Asymptotic wave function for three charged particles in the continuum

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We present an improved version of the wave function derived by Alt and Mukhamedzhanov [Phys. Rev. A **47**, 2004 (1993)] that satisfies the Schrödinger equation up to terms of order $O(1/\rho_{\alpha}^{2})$ in the region where the pair $\alpha = (\beta, \gamma)$ remains close, while the third particle α moves to infinity $(\rho_{\alpha} \rightarrow \infty)$. The new wave function contains the zeroth- and all the first-order $O(1/\rho_{\alpha})$ terms, and matches smoothly Redmond's asymptotics and the Redmond-Merkuriev wave function when all three particles are well separated. [S1050-2947(96)08110-3]

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I. INTRODUCTION

The problem of the wave function for the scattering of three charged particles has attracted the attention of theorists for a long time. An asymptotic wave function, valid in the region Ω_0 in which all three interparticle distances are large, was proposed by Redmond [1] (see Rosenberg [2]). This wave function, Redmond's asymptotics, has the form of a Coulomb-distorted three-particle plane wave. Redmond also proposed an extended wave function in which the three pairs of Coulomb-distorted factors are replaced by corresponding confluent hypergeometric functions. This wave function later considered by Merkuriev [3] has three desirable properties: it is also an asymptotic solution to the three-Coulomb Schrödinger equation in the region Ω_0 , satisfying it in the leading order; the leading term in its asymptotic expansion is the Coulomb-distorted three-particle plane wave, by design, and, if any one of the charges is set equal to zero, the resulting wave function becomes an exact solution to the Schrödinger equation (i.e., a Coulomb wave function for the charged pair multiplied by a plane wave for the neutral particle). However, this wave function does not possess the correct asymptotic behavior in other asymptotic regions of configuration different from the region Ω_0 . These regions are important when calculating cross sections for ionization processes such as

$$(12) + 3 \rightarrow 1 + 2 + 3.$$
 (1)

The ionization amplitude for this process contains the overlap of the initial bound-state wave function for the bound pair (12) and the three-body final state continuum wave function. The presence of the bound-state wave function cuts off the integration in the variable r_3 , the relative coordinate between particles 1 and 2, but the integration over the variable ρ_3 , the relative coordinate between the center of mass of the pair (12) and particle 3 is not "protected," and the region of integration extends to infinity, i.e., the integration region includes the whole of the asymptotic region we call Ω_3 : $r_3/\rho_3 \rightarrow 0$, $\rho_3 \rightarrow \infty$. In this region the Coulomb-distorted three-body plane wave is not the leading asymptotic term, hence the Redmond-Merkuriev wave function is not applicable. Nevertheless, this wave function has been employed in many applications (see, for example, [4–7]).

The asymptotic behavior of the three-body scattering wave function for three charged particles in the region Ω_3 has been found in work [8]. This wave function satisfies the asymptotic Schrödinger equation to leading order [up to terms $O(1/\rho_3^2)$]. But this wave function does not use up all the terms of order $O(1/\rho_3)$.

The aim of the present paper is to suggest an improved expression for the approximate three-body continuum wave function whose main asymptotic term in the region Ω_3 coincides with that found in Ref. [8], contains all the terms of order $O(1/\rho_3)$ which also satisfy the Schrödinger equation up to terms $O(1/\rho_3^2)$, while in the region Ω_0 this wave function joins smoothly with the Redmond-Merkuriev wave function and hence its leading term in Ω_0 is the Redmond asymptotics.

II. ASYMPTOTIC THREE-BODY WAVE FUNCTION IN Ω_{α}

A. Nonsingular directions

Consider a system of three particles with mass m_{α} and charge e_{α} , $\alpha = 1, 2, 3$, in the continuum. We use the notation for the Jacobi coordinates, kinetic energy operators, and potentials employed in Ref. [8]. The Schrödinger equation describing this system is

$$(E - T_{\mathbf{r}_{\alpha}} - T_{\boldsymbol{\rho}_{\alpha}} - V) \Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(+)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) = 0.$$
(2)

Before looking for the solution we would like to remind the reader that for pure Coulombic interactions in all three pairs, i.e., $V_{\nu} = V_{\nu}^{C}$, $\nu = 1, 2, 3$, an asymptotic solution satisfying (2) in the leading order $O(1/r_{\nu})$, $\nu = 1, 2, 3$, in Ω_0 in the nonsingular directions ($\hat{\mathbf{k}}_{\nu} \cdot \hat{\mathbf{r}}_{\nu} \neq 1$, $\nu = 1, 2, 3$) is the Redmond-Merkuriev wave function

$$\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{RM})(+)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) = e^{i \mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} e^{i \mathbf{k}_{\alpha}\cdot\mathbf{r}_{\alpha}} \times \prod_{\nu=1}^{3} N_{\nu}F(-i\eta_{\nu},1;i(k_{\nu}r_{\nu}-\mathbf{k}_{\nu}\cdot\mathbf{r}_{\nu})).$$
(3)

We note that

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$$\epsilon - \epsilon_{\nu\alpha} \rho_{\alpha} - \frac{m_{\nu}}{m_{\beta\gamma}} \mathbf{r}_{\alpha}, \quad \rho_{\nu} = -\frac{\mu_{\nu}}{m_{\gamma}} \rho_{\alpha} + \epsilon_{\nu\alpha} \frac{\mu_{\nu}}{M_{\alpha}} \mathbf{r}_{\alpha},$$
(4)

where $\nu = \beta$, γ , $\epsilon_{\nu\alpha} = -\epsilon_{\alpha\nu}$ is the antisymmetric symbol, with $\epsilon_{\nu\alpha} = 1$ for $(\nu\alpha)$ being a cyclic permutation of (1, 2, 3), and $\epsilon_{\alpha\alpha} = 0$; $\mu_{\alpha} = m_{\beta}m_{\gamma}/m_{\beta\gamma}$, $m_{\beta\gamma} = m_{\beta} + m_{\gamma}$, $M_{\alpha} = m_{\alpha}m_{\beta\gamma}/(m_1 + m_2 + m_3)$. The confluent hypergeometric function $F_{\nu}(i\zeta_{\nu}) \equiv F(-i\eta_{\nu}, 1; i\zeta_{\nu})$ is the solution for

$$\left(\frac{1}{2\mu_{\nu}}\Delta_{\mathbf{r}_{\nu}}+i\frac{1}{\mu_{\nu}}\mathbf{k}_{\nu}\cdot\nabla_{\mathbf{r}_{\nu}}-V_{\nu}^{C}\right)F_{\nu}(i\zeta_{\nu})=0,\qquad(5)$$

where

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 $\mathbf{r}_{\nu} =$

$$\eta_{\alpha} = \frac{e_{\beta} e_{\gamma} \mu_{\alpha}}{k_{\alpha}}, \quad N_{\alpha} = e^{-(\pi \eta_{\alpha}/2)} \Gamma(1 + i \eta_{\alpha}),$$
$$\zeta_{\alpha} = k_{\alpha} r_{\alpha} - \mathbf{k}_{\alpha} \cdot \mathbf{r}_{\alpha}. \tag{6}$$

We use the system of units such that $\hbar = c = 1$. Taking into account that [9]

$$N_{\nu}F(-i\eta_{\nu},1;i\zeta_{\nu}) = \mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) + \mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu}), \qquad (7)$$

$$\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) = e^{(\pi\eta_{\nu}/2)} (i\zeta_{\nu})^{-(1/2)} e^{(i\zeta_{\nu}/2)} W_{i\eta_{\nu}+1/2, 0}(i\zeta_{\nu}),$$

$$\mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu}) = -i \frac{\Gamma(1+i\eta_{\nu})}{\Gamma(-i\eta_{\nu})} e^{(\pi\eta_{\nu}/2)} (i\zeta_{\nu})^{-(1/2)} \times e^{(i\zeta_{\nu}/2)} W_{-i\eta_{\nu}-1/2, 0}(-i\zeta_{\nu}), \qquad (8)$$

and asymptotic behavior of the Whittaker function at $\zeta_{\nu} \rightarrow \infty$,

$$W_{\lambda,0}(i\zeta_{\nu}) = (i\zeta_{\nu})^{\lambda} e^{(-i\zeta_{\nu}/2)} \left[1 - \frac{(\lambda - \frac{1}{2})^2}{i\zeta_{\nu}} + O\left(\frac{1}{i\zeta_{\nu}^2}\right) \right],$$
(9)

we derive the well known asymptotic behavior

$$\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) \stackrel{\zeta_{\nu}\to\infty}{=} e^{i\eta_{\nu}\ln\zeta_{\nu}} \bigg[1 + O\bigg(\frac{1}{\zeta_{\nu}}\bigg) \bigg], \tag{10}$$

$$\mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu}) \stackrel{\zeta_{\nu}\to\infty}{=} f_{\nu}^{C} \frac{e^{i\zeta_{\nu}}}{r_{\nu}} e^{-i\eta_{\nu}\ln(2k_{\nu}r_{\nu})} \left[1 + O\left(\frac{1}{\zeta_{\nu}}\right)\right].$$
(11)

Correspondingly

$$N_{\nu}F(-i\eta_{\nu},1;i\zeta_{\nu}) \stackrel{\zeta_{\nu}\to\infty}{=} e^{i\eta_{\nu}\ln\zeta_{\nu}} \left[1+O\left(\frac{1}{\zeta_{\nu}}\right)\right] +f_{\nu}^{C}\frac{e^{i\zeta_{\nu}}}{r_{\nu}}e^{-i\eta_{\nu}\ln(2k_{\nu}r_{\nu})} \times \left[1+O\left(\frac{1}{\zeta_{\nu}}\right)\right], \quad (12)$$

where f_{ν}^{C} is the Coulomb scattering amplitude of particles of the pair ν . The leading term of the Redmond-Merkuriev wave function $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(0)+}(\mathbf{r}_{\alpha},\rho_{\alpha})$ in Ω_{0} also satisfying (2) in the leading order is the three-particle Coulomb-distorted plane wave (Redmond's asymptotics):

$$\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(0)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) = e^{i \mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} e^{i \mathbf{k}_{\alpha}\cdot\mathbf{r}_{\alpha}} \prod_{\nu=1}^{3} e^{i \eta_{\nu} \ln(k_{\nu} r_{\nu}-\mathbf{k}_{\nu}\cdot\mathbf{r}_{\nu})}.$$
(13)

Also note that the leading asymptotic term of the threebody wave function in Ω_{α} satisfying the Schrödinger equation in the leading order $O(1/\rho_{\alpha})$ is given by [8]

$$\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{as})(+)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) = e^{i \mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} e^{i \mathbf{k}_{\alpha}\cdot\mathbf{r}_{\alpha}} \mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})$$

$$\times \varphi_{\alpha}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha}) \qquad (14)$$

$$= e^{i \mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} \psi_{\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha})$$

$$\times \prod_{\nu=\beta,\gamma} e^{i\eta_{\nu}\ln(k_{\nu},\boldsymbol{\rho}_{\alpha}-\mathbf{k}_{\nu}\cdot\boldsymbol{\rho}_{\alpha})} + O\left(\frac{1}{\rho_{\alpha}}\right), \qquad (15)$$

where

$$\psi_{\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}) = e^{i\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})\cdot\mathbf{r}_{\alpha}} \varphi_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$$
(16)

is the continuum solution of the two-body Schrödinger equation

$$[E_{\alpha}(\boldsymbol{\rho}_{\alpha}) - T_{\mathbf{r}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})] \boldsymbol{\psi}_{\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha})] = 0, \qquad (17)$$

with the corresponding equation for $\varphi_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$,

$$\left[\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}}+i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})\cdot\nabla_{\mathbf{r}_{\alpha}}-V_{\alpha}(\mathbf{r}_{\alpha})\right]\varphi_{\alpha}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha})=0.$$
(18)

Equation (17) [or equivalently Eq. (18)] describes the relative motion of particles β and γ , with relative kinetic energy $E_{\alpha}(\boldsymbol{\rho}_{\alpha}) = k_{\alpha}^{2}(\boldsymbol{\rho}_{\alpha})/2\mu_{\alpha}$, interacting via the potential given by the sum of the Coulomb and short-range potentials $V_{\alpha} = V_{\alpha}^{C} + V_{\alpha}^{S}$ The relative "local momentum" $k_{\alpha}(\boldsymbol{\rho}_{\alpha})$ of particles β and γ in the Coulomb field of the third particle α at $r_{\alpha}/\rho_{\alpha} \ll 1$, introduced in [8], is given by

$$\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} + \sum_{\nu=\beta,\gamma} \frac{m_{\nu}}{m_{\beta\gamma}} \eta_{\nu} \frac{\hat{\mathbf{k}}_{\nu} - \hat{\mathbf{r}}_{\nu}}{1 - \hat{\mathbf{k}}_{\nu} \cdot \hat{\mathbf{r}}_{\nu}} \frac{1}{r_{\nu}}$$
(19)

$$=\mathbf{k}_{\alpha} + \frac{1}{\rho_{\alpha}} \sum_{\nu=\beta,\gamma} \frac{m_{\nu}}{m_{\beta\gamma}} \eta_{\nu} \frac{\hat{\mathbf{k}}_{\nu} - \boldsymbol{\epsilon}_{\alpha\nu} \hat{\boldsymbol{\rho}}_{\alpha}}{1 - \boldsymbol{\epsilon}_{\alpha\nu} \hat{\mathbf{k}}_{\nu} \cdot \hat{\boldsymbol{\rho}}_{\alpha}} + O\left(\frac{1}{\rho_{\alpha}^{2}}\right), \qquad (20)$$

where $\hat{\mathbf{k}} = \mathbf{k}/k$. Since the Coulomb interaction between particles α and ν , $\nu = \beta, \gamma$, falls off only as the inverse of the distance between them, the distortion of the motion of particles β and γ caused by the third particle α cannot be neglected even if $r_{\beta}, r_{\gamma} \rightarrow \infty$, which is equivalent to $\rho_{\alpha} \rightarrow \infty$ in the region Ω_{α} . This distortion causes the modification of the momentum of particles β and γ , which is represented in the local momentum of Eq. (20). If the potential V_{α} is pure Coulombic, $V_{\alpha} = V_{\alpha}^{C}$, then $\varphi_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ is given by

$$\varphi_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = N_{\alpha}(\boldsymbol{\rho}_{\alpha}) F(-i\eta_{\alpha}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}(\boldsymbol{\rho}_{\alpha})), (21)$$

where

$$\eta_{\alpha}(\boldsymbol{\rho}_{\alpha}) = \frac{e_{\beta}e_{\gamma}\mu_{\alpha}}{k_{\alpha}(\boldsymbol{\rho}_{\alpha})},$$
$$N_{\alpha}(\boldsymbol{\rho}_{\alpha}) = e^{-\pi\eta_{\alpha}(\boldsymbol{\rho}_{\alpha})/2} \Gamma(1 + i\eta_{\alpha}(\boldsymbol{\rho}_{\alpha})),$$
$$\zeta_{\alpha}(\boldsymbol{\rho}_{\alpha}) = k_{\alpha}(\boldsymbol{\rho}_{\alpha}) r_{\alpha} - \mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha}) \cdot \mathbf{r}_{\alpha}.$$
(22)

We note that Eq. (15) is valid in the nonsingular directions $(\hat{\mathbf{k}}_{\nu}, \hat{\boldsymbol{\rho}}_{\alpha} \neq 1, \nu = \beta, \gamma).$

Our aim now is to find an extension of $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{as})(+)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})$ satisfying the Schrödinger equation in Ω_{α} in the leading order $O(1/\rho_{\alpha})$ and containing not only the main term given by (14) but also all the terms of order $O(1/\rho_{\alpha})$. The derived wave function is the asymptotic term [up to order of $O(1/\rho_{\alpha}^{2})$] of the exact three-body wave function in Ω_{α} which should match smoothly with the leading asymptotics of the exact three-body wave function in the asymptotic region Ω_{0} .

We start our consideration from the Redmond-Merkuriev wave function (3). This wave function is an asymptotic solution to the Schrödinger equation in Ω_0 because in that region all $\zeta_{\nu} \rightarrow \infty$, $\nu = 1, 2, 3$, and, as follows from (7),

$$\left|\nabla_{\nu} F_{\nu}(i\zeta_{\nu})\right| = O\left(\frac{1}{\zeta_{\nu}}\right).$$
(23)

However, in Ω_{α} r_{α} , *a priori*, is limited (more strictly, it is allowed to grow, but slower than ρ_{α}), which is why Eq. (23) does not hold for $\nu = \alpha$ in Ω_{α} and the Schrödinger equation cannot be satisfied in Ω_{α} by (3) even in the leading order. Hence a proper modification of the Redmond-Merkuriev function should be done to get an asymptotic solution in Ω_{α} . To find it let us rewrite (3) in the form

$$\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{RM})(+)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) = e^{i \mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} e^{i \mathbf{k}_{\alpha}\cdot\mathbf{r}_{\alpha}} \left[\mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta}) \times \mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})N_{\alpha}F_{\alpha}(i\zeta_{\alpha}) + \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) \times \mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})N_{\alpha}F_{\alpha}(i\zeta_{\alpha}) + \mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta}) \times \mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma})N_{\alpha}F_{\alpha}(i\zeta_{\alpha}) + \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) \times \mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma})N_{\alpha}F_{\alpha}(i\zeta_{\alpha}) \right].$$
(24)

Compare the first term of (24) and (14). Taking into account that for the pure Coulombic interaction in the pair α , function $\varphi_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ is given by (21), one sees that the wave function of Alt and Mukhamedzhanov, $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{as})(+)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})$, Eq. (14), can be derived from the first term of (24) by substituting $N_{\alpha}(\boldsymbol{\rho}_{\alpha}) F(-i\eta_{\alpha}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}(\boldsymbol{\rho}_{\alpha}))$ for $N_{\alpha}F_{\alpha}(i\zeta_{\alpha})$. It was the main result of work [8]. Since the first term in (24) is the leading term (of the zeroth order) of the Redmond-Merkuriev wave function we may conclude that the wave function $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{as})}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})$ is the leading term of the asymptotic wave function in Ω_{α} satisfying Eq. (2) up to terms of order $O(1/\rho_{\alpha}^2)$. But there are three more terms in (24), which are of the next order. A proper modification of these terms in Ω_{α} provides the terms of order $O(1/\rho_{\alpha})$ of the asymptotic wave function satisfying Eq. (2) up to the terms $O(1/\rho_{\alpha}^2)$ in Ω_{α} . Our educated guess based on the results of [8] allows us to conclude that the asymptotic wave function in Ω_{α} can be derived from (24) by properly changing $N_{\alpha} F_{\alpha}(i\zeta_{\alpha})$. We will show, however, that the modification of $N_{\alpha} F_{\alpha}(i\zeta_{\alpha})$ in (24) depends on the preceding factors $\mathcal{F}_{\beta}^{(n)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(m)}(i\zeta_{\gamma}), n,m=1,2$, i.e., for each term in (24) the modification is different. That is why we are looking for the solution satisfying Eq. (2) in Ω_{α} in the leading order in the form

$$\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{as})(+)'}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) = e^{i\,\mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}}\,e^{i\,\mathbf{k}_{\alpha}\cdot\mathbf{r}_{\alpha}}\,[\mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma}) \\ \times\,\varphi_{\alpha}^{(11)}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha}) + \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma}) \\ \times\,\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha}) + \mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) \\ \times\,\varphi_{\alpha}^{(12)}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha}) + \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) \\ \times\,\varphi_{\alpha}^{(22)}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha})].$$
(25)

We assumed in (25) that the interaction potentials in pairs β and γ are pure Coulombic. Our idea is to single out explicitly the functions describing asymptotically [up to order $O(1/r_{\nu}^2)$, $\nu = \beta$, γ] the relative motion of the pairs $\beta = (\gamma \alpha)$ and $\gamma = (\beta, \alpha)$, respectively, and then to derive equations for the functions $\varphi_{\alpha}^{(nm)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ describing the relative motion of particles of the pair $\alpha = (\beta, \gamma)$ distorted by the presence of the third particle α . Then we will find asymptotic solutions to these equations in Ω_{α} which satisfy these equations in the first order $O(1/\rho_{\alpha})$.

When substituting Eq. (25) into (2) we assume that each term of the sum in (25) satisfies this equation. Then we derive four independent equations. For the first term in (25) we arrive at the equation

$$\begin{aligned} \mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma}) &\left(\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}} + \frac{1}{2M_{\alpha}}\Delta_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}\cdot\nabla_{\mathbf{r}_{\alpha}}\right. \\ &+ i\frac{1}{M_{\alpha}}\mathbf{q}_{\alpha}\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} + \frac{1}{\mu_{\alpha}}\sum_{\nu=\beta,\gamma}\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})\cdot\nabla_{\mathbf{r}_{\alpha}} \\ &+ \frac{1}{M_{\alpha}}\sum_{\nu=\beta,\gamma}\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha}) \\ &+ \frac{1}{\mu_{\alpha}}\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta})\cdot\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma}) \\ &+ \frac{1}{M_{\alpha}}\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma}) \\ &+ \frac{1}{M_{\alpha}}\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma}) \\ &\times \varphi_{\alpha}^{(11)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = 0. \end{aligned}$$

When deriving (26) we took into account that Eq. (5) is satisfied by $\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})$ in the leading order $O(1/\zeta_{\nu})$. It can be easily checked by the direct substitution of $\exp(i\eta_{\nu}\ln\zeta_{\nu})$ into Eq. (5). It is important to stress that we are looking for the asymptotic behavior of the three-body wave function in Ω_{α} in the nonsingular directions ($\hat{\mathbf{k}}_{\nu} \cdot \hat{\mathbf{r}}_{\nu} \neq 1$, $\nu = \beta$, γ ; in Ω_{α} $\hat{\mathbf{r}}_{\nu}$ can be replaced by $\hat{\boldsymbol{\rho}}_{\alpha}$). Taking into account the asymptotic behavior of $\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})$ we can write up to terms $O(1/r_{\nu}^2)$

$$\nabla_{\mathbf{r}_{\alpha}} \ln \mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) = i \eta_{\nu} \frac{m_{\nu}}{m_{\beta\gamma}} \frac{1}{r_{\nu}} \frac{\hat{\mathbf{k}}_{\nu} - \hat{\mathbf{r}}_{\nu}}{1 - \hat{\mathbf{k}}_{\nu} \cdot \hat{\mathbf{r}}_{\nu}} + O\left(\frac{1}{r_{\nu}^{2}}\right)$$
(27)

$$= i \eta_{\nu} \frac{m_{\nu}}{m_{\beta\gamma}} \frac{1}{\rho_{\alpha}} \frac{\hat{\mathbf{k}}_{\nu} - \boldsymbol{\epsilon}_{\alpha\nu} \hat{\boldsymbol{\rho}}_{\alpha}}{1 - \boldsymbol{\epsilon}_{\alpha\nu} \hat{\mathbf{k}}_{\nu} \cdot \hat{\boldsymbol{\rho}}_{\alpha}} + O\left(\frac{1}{\rho_{\alpha}^{2}}\right),$$
(28)

and

$$\nabla_{\boldsymbol{\rho}_{\alpha}} \ln \mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) = i \,\eta_{\nu} \frac{1}{r_{\nu}} \,\boldsymbol{\epsilon}_{\nu\alpha} \,\frac{\hat{\mathbf{k}}_{\nu} - \hat{\mathbf{r}}_{\nu}}{1 - \hat{\mathbf{k}}_{\nu} \cdot \hat{\mathbf{r}}_{\nu}} + O\left(\frac{1}{r_{\nu}^{2}}\right) \tag{29}$$

$$= i \eta_{\nu} \epsilon_{\nu\alpha} \frac{1}{\rho_{\alpha}} \frac{\hat{\mathbf{k}}_{\nu} - \epsilon_{\alpha\nu} \hat{\boldsymbol{\rho}}_{\alpha}}{1 - \epsilon_{\alpha\nu} \hat{\mathbf{k}}_{\nu} \cdot \hat{\boldsymbol{\rho}}_{\alpha}} + O\left(\frac{1}{\rho_{\alpha}^{2}}\right).$$
(30)

Equations (28) and (30) are valid only in Ω_{α} , where both gradients are of order $O(1/r_{\nu}) = O(1/\rho_{\alpha})$, while Eqs. (27) and (29) are valid both in Ω_0 and Ω_{α} .

Since we are seeking the solution of Eq. (26) which is valid up to terms $O(1/\rho_{\alpha}^2)$, we may drop the last two terms in Eq. (26) and rewrite it in the form

$$\left(\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}} + \frac{1}{2M_{\alpha}}\Delta_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}\cdot\nabla_{\mathbf{r}_{\alpha}} + i\frac{1}{M_{\alpha}}\mathbf{q}_{\alpha}\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} + \frac{1}{\mu_{\alpha}}\sum_{\nu=\beta,\gamma}\nabla_{\mathbf{r}_{\alpha}}\ln\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})\cdot\nabla_{\mathbf{r}_{\alpha}} + \frac{1}{M_{\alpha}}\sum_{\nu=\beta,\gamma}\nabla_{\boldsymbol{\rho}_{\alpha}}\ln\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})\right) \times \varphi_{\alpha}^{(11)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = 0.$$
(31)

This equation can be further simplified. According to (28) and (30) the coefficients in this equation actually depend on $1/\rho_{\alpha}$. Hence the solution $\varphi_{\alpha}^{(11)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ will also depend on $1/\rho_{\alpha}$ and we may drop the second, fourth, and sixth terms, because their contribution will be only of order $O(1/\rho_{\alpha}^2)$. Besides, since we are interested only in solutions satisfying Eq. (31) in the leading order $O(1/\rho_{\alpha})$, the function $\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})$ can be approximated by its leading term $\exp(i\eta_{\nu}\ln\zeta_{\nu})$ at $\zeta_{\nu}\rightarrow\infty$. Nevertheless we save $\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})$, keeping in mind that we need to take into account its leading term. We thus arrive at the final equation

$$\left(\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}}+i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}\cdot\nabla_{\mathbf{r}_{\alpha}}+\frac{1}{\mu_{\alpha}}\sum_{\nu=\beta,\gamma}\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu})\cdot\nabla_{\mathbf{r}_{\alpha}}\right)-V_{\alpha}(\mathbf{r}_{\alpha})\left(\varphi_{\alpha}^{(11)}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})=0,\right)$$
(32)

which can be written more compactly if we introduce the local momentum of the relative motion of particles β and γ in the Coulomb field of the third particle α :

$$\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} - i \sum_{\nu=\beta,\gamma} \nabla_{\mathbf{r}_{\alpha}} \ln \mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}).$$
(33)

Taking into account (28) we arrive at the conclusion that in the leading order $\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})$, i.e., $\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha})$ is nothing but the local momentum (20) introduced in [8]. Then Eq. (32) reduces to (18), i.e.,

$$\varphi_{\alpha}^{(11)}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha}) = \varphi_{\alpha}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha}), \qquad (34)$$

where $\varphi_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ is the solution to Eq. (18). We note that (19) follows from (33) both in Ω_{α} and in Ω_{0} [when deriving Eq. (19) from (33) we did not use the condition $r_{\alpha}/\rho_{\alpha} \rightarrow 0$]. Hence we may consider $\varphi_{\alpha}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ even in Ω_{0} .

The second term of (25) satisfies the equation

$$\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})\left(\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}}+\frac{1}{2M_{\alpha}}\Delta_{\boldsymbol{\rho}_{\alpha}}+i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}\cdot\nabla_{\mathbf{r}_{\alpha}}\right)$$

$$+i\frac{1}{M_{\alpha}}\mathbf{q}_{\alpha}\cdot\nabla_{\boldsymbol{\rho}_{\alpha}}+\frac{1}{\mu_{\alpha}}\left[\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\right]$$

$$+\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})\right]\cdot\nabla_{\mathbf{r}_{\alpha}}+\frac{1}{M_{\alpha}}\left[\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\right]$$

$$+\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})\right]\cdot\nabla_{\boldsymbol{\rho}_{\alpha}}-V_{\alpha}(\mathbf{r}_{\alpha})$$

$$+\frac{1}{\mu_{\alpha}}\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\cdot\nabla_{\mathbf{r}_{\alpha}}\mathrm{ln}\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})$$

$$+\frac{1}{M_{\alpha}}\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}}\mathrm{ln}\mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})$$

$$\times\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha},\,\boldsymbol{\rho}_{\alpha})=0.$$
(35)

When deriving this equation we took into account that $\mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu})$ satisfies Eq. (5) in the leading order $O(1/\zeta_{\nu})$ at $\zeta_{\nu} \rightarrow \infty$ [up to terms $O(1/\zeta_{\nu}^2)$]:

$$\left(\frac{1}{2\mu_{\nu}}\Delta_{\mathbf{r}_{\nu}}+i\frac{1}{\mu_{\nu}}\mathbf{k}_{\nu}\cdot\nabla_{\mathbf{r}_{\nu}}-V_{\nu}^{C}\right)\mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu})$$

$$\approx f_{\nu}^{C}\frac{1}{r_{\nu}}e^{-i\eta_{\nu}\ln(2k_{\nu}r_{\nu})}\left(\frac{1}{2\mu_{\nu}}\Delta_{\mathbf{r}_{\nu}}+i\frac{1}{\mu_{\nu}}\mathbf{k}_{\nu}\cdot\nabla_{\mathbf{r}_{\nu}}\right)e^{i\zeta_{\nu}}$$

$$=O\left(\frac{1}{r_{\nu}^{2}}\right).$$
(36)

We note that in $\Omega_{\alpha} = O(1/r_{\nu}^2) = O(1/\rho_{\alpha}^2), \nu \neq \alpha$. According to (11) $\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) = O(1/\rho_{\alpha})$ at $\rho_{\alpha} \to \infty$ in Ω_{α} . Hence it is enough to satisfy the equation for $\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ in the leading order $O(1/\rho_{\alpha})$. Besides, it follows from (11) that up to terms $O(1/r_{\nu})$ we have

$$\nabla_{\mathbf{r}_{\alpha}} \ln \mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu}) \approx \frac{m_{\nu}}{m_{\beta\gamma}} \nabla_{\mathbf{r}_{\alpha}} \zeta_{\nu} = i \frac{m_{\nu}}{m_{\beta\gamma}} (-k_{\nu} \hat{\mathbf{r}}_{\nu} + \mathbf{k}_{\nu})$$
(37)

$$\approx i \frac{m_{\nu}}{m_{\beta\gamma}} (\epsilon_{\nu\alpha} k_{\nu} \hat{\boldsymbol{\rho}}_{\alpha} + \mathbf{k}_{\nu}), \quad \nu = \beta, \gamma$$
(38)

and

$$\nabla_{\boldsymbol{\rho}_{\alpha}} \ln \mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu}) \approx i \nabla_{\boldsymbol{\rho}_{\alpha}} \zeta_{\nu} = i \boldsymbol{\epsilon}_{\nu\alpha} (-k_{\nu} \hat{\mathbf{r}}_{\nu} + \mathbf{k}_{\nu})$$
(39)

$$\approx i(k_{\nu}\hat{\boldsymbol{\rho}}_{\alpha} + \boldsymbol{\epsilon}_{\nu\alpha} \mathbf{k}_{\nu}), \quad \nu = \boldsymbol{\beta}, \boldsymbol{\gamma}.$$
(40)

Equations (38) and (40) are valid only in Ω_{α} . Since in $\Omega_{\alpha} \quad \mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu}) = O(1/\rho_{\alpha})$, to satisfy Eq. (35) up to terms of order $O(1/\rho_{\alpha}^2)$ we are seeking the solution $\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ which is valid in the leading order $O(1/\rho_{\alpha})$. Hence, we may drop all the terms in Eq. (35) containing $\nabla_{\mathbf{r}_{\alpha}} \ln \mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})$ and $\nabla_{\boldsymbol{\rho}_{\alpha}} \ln \mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma})$ because they are of order $O(1/\rho_{\alpha})$. Taking into account (37) and (39) gives the equation [up to terms of order $O(1/\rho_{\alpha})$]

$$\left(\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}} + \frac{1}{2M_{\alpha}}\Delta_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}\cdot\nabla_{\mathbf{r}_{\alpha}} + i\frac{1}{M_{\alpha}}\mathbf{q}_{\alpha}\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\frac{m_{\beta}}{m_{\beta}\gamma}(\boldsymbol{\epsilon}_{\beta\alpha}k_{\beta}\hat{\boldsymbol{\rho}}_{\alpha} + \mathbf{k}_{\beta})\cdot\nabla_{\mathbf{r}_{\alpha}} + i\frac{1}{M_{\alpha}}\times(k_{\beta}\hat{\boldsymbol{\rho}}_{\alpha} + \boldsymbol{\epsilon}_{\beta\alpha}\mathbf{k}_{\beta})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})\right)\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = 0.$$
(41)

The coefficients of this equation depend on $\hat{\rho}_{\alpha}$. From $\nabla_{\rho_{\alpha}} \cdot \hat{\rho}_{\alpha} = O(1/\rho_{\alpha})$ it follows that $|\nabla_{\rho_{\alpha}} \varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \rho_{\alpha})| = O(1/\rho_{\alpha})$. Hence when looking for the solution of Eq. (41) up to order $O(1/\rho_{\alpha})$ the second, fourth, and sixth terms containing derivatives over ρ_{α} can be dropped. We can introduce a new local momentum

$$\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} - i\chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha})\nabla_{\mathbf{r}_{\alpha}}\ln\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})$$
$$= \mathbf{k}_{\alpha} + \chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha})\frac{m_{\beta}}{m_{\beta\gamma}}(\boldsymbol{\epsilon}_{\beta\alpha}k_{\beta}\boldsymbol{\hat{\rho}}_{\alpha} + \mathbf{k}_{\beta}). \quad (42)$$

From

$$\mathbf{k}_{\alpha} = \boldsymbol{\epsilon}_{\beta\alpha} \frac{\mu_{\beta}}{M_{\alpha}} \mathbf{q}_{\beta} - \frac{m_{\beta}}{m_{\beta\gamma}} \mathbf{k}_{\beta} \tag{43}$$

it follows that in Ω_{α}

$$\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}) = \boldsymbol{\epsilon}_{\beta\alpha} \frac{\mu_{\beta}}{M_{\alpha}} \mathbf{q}_{\beta} - \frac{m_{\beta}}{m_{\beta\gamma}} \boldsymbol{\epsilon}_{\alpha\beta} k_{\beta} \hat{\boldsymbol{\rho}}_{\alpha}, \quad \mathbf{r}_{\alpha}, \ \boldsymbol{\rho}_{\alpha} \in \Omega_{\alpha}.$$
(44)

To stress that the approximation (40) and correspondingly the definitions of the local momentum (42) and (44) are valid only in Ω_{α} we introduced the cutoff function $\chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha})$ such that $\chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}) = 1$ in Ω_{α} and $\chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}) = 0$ out of Ω_{α} . Comparison of (43) and (44) shows that in Ω_{α} , $\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})$ can be derived from \mathbf{k}_{α} by the replacement in (43) of \mathbf{k}_{β} by $\epsilon_{\alpha\beta}k_{\beta}\hat{\boldsymbol{\rho}}_{\alpha}$. Then the equation for $\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ reduces to Eq. (18) with $\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})$ instead of $\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})$. The solution of this equation,

$$\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = e^{-i\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})\cdot\mathbf{r}_{\alpha}}\psi_{\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}), \qquad (45)$$

where $\psi_{\mathbf{k}_{\alpha}^{(1)}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha})$ is the scattering wave function describing the relative motion of particles β and γ , with the relative kinetic energy $E_{\alpha}(\boldsymbol{\rho}_{\alpha}) = k_{\alpha}^{(21)^2}(\boldsymbol{\rho}_{\alpha})/2\mu_{\alpha}$, interacting via the potential V_{α} . Similarly for the wave function $\varphi_{\alpha}^{(12)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ we derive Eq. (18) with the local momentum $\mathbf{k}_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha})$ instead of $\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})$, where $\mathbf{k}_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha})$ is given by

$$\mathbf{k}_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} - i\chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}) \nabla_{\mathbf{r}_{\alpha}} \ln \mathcal{F}_{\gamma}^{(2)}(i\xi_{\gamma})$$
$$= \mathbf{k}_{\alpha} + \chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}) \frac{m_{\gamma}}{m_{\beta\gamma}} (\boldsymbol{\epsilon}_{\gamma\alpha} k_{\gamma} \hat{\boldsymbol{\rho}}_{\alpha} + \mathbf{k}_{\gamma})$$
(46)

$$= \boldsymbol{\epsilon}_{\gamma\alpha} \frac{\mu_{\gamma}}{M_{\alpha}} \mathbf{q}_{\gamma} - \frac{m_{\gamma}}{m_{\beta\gamma}} \boldsymbol{\epsilon}_{\alpha\gamma} k_{\gamma} \hat{\boldsymbol{\rho}}_{\alpha}, \quad \mathbf{r}_{\alpha}, \ \boldsymbol{\rho}_{\alpha} \in \Omega_{\alpha}.$$
(47)

The fourth equation derived when substituting the last term of (25) into (2) is satisfied automatically up to terms $O(1/\rho_{\alpha}^2)$ in Ω_{α} , because the product $\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta})\mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) = O(1/\rho_{\alpha}^2)$. Since we are looking for the asymptotics of the exact three-body wave function in Ω_{α} containing the terms up to order $O(1/\rho_{\alpha}^2)$ [i.e., terms not exceeding $O(1/\rho_{\alpha})$] the last term of (25), containing $\varphi_{\alpha}^{(22)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$, can be disregarded. Nevertheless we will keep that term also to provide the matching of the asymptotic wave function $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(as)(+)'}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})$ with the Redmond-Merkuriev wave function $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(as)(+)'}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})$ in Ω_{0} . The fourth term in (25) gives rise to an equation for $\varphi_{\alpha}^{(22)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$:

$$\left(\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}} + \frac{1}{2M_{\alpha}}\Delta_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}\cdot\nabla_{\mathbf{r}_{\alpha}} + i\frac{1}{M_{\alpha}}\mathbf{q}_{\alpha}\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\sum_{\nu=\beta,\gamma}\frac{m_{\nu}}{m_{\beta\gamma}}(\boldsymbol{\epsilon}_{\nu\alpha}k_{\nu}\hat{\boldsymbol{\rho}}_{\alpha} + \mathbf{k}_{\nu})\cdot\nabla_{\mathbf{r}_{\alpha}} + i\frac{1}{M_{\alpha}}\sum_{\nu=\beta,\gamma}\left(k_{\nu}\hat{\boldsymbol{\rho}}_{\alpha} + \boldsymbol{\epsilon}_{\nu\alpha}\mathbf{k}_{\nu})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})\right) \times\varphi_{\alpha}^{(22)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = 0.$$
(48)

Using the same arguments we have used to simplify (41) we may drop all the terms containing derivatives over ρ_{α} when looking for the solution of this equation in the leading order. We can introduce now a new local momentum

$$\mathbf{k}_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} + \chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha}) \sum_{\nu=\beta,\gamma} \frac{m_{\nu}}{m_{\beta\gamma}} (\boldsymbol{\epsilon}_{\nu\alpha} k_{\nu} \hat{\boldsymbol{\rho}}_{\alpha} + \mathbf{k}_{\nu}).$$
(49)

Then the equation for $\varphi_{\alpha}^{(22)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ reduces to (18) with $\mathbf{k}_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha})$ instead of $\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})$.

Thus we have found all the unknown functions $\varphi_{\alpha}^{(nm)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ in (25). Hence we have shown that the asymptotic solution to the Schrödinger equation (2) in Ω_{α} , satisfying it up to order $O(1/\rho_{\alpha}^2)$ and containing the zerothand all first-order terms $O(1/\rho_{\alpha})$, can be written in the form (25), where each $\mathcal{F}_{\nu}^{(j)}(i\zeta_{\nu})$ is given by its leading term in Ω_{α} , Eqs. (10) and (11). Functions $\varphi_{\alpha}^{(nm)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ are the solutions of Eq. (18) with the local momenta $\mathbf{k}_{\alpha}^{(nm)}(\boldsymbol{\rho}_{\alpha})$ instead of $\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})$. Equation (25) is our main result.

The other convenient forms can be derived from it. Equa-

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tion (25) is valid for pure Coulombic interactions in the pairs β and γ , while the interaction in the pair α may contain a short-range term. Suppose now that $V_{\alpha} = V_{\alpha}^{C}$, i.e., there is the pure Coulombic interaction between particles of the pair

 α . Then functions $\varphi_{\alpha}^{(nm)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ are given by (21) with $\mathbf{k}_{\alpha}^{(nm)}(\boldsymbol{\rho}_{\alpha})$ instead of $\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})$ in (22) and the asymptotics of the three-body wave function satisfying the Schrödinger equation in the leading order $O(1/\rho_{\alpha})$ takes the form

$$\begin{split} \Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{as})(+)'}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) &= e^{i \,\mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} \, e^{i \,\mathbf{k}_{\alpha}\cdot\mathbf{r}_{\alpha}} \left[\mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta}) \, \mathcal{F}_{\gamma}^{(1)}(i\zeta_{\gamma}) N_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})) \\ &+ \mathcal{F}_{\beta}^{(1)}(i\zeta_{\beta}) \, \mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) \, N_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha})) \\ &+ \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) \, \mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) \, N_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha})) \\ &+ \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) \, \mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) \, N_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha})) \\ &+ \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) \, \mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) \, N_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha})) e^{i \eta_{\beta} \ln \zeta_{\beta \alpha}} \, e^{i \eta_{\gamma} \ln \zeta_{\gamma \alpha}} \\ &+ \mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) \, \mathcal{F}_{\gamma}^{(2)}(i\zeta_{\gamma}) \, N_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})) e^{i \eta_{\beta} \ln \zeta_{\beta \alpha}} \, e^{-i \eta_{\beta} \ln (2k_{\beta \rho_{\alpha}})} \, e^{i \eta_{\gamma} \ln \zeta_{\gamma \alpha}} \\ &+ e^{i \,\mathbf{k}_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha}) \cdot \mathbf{r}_{\alpha}} \, N_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})) \, e^{i \eta_{\beta} \ln \zeta_{\beta \alpha}} \, f_{\gamma}^{C} \, \frac{e^{i \zeta_{\gamma \alpha}}}{\boldsymbol{\rho}_{\alpha}} \, e^{-i \eta_{\gamma} \ln (2k_{\gamma \rho_{\alpha}})} \\ &+ e^{i \,\mathbf{k}_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha}) \cdot \mathbf{r}_{\alpha}} \, N_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha})) \, e^{i \eta_{\beta} \ln \zeta_{\beta \alpha}} \, f_{\gamma}^{C} \, \frac{e^{i \zeta_{\gamma \alpha}}}{\boldsymbol{\rho}_{\alpha}} \, e^{-i \eta_{\gamma} \ln (2k_{\gamma \rho_{\alpha}})} \\ &+ e^{i \,\mathbf{k}_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \cdot \mathbf{r}_{\alpha}} \, N_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha})) \, f_{\beta}^{C} \, \frac{e^{i \zeta_{\beta \alpha}}}{\boldsymbol{\rho}_{\alpha}} \\ &+ e^{i \,\mathbf{k}_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \cdot \mathbf{r}_{\alpha}} \, N_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha})) \, f_{\beta}^{C} \, \frac{e^{i \zeta_{\beta \alpha}}}{\boldsymbol{\rho}_{\alpha}} \\ &+ e^{i \,\mathbf{k}_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \cdot \mathbf{r}_{\alpha}} \, N_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \, F(-i \,\eta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}), 1; i\zeta_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha})) \, f_{\beta}^{C} \, \frac{e^{i \zeta_{\beta \alpha}}}{\boldsymbol{\rho}_{\alpha$$

Here $N_{\alpha}^{(nm)}(\boldsymbol{\rho}_{\alpha})$, $\eta_{\alpha}^{(nm)}$, and $\zeta_{\alpha}^{(nm)}$ are given by (22) with $\mathbf{k}_{\alpha}^{(nm)}(\boldsymbol{\rho}_{\alpha})$ instead of $\mathbf{k}_{\alpha}(\boldsymbol{\rho}_{\alpha})$. When deriving (51) we approximated $\mathcal{F}_{\nu}^{(j)}(i\zeta_{\nu})$ by their leading terms, Eqs. (10) and (11), and expressed ζ_{ν} in terms of $\zeta_{\nu\alpha}$:

$$\boldsymbol{\zeta}_{\nu} = \boldsymbol{\zeta}_{\nu\alpha} + \boldsymbol{\epsilon}_{\nu\alpha} \frac{m_{\nu}}{m_{\beta\gamma}} \boldsymbol{k}_{\nu} \, \boldsymbol{\mathbf{r}}_{\alpha} \cdot \boldsymbol{\hat{\rho}}_{\alpha} + \frac{m_{\nu}}{m_{\beta\gamma}} \, \boldsymbol{\mathbf{k}}_{\nu} \cdot \, \boldsymbol{\mathbf{r}}_{\alpha} + O\left(\frac{1}{\rho_{\alpha}}\right), \quad \boldsymbol{\zeta}_{\nu\alpha} = \boldsymbol{k}_{\nu} \rho_{\alpha} - \boldsymbol{\epsilon}_{\alpha\nu} \, \boldsymbol{\mathbf{k}}_{\nu} \cdot \boldsymbol{\rho}_{\alpha} \,. \tag{52}$$

This approximation is valid in Ω_{α} . If the interactions in all three pairs are given by the sum of the short-range and Coulombic potentials, $V_{\nu} = V_{\nu}^{C} + V_{\nu}^{S}$, $\nu = 1, 2, 3$, then by replacing in Eq. (51) the Coulomb scattering amplitudes f_{ν}^{C} of particles of the pairs $\nu = \beta, \gamma$ by the scattering amplitudes f_{ν} of these particles interacting via potential V_{ν} we derive the asymptotic wave function

$$\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(\mathrm{as})(+)'}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha}) = e^{i \mathbf{q}_{\alpha}\cdot\boldsymbol{\rho}_{\alpha}} \left(\psi_{\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}) \ e^{i \eta_{\beta} \ln \zeta_{\beta\alpha}} \ e^{i \eta_{\gamma} \ln \zeta_{\gamma\alpha}} + \psi_{\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}) \ f_{\beta} \ \frac{e^{i \zeta_{\beta\alpha}}}{\boldsymbol{\rho}_{\alpha}} \ e^{-i \eta_{\beta} \ln (2k_{\beta}\boldsymbol{\rho}_{\alpha})} \ e^{i \eta_{\gamma} \ln \zeta_{\gamma\alpha}} + \psi_{\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})}^{(+)}(\mathbf{r}_{\alpha}) \ f_{\beta} \ \frac{e^{i \zeta_{\beta\alpha}}}{\boldsymbol{\rho}_{\alpha}} \ e^{-i \eta_{\beta} \ln (2k_{\beta}\boldsymbol{\rho}_{\alpha})} \ f_{\gamma} \ \frac{e^{i \zeta_{\gamma\alpha}}}{\boldsymbol{\rho}_{\alpha}} \ e^{-i \eta_{\gamma} \ln (2k_{\gamma}\boldsymbol{\rho}_{\alpha})} + \psi_{\mathbf{k}_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha})}^{(+)} \\ \times (\mathbf{r}_{\alpha}) \ f_{\beta} \ \frac{e^{i \zeta_{\beta\alpha}}}{\boldsymbol{\rho}_{\alpha}} \ e^{-i \eta_{\beta} \ln (2k_{\beta}\boldsymbol{\rho}_{\alpha})} \ f_{\gamma} \ \frac{e^{i \zeta_{\gamma\alpha}}}{\boldsymbol{\rho}_{\alpha}} \ e^{-i \eta_{\gamma} \ln (2k_{\gamma}\boldsymbol{\rho}_{\alpha})} \right).$$
(53)

B. Matching with the Redmond-Merkuriev wave function in Ω_0

Let us discuss the problem of matching the wave function (50) with the Redmond-Merkuriev wave function (3) in Ω_0 . From the derivation of (50) it is clear that it defines the asymptotic solution to the Schrödinger equation (2) up to terms $O(1/\rho_{\alpha}^2)$ only in the asymptotic domain Ω_{α} and is not

valid in Ω_0 . The first term of (50) can be extrapolated in Ω_0 where its leading part joins smoothly with the leading part of the Redmond-Merkuriev wave function [three-particle Coulomb-distorted wave (13)] due to the disappearance of the addend to \mathbf{k}_{α} in (33). But it is not the case for the second, third, and fourth terms of (50). To see it consider, for example, Eq. (41). This equation is valid only in Ω_{α} : when

deriving it we used Eqs. (38) and (40) valid in Ω_{α} . In Ω_0 , instead of (41), we derive using (37) and (39)

$$\left(\frac{1}{2\mu_{\alpha}}\Delta_{\mathbf{r}_{\alpha}} + \frac{1}{2M_{\alpha}}\Delta_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\mathbf{k}_{\alpha}\cdot\nabla_{\mathbf{r}_{\alpha}} + i\frac{1}{M_{\alpha}}\mathbf{q}_{\alpha}\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} + i\frac{1}{\mu_{\alpha}}\frac{m_{\beta}}{m_{\beta\gamma}}(-k_{\beta}\hat{\mathbf{r}}_{\beta} + \mathbf{k}_{\beta})\cdot\nabla_{\mathbf{r}_{\alpha}} + i\frac{1}{M_{\alpha}}\epsilon_{\beta\alpha} \times (-k_{\beta}\hat{\mathbf{r}}_{\beta} + \mathbf{k}_{\beta})\cdot\nabla_{\boldsymbol{\rho}_{\alpha}} - V_{\alpha}(\mathbf{r}_{\alpha})\right)\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = 0.$$
(54)

This equation in contrast to (41) is valid both in Ω_{α} and Ω_0 . But now coefficients in this equation depend on \mathbf{r}_{β} , and not on ρ_{α} as in (41). That is why we cannot integrate over \mathbf{r}_{α} assuming coefficients to be constants. However, we recall that $\mathcal{F}_{\beta}^{(2)}(i\zeta_{\beta}) = O(1/r_{\nu})$, hence to satisfy Eq. (2) up to terms of the second order $O(1/(r_{\alpha}r_{\beta}))$ in Ω_0 it is enough to find a solution to (54) satisfying it up to terms $O(1/r_{\alpha})$. In the domain Ω_0 , $|\nabla_{\mathbf{r}_{\alpha}} \varphi_{\alpha}^{(0)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})| = O(1/r_{\alpha})$, where $\varphi_{\alpha}^{(0)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ is the solution of Eq. (18) with the asymptotic momentum \mathbf{k}_{α} . Hence it is evident that $\varphi_{\alpha}^{(0)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ satisfies (54) up to terms $O(1/r_{\alpha})$, just what we need to satisfy (2) in the second order [up to terms $O(1/(r_{\nu}r_{\alpha}))$]. That is why to provide a smooth matching of $\varphi_{\alpha}^{(21)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ with $\varphi_{\alpha}^{(0)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ in Ω_0 we introduced a cutoff function $\chi(\boldsymbol{\rho}_{\alpha}, \mathbf{r}_{\alpha})$ in (42). Similarly, to provide a smooth join in Ω_0 of $\varphi_{\alpha}^{(12)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ and $\varphi_{\alpha}^{(22)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ with $\varphi_{\alpha}^{(0)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ we introduced the cutoff function in (46) and (49). For pure Coulombic interaction $\varphi_{\alpha}^{(0)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha}) = N_{\alpha} F(-i \eta_{\alpha}, 1; i(k_{\alpha} r_{\alpha} - \mathbf{k}_{\alpha} \cdot \mathbf{r}_{\alpha}))$. Since all the functions $\varphi_{\alpha}^{(nm)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ go to $\varphi_{\alpha}^{(0)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$ in Ω_0 , we easily see that in Ω_0 due to (7) the wave function $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(as)(+)'}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})$ given by (50) matches smoothly to the Redmond-Merkuriev wave function (3). It is evident that to provide that joining we should keep the last term in (25).

C. Singular directions

We note that (25), (50), (51), and (53) are valid only in the nonsingular directions $(\hat{\mathbf{k}}_{\nu} \cdot \hat{\boldsymbol{\rho}}_{\alpha} \neq 1, \nu = \beta, \gamma)$. For practical applications it is important to know how to overcome the problem of the singular directions although a small contribution to the ionization amplitude arises from the singular directions, because the exact wave function is finite in the singular directions. The most serious problem here is the divergent of $\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha})$ given by (33) in the singular directions. To get rid of that divergency we redefine (33) using a characteristic function of the singular direction $\hat{\mathbf{k}}_{\nu} \cdot \hat{\mathbf{r}}_{\nu} = 1$ $\omega_{\nu}(\mathbf{r}_{\nu}), \nu = \beta, \gamma, [3]$ such that

$$\omega_{\nu}(\mathbf{r}_{\nu}) = 0, \quad \zeta_{nu} \leq (k_{\nu}r_{\nu})^{\lambda}, \quad 0 < \lambda < 1,$$
$$\omega_{\nu}(\mathbf{r}_{\nu}) = 1, \quad \zeta_{\nu} \geq (k_{\nu}r_{\nu})^{\lambda'}, \quad \lambda < \lambda' < 1 \qquad (55)$$

i.e., $\omega_{\nu}(\mathbf{r}_{\nu})$ disappears in the vicinity of the singular direction and goes to 1 beyond it.

Surely the procedure of the redefinition of $\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha})$ in (33) is not unique and we consider here two possible ways it could be done.

(1) Let us introduce

$$\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} - i \sum_{\nu=\beta,\gamma} \omega_{\nu}(\mathbf{r}_{\nu}) \nabla_{\mathbf{r}_{\alpha}} \ln \mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}).$$
(56)

Due to the presence of the characteristic functions in (56) in the vicinity of the singular direction $\hat{\mathbf{k}}_{\nu} \cdot \hat{\mathbf{r}}_{\nu} \rightarrow 1$, $\omega_{\nu}(\mathbf{r}_{\nu}) \nabla_{\mathbf{r}_{\alpha}} \ln \mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) \rightarrow 0$. If $\hat{\mathbf{k}}_{\beta} \cdot \hat{\mathbf{r}}_{\beta} \rightarrow 1$ and $\hat{\mathbf{k}}_{\gamma} \cdot \hat{\mathbf{r}}_{\gamma} \rightarrow 1$ simultaneously, then all the "local momenta" $\mathbf{k}_{\alpha}^{(nm)}(\boldsymbol{\rho}_{\alpha})$ $\rightarrow \mathbf{k}_{\alpha}$ [it is clear from (37) that in that case $\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})$, $\mathbf{k}_{\alpha}^{(12)}(\boldsymbol{\rho}_{\alpha}), \mathbf{k}_{\alpha}^{(22)}(\boldsymbol{\rho}_{\alpha}) \rightarrow \mathbf{k}_{\alpha}$].

(2) One can introduce another local momentum

$$\mathbf{k}_{\alpha}^{(11)}(\boldsymbol{\rho}_{\alpha}) = \mathbf{k}_{\alpha} - i \sum_{\nu=\beta,\gamma} \\ \times \frac{\nabla_{\mathbf{r}_{\alpha}} \mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) + [1 - \omega_{\nu}(\mathbf{r}_{\nu})] \nabla_{\mathbf{r}_{\alpha}} \mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu})}{\mathcal{F}_{\nu}^{(1)}(i\zeta_{\nu}) + [1 - \omega_{\nu}(\mathbf{r}_{\nu})] \mathcal{F}_{\nu}^{(2)}(i\zeta_{\nu})}.$$
(57)

Away from the singular directions, the local momentum coincides with the previous definition (33), while in the vicinity of the singular directions it is regular due to (7) and regularity of $\nabla_{\mathbf{r}_{\alpha}} \ln F(-i\eta_{\nu}1; i\zeta_{\nu})$ at $\zeta_{\nu} \rightarrow 0$. With either definition of the local momentum, (56) or (57), the wave function $\Psi_{\mathbf{k}_{\alpha},\mathbf{q}_{\alpha}}^{(as)(+)'}(\mathbf{r}_{\alpha},\boldsymbol{\rho}_{\alpha})$, Eq. (50), goes to the Redmond-Merkuriev wave function (3). Surely such a wave function is not an asymptotic solution to the Schrödinger equation in Ω_{α} in the singular directions and can be considered only as a way out for the practical calculations to avoid the divergence of the local momentum $\mathbf{k}_{\alpha}^{(21)}(\boldsymbol{\rho}_{\alpha})$ in the singular directions in Ω_{α} . The question about an asymptotic solution to the Schrödinger equation in the singular directions in Ω_{α} remains open.

III. SUMMARY

Summarizing the result obtained in this work, we have derived the asymptotic continuum wave function for three charged particles [Eq. (25)] which satisfies the Schrödinger equation up to terms of order $O(1/\rho_{\alpha}^2)$ in the domain Ω_{α} in the nonsingular directions. This wave function is an extension of the one derived in [8]. It would be of interest, for example, to evaluate the so-called post-Coulomb acceleration (PCA) in the atomic ionization processes and nuclear breakup reactions using our wave function $\Psi_{\mathbf{k}_{\alpha}\mathbf{q}_{\alpha}}^{(+)'}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$. The appearance of the local momenta $\mathbf{k}_{\alpha}^{(nm)}(\boldsymbol{\rho}_{\alpha})$ in $\varphi_{\alpha}^{(nm)}(\mathbf{r}_{\alpha}, \boldsymbol{\rho}_{\alpha})$, instead of the asymptotic momentum \mathbf{k}_{α} , is a genuine three-body effect which can be important when calculating PCA at low relative kinetic energies of the final particles β and γ . We note that the method used here can be applied to obtain the asymptotic wave function which satisfies the Schrödinger equation up to terms of order $O(1/\rho_{\alpha}^{3})$ in the region Ω_{α} .

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