LM}(\widehat{\boldsymbol{\rho}}_\alpha). \tag{6.47}$$

We also took into account that $\xi_\beta \approx \xi_{\beta\alpha}$ and $\xi_\gamma \approx \xi_{\gamma\alpha}$, where $\xi_{\nu\alpha} = k_\nu \rho_\alpha - \epsilon_{\alpha\nu} \mathbf{k}_\nu \cdot \boldsymbol{\rho}_\alpha$, and $\nu = \beta, \gamma$. Now we can separate the integrations over $\mathbf{r}_\alpha$ and $\boldsymbol{\rho}_\alpha$ in the matrix element (6.24):

$$\mathcal{M}_{if} = \sum_{LM} \frac{4\pi}{2L+1} Q_{LM} \mathcal{Q}_{LM}, \tag{6.48}$$

where

$$Q_{LM} = e\mu_\alpha^L((-1)^L \frac{z_\beta}{m_\beta^L} + \frac{z_\gamma}{m_\gamma^L}) \int \frac{d\mathbf{r}_\alpha}{(2\pi)^{3/2}} \Phi^*_{\lambda J_f M_f I_f} r_\alpha^L Y^*_{LM}(\widehat{\mathbf{r}}_\alpha) \Phi_{\lambda J_i M_i I_i} \tag{6.49}$$

is the multipole moment for ^{7}Be$(p,\gamma)^8$B capture and

$$\begin{aligned} \mathcal{Q}_{LM} &= z_\alpha e \int \frac{d\vec{\rho}_\alpha}{(2\pi)^3} \frac{e^{i(\mathbf{q}_\alpha - \mathbf{q}'_\alpha)\cdot\vec{\rho}_\alpha}}{\rho_\alpha^{L+1}} NF(-i\eta, 1, i\xi) Y_{LM}(\widehat{\rho}_\alpha) \\ &\times \prod_{\nu=\beta,\gamma} N_\nu F(-i\eta_\nu, 1, i\xi_\nu). \end{aligned} \tag{6.50}$$

Let us investigate the matrix element (6.49) for further simplifications. As $\mathbf{q}'_\alpha$ is reasonably large in the final state wave function, we replace $NF(-i\eta,1,i\xi)$ by its asymptotic form $e^{i\eta \ln \xi}$. Similarly we replace the $N_\beta F(-i\eta_\beta, 1, i\xi_\beta)$ function describing the scattering of two protons in the initial state by its asymptotic form $e^{i\eta_\beta \ln \xi_{\beta\alpha}}$. As usual the dipole moment contribution in Eq. (6.48) will dominate so we keep only the $L=1$ term. After substituting $\Phi^*_{\lambda J_f M_f I_f}$, and $\Phi_{\lambda J_i M_i I_i}$ into Eq.(6.49) we have

$$Q_{1M} = \mu_\alpha(\frac{Z_\gamma}{m_\gamma} - \frac{Z_\beta}{m_\beta})(-1)^M C^{J_f M_f}_{J_i M_i L -M} \int \frac{r_\alpha^2 dr_\alpha}{(2\pi)^{3/2}} \phi^*_{\lambda l_f} r_\alpha^L \psi_{\lambda l_i}, \tag{6.51}$$

where $\psi_{\lambda l_i}$ is the radial part of the initial wave function of the reacting pair and the radial part of the bound state $\phi^*_{\lambda l_f}$ is given by (6.13). Using the following relation for the Clebsch-Gordan coefficients

$$\sum_{M_i M_f} C^{J_f M_f}_{J_i M_i L -M} C^{J_f M_f}_{J_i M_i L -M'} = \sum_{M_i M_f} C^{J_f M_f}_{J_i M_i L x} C^{J_f M_f}_{J_i M_i L x'} = \frac{2J_f+1}{2L+1} \delta_{MM'}, \tag{6.52}$$

averaging $|\mathcal{M}_{if}|^2$ over the initial state projections M_i and summing over the final state projections M_f, we can write down Eq. (6.48) in the following form:

$$|\mathcal{M}_{if}|^2 \approx (\frac{4\pi}{2L+1})^2 \sum_M |Q_{LM}|^2 \, |\mathcal{Q}_{LM}|^2 \,. \tag{6.53}$$

The angular integration in the matrix element $\mathcal{Q}_{LM}$ can be performed using the following relation for the plane

$$e^{i\mathbf{p}\cdot\boldsymbol{\rho}_\alpha} \sim \frac{2\pi}{ip\rho_\alpha}[\delta(\widehat{\mathbf{p}}-\widehat{\boldsymbol{\rho}}_\alpha)e^{ip\rho_\alpha} - \delta(\widehat{\mathbf{p}}+\widehat{\boldsymbol{\rho}}_\alpha)e^{-ip\rho_\alpha}], \tag{6.54}$$

where $\mathbf{p} = \mathbf{q}_\alpha - \mathbf{q}'_\alpha$. Then keeping the leading term in the direction $-\widehat{\mathbf{p}}$, we integrate over $\boldsymbol{\rho}_\alpha$ [101, 102]:

$$\begin{aligned}\mathcal{Q}_{1M} \quad &\approx \quad -\frac{2\pi Z_\alpha e Y_{1M}(-\widehat{\mathbf{p}})}{i\,|\mathbf{p}|} N_\gamma e^{i\eta_\beta \ln(k_\beta+\epsilon_{\beta\alpha}\mathbf{k}_\beta\cdot(-\widehat{\mathbf{p}}))+i\eta\ln(q+\mathbf{q}\cdot(-\widehat{\mathbf{p}}))} e^{-i(\eta_\beta+\eta)\ln|\mathbf{q}_\alpha-\mathbf{q}|} \\ &\times\Gamma(i(\eta_\beta+\eta))e^{\frac{\pi}{2}(\eta_\beta+\eta)}F(-i\eta_\gamma, i(\eta_\beta+\eta), 1, \frac{\xi'_\gamma(-\widehat{\mathbf{p}})}{|\mathbf{p}|}).\end{aligned} \tag{6.55}$$

So finally Eq. (6.55) takes the following form

$$\mathcal{Q}_{1M} = G Y_{1M}(-\widehat{\mathbf{p}}), \tag{6.56}$$

where for simplicity we have defined

$$\begin{aligned}G = \frac{2\pi\, i\, z_\alpha e}{|\mathbf{p}|} N_\gamma e^{i\eta_\beta \ln(k_\beta+\epsilon_{\beta\alpha}\mathbf{k}_\beta\cdot(-\widehat{\mathbf{p}}))+i\eta\ln(q+\mathbf{q}\cdot(-\widehat{\mathbf{p}}))} e^{-i(\eta_\beta+\eta)\ln|\mathbf{q}_\alpha-\mathbf{q}|} \\ \times\Gamma(i(\eta_\beta+\eta))e^{\frac{\pi}{2}(\eta_\beta+\eta)}F(-i\eta_\gamma, i(\eta_\beta+\eta), 1, \frac{\xi'_\gamma(-\widehat{\mathbf{p}})}{|\mathbf{p}|}).\end{aligned} \tag{6.57}$$

All phase factors will disappear when we multiply Eq. (6.57) by its complex conjugate:

$$\begin{aligned}G^*G \quad &= \quad \frac{4\pi^2 z_\alpha^2 e^2}{|\mathbf{p}|^2} \frac{2\pi}{e^{2\pi\eta_\gamma}-1} \frac{2\pi}{1-e^{-2\pi(\eta_\beta+\eta)}} \frac{\eta_\gamma}{(\eta_\beta+\eta)} \\ &\times \left| F(-i\eta_\gamma, i(\eta_\beta+\eta), 1, \frac{\xi'_\gamma(-\widehat{\mathbf{p}})}{|\mathbf{p}|}) \right|^2 .\end{aligned} \tag{6.58}$$

Finally, Eq. (6.53) boils down to

$$\sum_{M_i,M_f} |\mathcal{M}_{if}|^2 \approx \frac{3}{4\pi}(\frac{4\pi}{2L+1})^2 \frac{2J_f+1}{2L+1} |X|^2 |G|^2 , \tag{6.59}$$

where X comes from the matrix element of the dipole moment, Eq. (6.51), and is defined by

$$|X|^2 = \mu_\alpha^2(-\frac{z_\beta}{m_\beta} + \frac{z_\gamma}{m_\gamma})^2 e^2 \left| \int r_\alpha^2 dr_\alpha \phi^*_{\lambda l_f} r_\alpha \psi_{\lambda l_i} \right|^2 \tag{6.60}$$

$$= \mu_\alpha^2(-\frac{z_\beta}{m_\beta} + \frac{z_\gamma}{m_\gamma})^2 e^2 \frac{C^2_{Il_f}}{k_\alpha^2} \left| \int r_\alpha dr_\alpha W^*_{l_f}(r_\alpha) F_{l_i}(-i\eta_\alpha, k_\alpha r_\alpha) \right|^2 \tag{6.61}$$

The final equation which we use to estimate the reaction rates of the ^{7}Be$(pp,p)^8$B nonradiative triple collision takes the following form:

$$\begin{aligned} \langle \Sigma(T) \rangle_p = A \int & \left| \int r_\alpha dr_\alpha W^*_{l_f}(r_\alpha) F_{l_i}(-i\eta_\alpha, k_\alpha r_\alpha) \right|^2 e^{-\frac{(\hbar c)^2 k_\alpha^2}{2\mu c^2 k_B T}} dk_\alpha \\ \times \int & q_\alpha^2 dq_\alpha \sqrt{(\varepsilon_b + \frac{(\hbar c)^2 k_\alpha^2}{2\mu_\alpha} + \frac{(\hbar c)^2 q_\alpha^2}{2M_\alpha})} e^{-\frac{(\hbar c)^2 q_\alpha^2}{2M_\alpha c^2 k_B T}} \\ \times \int\int & \sin\theta d\theta \sin\delta d\delta d\phi \frac{1}{|\mathbf{p}|^2} \frac{1}{e^{2\pi\eta_\gamma} - 1} \frac{k_\beta}{k_\gamma} \frac{e_\beta \mu_\gamma}{(e_\gamma \mu_\beta + \frac{k_\beta}{q}(e_\beta + e_\gamma)\mu)} \\ \times & \left| F(-i\eta_\gamma, i(\eta_\beta + \eta), 1, \frac{\xi'_\gamma(-\widehat{\mathbf{p}})}{|\mathbf{p}|}) \right|^2 , \end{aligned} \tag{6.62}$$

where A is constant factor

$$\begin{aligned} A = \frac{(\hbar c)^4}{(k_B T)^3} c \frac{16\pi^2}{3} \frac{2J_f+1}{2L+1} \frac{\mu c^2 \sqrt{2\mu c^2}}{(M_\alpha c^2 \mu_\alpha c^2)^{\frac{3}{2}}} \mu^2_{\beta\gamma} (-\frac{z_\beta}{m_\beta} + \frac{z_\gamma}{m_\gamma})^2 \\ \times z_\alpha^2 (\frac{e^2}{\hbar c})^2 \sum_{J_i} \frac{C^2_{Il_f}}{(2J_i+1)} . \end{aligned} \tag{6.63}$$

The reaction rates for the ^{7}Be$(pp,p)^8$B nonradiative triple collisions are given in the Table I.

D. Results and discussions

We calculated reaction rates for the ^{7}Be$(pe,e)^8$B and ^{7}Be$(pp,p)^8$B nonradiative reactions using Eqs.(6.44) and (6.62) for temperatures T ranging from $1.4 \times 10^7\,K$ to $10^9\,K$. The results of our calculations are given in Table I. We present the results for the triple reaction rate per particle triplet multiplied by the square of Avagadro's number, $N_A^2 \langle \Sigma(T) \rangle_s$, with units $(cm^6 mol^{-2} s^{-1})$. In this form our results can be used not only for solar conditions but also for any stellar objects with different particle densities and temperatures. Any specific reaction rate for a particular stellar object can be calculated from Table I by multiplying the rate by $n_{^7\mathrm{Be}} n_p n_s / N_A^2$, where n_s is number density of either the electron or proton spectator. The four columns give temperature, binary rection rate and the nonradiative triple reaction rates for electron and proton spectator cases, respectively. The temperature dependence of the binary and triple reaction rates, normalized to the same value at $T = 1.4 \times 10^7 K$ are shown in Figure 3. We have defined $NR(T) = N_A \langle \sigma v \rangle \times 10^{12}$, for the binary reaction rate, and $NR(T) = N_A^2 \langle \Sigma(T) \rangle_s N_A \langle \sigma v \rangle_{T_0} / (N_A^2 \langle \Sigma(T_0) \rangle_s) \times 10^{12}$ as the rate for the triple reaction normalized to the rate at $T_0 = 1.4 \times 10^7$, and $s = e, p$ for the electron and proton spectators, respectively.

The ^{7}Be$(pp,p)^8$B reaction has the strongest temperature dependence at low temperatures, as is expected, since all particles are positively charged and have a strong Coulomb barrier. At high temperatures the reaction rate is practically a flat function of temperature for all reactions and triple rates with electron and proton spectators have the same order. As has been anticipated the nonradiative reaction rates are small compared to the corresponding binary radiative fusion rates in the solar core. A supernova's envelope has similar conditions as the core of a normal hydrogen burning star. Therefore the triple to binary reaction rate ratios have almost the same order

Table I. Temperature dependence of the reaction rates of the binary radiative ^{7}Be$(p,\gamma)^8$B, and nonradiative triple ^{7}Be$(ep,e)^8$B, and ^{7}Be$(pp,p)^8$B reactions

T_7 $(10^7 K)$	$N_A \langle\sigma v\rangle$ $(cm^3 mol^{-1} s^{-1})$	$N_A^2 \langle\Sigma(T)\rangle_e$ $(cm^6 mol^{-2} s^{-1})$	$N_A^2 \langle\Sigma(T)\rangle_p$ $(cm^6 mol^{-2} s^{-1})$
1.4	1.7×10^{-12}	1.7×10^{-19}	1.2×10^{-26}
1.5	4.2×10^{-12}	4.2×10^{-19}	4.3×10^{-26}
1.6	9.9×10^{-12}	9.6×10^{-19}	1.4×10^{-25}
1.8	4.5×10^{-11}	4.1×10^{-18}	1.0×10^{-24}
2	1.7×10^{-10}	1.4×10^{-17}	5.5×10^{-24}
3	1.7×10^{-8}	1.1×10^{-15}	2.0×10^{-21}
4	3.2×10^{-7}	1.7×10^{-14}	7.8×10^{-20}
6	1.3×10^{-5}	4.5×10^{-13}	9.3×10^{-18}
8	1.4×10^{-4}	3.4×10^{-12}	2.3×10^{-16}
10	7.6×10^{-4}	1.4×10^{-11}	2.6×10^{-15}
20	7.7×10^{-2}	4.6×10^{-10}	1.6×10^{-12}
30	7.9×10^{-1}	2.1×10^{-9}	3.3×10^{-11}
40	3.6	5.0×10^{-9}	2.1×10^{-10}
50	10.8	8.8×10^{-9}	7.7×10^{-10}
60	25.4	1.3×10^{-8}	2.0×10^{-9}
80	90.9	2.1×10^{-8}	7.1×10^{-9}
90	149.1	2.5×10^{-8}	1.1×10^{-8}
100	229.2	2.8×10^{-8}	1.7×10^{-8}

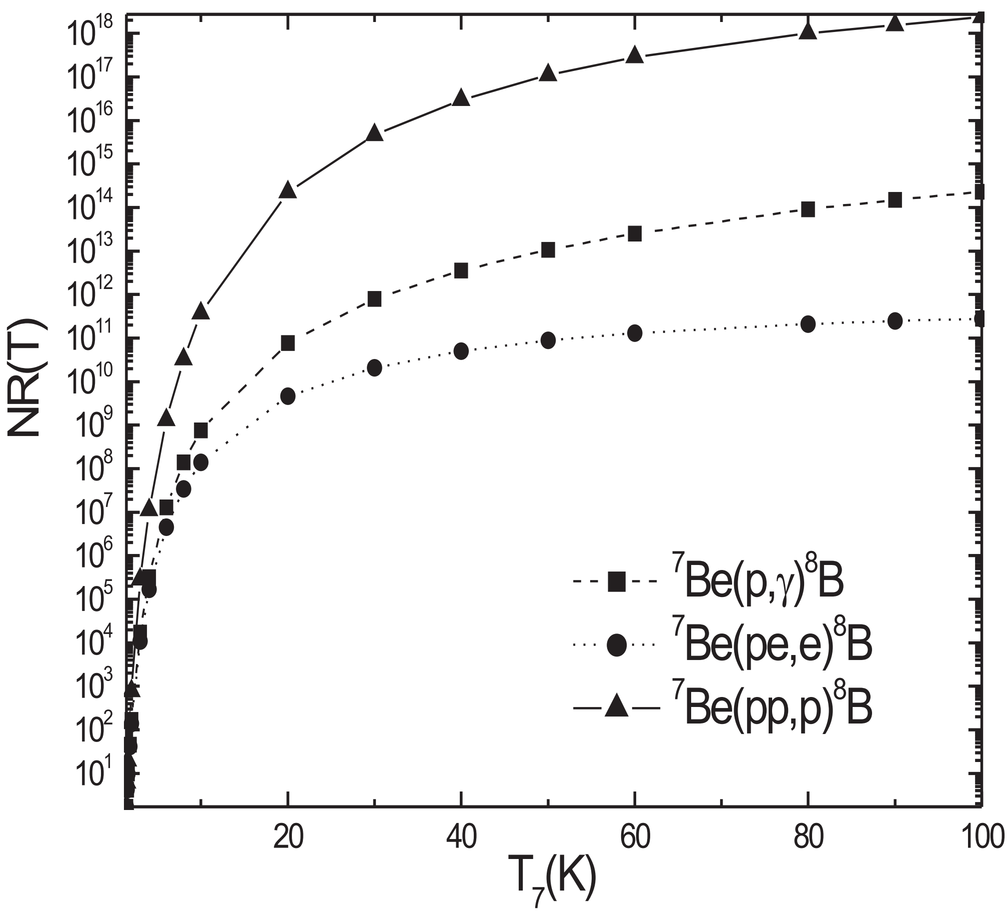

Fig. 3. Temperature dependence of the binary and triple reaction rates.

as for the Sun, as shown in Table II. This smallness is due to the small probability of triple collisions for the low density of spectator particles and to the Coulomb barrier for the proton spectators at low temperatures. We can use the results of Table I to estimate triple reaction rates in other stellar objects where high temperatures and densities exist. Even though the triple reaction rates are small at low temperatures and densities the calculations performed here give some insight into conditions when triple collisions might be important. Triple collisions have larger probability at high temperatures due to the smaller effect of the Coulomb barrier and at high densities of the spectator particles since the probability of the triple collisions is proportional to the number densities of the spectator particles.

Now let us consider some other stellar objects, where high temperature and high density conditions exist. These objects are novae events in binary systems, X-ray bursts and X-ray Superbursts. In [92] the reaction rate uncertainties in nova nucleosynthesis were investigated for a wide range of reactions. These investigations cover temperatures ranging from $0.145 \times 10^9\, K$ to $0.418 \times 10^9\, K$ and densities from $10\, gcm^{-3}$ to $10^5\, gcm^{-3}$. Another object of interest is an X-ray burst in a binary system. Type I X-ray bursts are thermonuclear flashes of accumulated hydrogen and helium on an accreting neutron star. The X-ray emission in binary systems with compact objects is due to accretion. Densities in an X-ray binary system are much higher than that in a nova binary.

Finally, we need to mention the stellar objects, called Superburst, with densities higher than X-ray bursts. Superbursts are rare and powerful nuclear explosions on the surface of neutron stars. Superbursts are energetic ($10^{42} - 10^{43}$ ergs) thermonuclear flashes on the surface of accreting neutron stars and are thought to be caused by unstable carbon burning and photodisintegration of heavy elements produced during the rapid proton capture process. Superbursts provide a new way to study the physics

Table II. Ratio of the nonradiative triple to radiative binary rates in different environments

Stellar Object	T_9	$n_e\ (cm^{-3})$	$n_p\ (cm^{-3})$	$\frac{\langle R_3(T)\rangle_e}{\langle R_2(T)\rangle}$	$\frac{\langle R_3(T)\rangle_p}{\langle R_2(T)\rangle}$
The Sun	0.0156	6×10^{25}	4.8×10^{25}	10^{-5}	10^{-12}
Supernova	0.02	7×10^{25}	5.4×10^{25}	9.6×10^{-6}	3×10^{-12}
Big bang	$0.8 \div 0.3$	3.6×10^{24}	3×10^{24}	2×10^{-7}	3.6×10^{-12}
Nova surface	$0.1 \div 0.4$	2.5×10^{28}	2×10^{28}	6×10^{-5}	2×10^{-6}
X-Ray burst	> 1	7.3×10^{29}	6×10^{29}	1.5×10^{-4}	7×10^{-5}
Superburst	> 1	6×10^{32}	$\sim 10^{25}$	0.1	$\sim 10^{-7}$

of nuclear burning at high temperatures and densities, as well as a new probe of the neutron star interior [93]. In a superburst the density reaches $\rho \approx 10^9\, g\, cm^{-3}$ and temperature $T > 10^9\, K$. Results of estimates for triple to binary rates are shown in Table II. These results depend on temperature, density and abundances of the elements in the stellar environment. As we see triple reactions are larger at high temperatures and densities than earlier thought. We have chosen here nonradiative triple reactions as examples. If the charges of interacting particles are small, and if there are some low lying resonances at high temperature and densities, such triple reactions might play an important role in stellar nucleosynthesis.

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