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Asymptotic solution of the Schrödinger equation for three charged particles

E. O. Alt and A. M. Mukhamedzhanov*
Institut für Physik, Universität Mainz, Mainz, Germany
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The Schrödinger equation for three charged particles in the continuum is considered in the region $\rho_\alpha \to \infty$, $r_\alpha/\rho_\alpha \to 0$, where r_α is the distance between the particles β and γ, and ρ_α denotes the distance between the center of mass of the pair (β,γ) and particle α, $\alpha \neq \beta \neq \gamma$. The asymptotic Schrödinger equation valid in this domain is found to have at least two types of solutions. The first, exact one which is of the familiar product form, however, does not connect to the known asymptotic expression for the solution of the original Schrödinger equation in the region where all interparticle distances r_1, r_2, and r_3 go to infinity. Therefore a second type of asymptotic wave function is derived which satisfies the asymptotic Schrödinger equation to leading order. It has a surprisingly simple form, being the product of asymptotic Coulomb distortion factors for the relative motion of the particles within each of the pairs (α,β) and (α,γ), and an ordinary two-particle scattering state for the third pair (β,γ) but belonging to an effective two-particle relative momentum which depends on the relative coordinate $\boldsymbol{\rho}_\alpha$. This constitutes a genuine three-body effect. Based on this result, we present an expression for the asymptotic wave function which is the asymptotic solution of the three-charged-particle Schrödinger equation in all asymptotic regions: where all three interparticle distances are large where it goes over into the standard asymptotic wave function, as well as if only any two interparticle distances, say r_β and r_γ, are large and the third one satisfies the condition $r_\alpha/\rho_\alpha \to 0$.

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I. INTRODUCTION

One of the intriguing problems in three-body physics concerns the incorporation in a useful manner of long-ranged Coulomb forces into the theoretical description of three-body processes. In recent years, though, there has been considerable progress in the theoretical formulation of three-body equations which render feasible the calculation of reactions involving charged particles. But none of them can at present be made use of without approximations, the reliability of which is often difficult to estimate. This is, in particular, true when three charged particles are in the continuum.

A much less involved task consists of deriving approximate but analytic forms for the scattering wave functions of the system of interest which are valid in some, in general asymptotic, domain. Not only is their knowledge required as the boundary condition to be imposed on the acceptable solutions of the Schrödinger equation, but for many practical applications it may be sufficient to substitute for the exact three-charged-particle scattering wave function a suitable asymptotic approximation in order to obtain physically reasonable, and in particular calculable, expressions for reaction amplitudes.

The investigation of the asymptotic behavior of the three-charged-particle wave function when all three particles are in the continuum has a long history. Redmond [1], as cited in Rosenberg [2], and Peterkop [3] have proposed an asymptotic wave function as a product of three-body plane waves times a Coulomb distortion factor for each of the three pairs of particles, which is valid provided all three interparticle distances tend to infinity, in the so-called nonsingular regions, i.e., except for directions where one or more of the interparticle relative coordinates is parallel to the corresponding canonically conjugated momentum. An extension of this result which remains sensible even in the singular directions has been stated by Merkuriev [4]; see also Brauner, Briggs, and Klar [5]. However, when using these asymptotic three-particle wave functions to evaluate approximate ionization amplitudes the integrations involved often extend over domains which are outside the range of validity of the aforementioned expressions. For such purposes it would be advantageous to have at one's disposal a three-particle wave function which is the solution of the Schrödinger equation also when two particles are still relatively close to each other while the third one is already very far from their center of mass. (In an ionization amplitude such a limitation in the variation of an interparticle distance is provided by the wave function of the pair bound in the initial state.)

The derivation of an asymptotic solution of the three-charged-particle Schrödinger equation in regions of the configuration space where the distance between two of the particles is much smaller than the distance of their center of mass from the third, the remaining particle constitutes a long-standing and important problem in atomic and nuclear physics, the solution of which will be presented in this paper. We mention that an asymptotic wave function valid in this domain has been proposed in [6], however, only for partial waves, for monopole and monopole-plus-dipole electron-electron interactions. Furthermore, a formal scheme which would yield the desired asymptotic solution of the Schrödinger equation was suggested in [7] but no concrete realization leading to an analytical wave function was attempted.

The problem is stated and discussed in a more detailed manner in Sec. II. In Sec. III we develop our method of solution at the example of a simplified model of two noninteracting charged particles moving in the Coulomb field of an infinitely massive charged core. The results obtained there are used in Sec. IV to find the asymptotic solution of the Schrödinger equation for three arbitrarily interacting charged particles in the region where the distance between one of the particles and the center of mass of the other two is much larger than the interparticle distance within this pair, with the exception of the singular directions. Moreover, generalizations of the asymptotic solution are proposed which are simultaneously valid in all asymptotic domains, i.e., where all three interparticle distances tend to infinity arbitrarily as well as where the ratio of the distance between any two particles to the distance between their center of mass and the third particle goes to zero. Section V contains a summary of the results and a discussion of some of the physical implications of the derived wave functions. In the Appendix we finally describe a procedure of how the latter can be smoothly continued into the singular directions.

We use units such that $\hbar = c = 1$. Furthermore, unit vectors will be denoted by a hat, i.e., $\hat{\mathbf{a}} \equiv \mathbf{a}/a$.

II. STATEMENT OF THE PROBLEM

In order to elucidate the problem more clearly let us consider a system of three particles of mass m_α and charge e_α, $\alpha = 1,2,3$, in the continuum. We use Jacobi variables: $\mathbf{r}_\alpha$ for the relative coordinate, and $\mathbf{k}_\alpha$ for the relative momentum, between particles β and γ, the reduced mass being $\mu_\alpha = m_\beta m_\gamma/(m_\beta + m_\gamma)$; $\boldsymbol{\rho}_\alpha$ for the relative coordinate between the center of mass of the pair (β,γ) and particle α, with $\mathbf{q}_\alpha$ denoting the canonically conjugated relative momentum (cf. Fig. 1). The corresponding reduced mass is denoted by $M_\alpha = m_\alpha(m_\beta + m_\gamma)/(m_1 + m_2 + m_3)$. Here and in the following the conventional notation for two-body quantities, $A_\alpha \equiv A_{\beta\gamma}$, with $\alpha \neq \beta \neq \gamma$, is being used. Frequently we will need the relations between the coordinates, respectively momenta for a channel $\beta \neq \alpha$ and the corresponding α-channel variables. They are given by

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

$$\begin{pmatrix} \mathbf{q}_\beta \\ \mathbf{k}_\beta \end{pmatrix} = \begin{pmatrix} -\frac{\mu_\alpha}{m_\gamma} & \epsilon_{\beta\alpha} \\ -\epsilon_{\beta\alpha}\frac{\mu_\alpha}{M_\beta} & -\frac{\mu_\beta}{m_\gamma} \end{pmatrix} \begin{pmatrix} \mathbf{q}_\alpha \\ \mathbf{k}_\alpha \end{pmatrix}. \tag{1}$$

For convenience we have introduced the antisymmetric symbol $\epsilon_{\alpha\beta} = -\epsilon_{\beta\alpha}$, with $\epsilon_{\alpha\beta} = 1$ for (α,β) being a cyclic permutation of (1, 2, 3), and $\epsilon_{\alpha\alpha} = 0$.

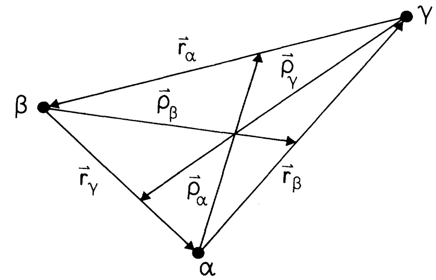

FIG. 1. Graphical representation of the Jacobi coordinates used.

The Schrödinger equation describing this system is

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

with

$$\begin{aligned} V &= \sum_{\nu=1}^{3} V_\nu(\mathbf{r}_\nu), \\ V_\alpha(\mathbf{r}_\alpha) &= V_\alpha^C(\mathbf{r}_\alpha) + V_\alpha^N(\mathbf{r}_\alpha), \\ V_\alpha^C(\mathbf{r}_\alpha) &= \frac{e_\beta e_\gamma}{r_\alpha}. \end{aligned} \tag{3}$$

Here, V_α^C (V_α^N) is the Coulomb (short-range, henceforth called nuclear) interaction between the particles β and γ. $T_{\mathbf{r}_\alpha}$ is the kinetic-energy operator for the relative motion of the pair of particles β and γ, and T_{ρ_α} the one for the motion of particle α relative to the center of mass of the pair (β,γ). They are defined as

$$T_{\mathbf{r}_\alpha} = -\frac{\Delta_{\mathbf{r}_\alpha}}{2\mu_\alpha}, \quad T_{\rho_\alpha} = -\frac{\Delta_{\rho_\alpha}}{2M_\alpha}. \tag{4}$$

Together with the other two pair coordinates $\mathbf{r}_\beta$ and $\mathbf{r}_\gamma$, the meaning of which can also be inferred from Fig. 1, we can define various asymptotic regimes.

(1) Ω_0: all three interparticle distances tend to infinity in an arbitrary manner, i.e., $r_1 \to \infty$, $r_2 \to \infty$, and $r_3 \to \infty$, but *not* $r_\nu/\rho_\nu \to 0$ for $\nu = 1$, 2, or 3.

(2) Ω_α, for $\alpha = 1, 2$, or 3: the distance between particle α and the center of mass of the pair (β,γ) tends to infinity, i.e., $\rho_\alpha \to \infty$, while the distance between particles β and γ satisfies the constraint $r_\alpha/\rho_\alpha \to 0$.

Let us make two remarks. First, we point out that none of the regions Ω_1, Ω_2, or Ω_3 is disjoint from Ω_0. Hence, any acceptable solution of Eq. (2) in Ω_α should connect smoothly to the asymptotic solution in Ω_0. Second, we note that the condition $\rho_\alpha \to \infty$ in Ω_α implies that the two interparticle distances r_β and r_γ go to infinity as well [cf. Eq. (1)]. But the converse is not true: there exists the possibility that r_β and r_γ go to infinity but ρ_α remains finite. Since in this case r_α goes to infinity as well this region is contained in Ω_0.

We are interested in solutions of Eq. (2) in regions where all three or only two of the interparticle distances r_ν become large. If the potentials were of short range the leading term of the solution of Eq. (2) would be a product of a plane wave describing the free motion of particle α relative to the center of mass of the pair (β,γ) times a plane wave in Ω_0, or a scattering state in Ω_α, for the internal motion of the latter pair. However, since the Coulombian part of V does not decrease fast enough to be negligible even for infinite separation of some or all three particles we must find wave functions such that they satisfy Eq. (2) in leading order. Solutions with this property will be called asymptotic. [We remark that this has to be distinguished from the notion of the asymptotic behavior of the wave function: for three charged particles in the continuum this has been described in [3, 4, 8] as a sum of "Coulomb-distorted plane waves," see Eq. (5), plus single- and double-scattering terms plus an outgoing spherical wave.]

As mentioned above the asymptotic solution of Eq. (2) in the region Ω_0 is well known. Except for the so-called singular directions, which are defined by the property that at least one of the relative momenta $\mathbf{k}_\nu$ is parallel to the corresponding relative coordinate $\mathbf{r}_\nu$, it is given as

$$\Psi^{(+)}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)\underset{\Omega_0}{\longrightarrow}\Psi_0^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$$

$$= e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha+i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\prod_{\nu=1}^{3}e^{i\eta_\nu\ln(k_\nu r_\nu-\mathbf{k}_\nu\cdot\mathbf{r}_\nu)} +O\left(\frac{1}{r_1},\frac{1}{r_2},\frac{1}{r_3}\right). \tag{5}$$

Here, $\mathbf{r}_1,\mathbf{r}_2$, and $\mathbf{r}_3$ are considered to be expressed in terms of the independent set of variables $\mathbf{r}_\alpha$ and $\boldsymbol{\rho}_\alpha$. We remark that in Ω_0 the form (5) is equivalent, in the sense of being an asymptotic solution of Eq. (2), to [4, 5]

$$\Psi_0^{\mathrm{as}(+)\prime}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)=e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha+i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\prod_{\nu=1}^{3}N_\nu F(-i\eta_\nu,1;i(k_\nu r_\nu-\mathbf{k}_\nu\cdot\mathbf{r}_\nu)). \tag{6}$$

We have introduced the usual notation

$$\eta_\alpha=\frac{e_\beta e_\gamma\mu_\alpha}{k_\alpha},\quad N_\alpha=e^{-\pi\eta_\alpha/2}\,\Gamma(1+i\eta_\alpha), \tag{7}$$

$F(a,b;x)$ is the confluent hypergeometric function, and $\Gamma(\,)$ the gamma function. But it is clear, however, that neither $\Psi_0^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ nor $\Psi_0^{\mathrm{as}(+)\prime}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ are asymptotic solutions of (2) in any of the domains Ω_1,Ω_2, or Ω_3.

The conventional procedure to find asymptotic solutions in Ω_α, $\alpha=1,2$, or 3, consists of investigating the asymptotic form of the Schrödinger equation (2) valid in this region. For this purpose we define an asymptotic Hamiltonian H_α^{as} via

$$\begin{aligned}H_\alpha^{\mathrm{as}}&=\lim_{\rho_\alpha\to\infty,\,r_\alpha/\rho_\alpha\to0}H\\&=T_{\mathbf{r}_\alpha}+T_{\boldsymbol{\rho}_\alpha}+V_\alpha(\mathbf{r}_\alpha)+v_\alpha^C(\boldsymbol{\rho}_\alpha),\end{aligned} \tag{8}$$

where

$$\begin{aligned}v_\alpha^C(\boldsymbol{\rho}_\alpha)&=\lim_{\rho_\alpha\to\infty,\,r_\alpha/\rho_\alpha\to0}\{V_\beta(\mathbf{r}_\beta)+V_\gamma(\mathbf{r}_\gamma)\}\\&=\frac{e_\alpha\,(e_\beta+e_\gamma)}{\rho_\alpha}\end{aligned} \tag{9}$$

is the Coulomb potential between the charge e_α of particle α and the total charge $(e_\beta+e_\gamma)$ of the particles β and γ concentrated in their center of mass. Because of this property $v_\alpha^C(\boldsymbol{\rho}_\alpha)$ will be termed the "center-of-mass Coulomb potential for channel α." Note that since in Eq. (9) the limit of ρ_α becoming large implies the same for r_β and r_γ, we could neglect the nuclear interactions between particles α and γ, and α and β, completely and, because of $r_\alpha/\rho_\alpha\to0$, terms $\sim r_\alpha/\rho_\alpha^2$ in the corresponding Coulombian parts.

It is a simple task to find solutions of the asymptotic Schrödinger equation

$$\{E-H_\alpha^{\mathrm{as}}\}\,\Phi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)=0 \tag{10}$$

belonging to the three-body energy $E=\mathbf{k}_\alpha^2/2\mu_\alpha+\mathbf{q}_\alpha^2/2M_\alpha$, since H_α^{as} is a sum of two commuting subsystem Hamiltonians

$$\begin{aligned}H_\alpha^{\mathrm{as}}&=H_{\rho_\alpha}^{\mathrm{as}}+H_{\mathbf{r}_\alpha},\\H_{\rho_\alpha}^{\mathrm{as}}&=\{T_{\rho_\alpha}+v_\alpha^C(\boldsymbol{\rho}_\alpha)\},\\H_{\mathbf{r}_\alpha}&=\{T_{\mathbf{r}_\alpha}+V_\alpha(\mathbf{r}_\alpha)\}.\end{aligned} \tag{11}$$

We introduce the eigenfunctions of the two-body Hamiltonian $H_{\mathbf{r}_\alpha}$ (we use the same symbols for operators acting in the two- and in the three-particle space) via

$$\left\{\frac{\mathbf{k}_\alpha^2}{2\mu_\alpha}-H_{\mathbf{r}_\alpha}\right\}\psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)=0, \tag{12}$$

and of the effective two-body Hamiltonian $H_{\rho_\alpha}^{\mathrm{as}}$

$$\left\{\frac{\mathbf{q}_\alpha^2}{2M_\alpha}-H_{\rho_\alpha}^{\mathrm{as}}\right\}\bar{\psi}^{(+)}_{C,\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)=0. \tag{13}$$

Solutions of the latter equation are the "center-of-mass Coulomb scattering states"

$$\bar{\psi}^{(+)}_{C,\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)=e^{i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\bar{N}_\alpha F(-i\bar{\eta}_\alpha,1;i(q_\alpha\rho_\alpha-\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha)), \tag{14}$$

with

$$\bar{\eta}_\alpha=\frac{e_\alpha(e_\beta+e_\gamma)M_\alpha}{q_\alpha},\quad \bar{N}_\alpha=e^{-\pi\bar{\eta}_\alpha/2}\,\Gamma(1+i\bar{\eta}_\alpha). \tag{15}$$

It is a well-known fact that the exact solution

$$\Phi^{as(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) = \psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\,\bar{\psi}^{(+)}_{C,\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha) \tag{16}$$

of the asymptotic Schrödinger equation (10) generally does not, when r_α becomes large, connect smoothly to the asymptotic solution (5) valid in Ω_0. In fact, this is most easily seen by taking into account that for large r_α in Eq. (12) the nuclear part of the interaction V_α can be neglected so that also this equation reduces to a Coulomb Schrödinger equation for which the solution takes a form similar to Eq. (14). Replacing the hypergeometric functions there and in Eq. (14) by their leading asymptotic terms [cf. Eq. (31)] the above assertion can be readily verified.

Furthermore, the question arises whether the solution (16) of the asymptotic Schrödinger equation (10) is the limit in Ω_α of the solution $\Psi^{(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ of the original Schrödinger equation (2), i.e., whether we also have, similarly to Eq. (8), the relation

$$\Phi^{as(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) \overset{?}{=} \lim_{\rho_\alpha\to\infty,\, r_\alpha/\rho_\alpha\longrightarrow 0} \Psi^{(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha). \tag{17}$$

In fact, we will show explicitly in a somewhat simplified model that this is *not generally* the case.

Realization of these facts motivates us to investigate whether the asymptotic Schrödinger equation also has another type of solution which then, of course, cannot have the structure (16); but instead it should possess the property (17) of being the leading term in Ω_α of the solution of the original Schrödinger equation (2), and it should allow a continuous matching to the asymptotic solution (5) in Ω_0.

In the present paper we proffer an explicit wave function which possesses all the desired properties. The goal is achieved by deriving a new analytical expression for an asymptotic solution of Eq. (10) which satisfies this asymptotic equation up to terms of the order $O(\rho_\alpha^{-2}, r_\alpha/\rho_\alpha^2)$. Moreover, it can be continued into the asymptotic regime Ω_0 where it coincides with the result (5) (in fact, it can even be continued into $\Omega_\beta, \beta \neq \alpha$). Hence this wave function is the leading term in the asymptotic expansion of the full wave function $\Psi^{(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ in Ω_α (in the model mentioned before this will be verified explicitly). As was to be expected the new asymptotic solution, although being an eigenfunction of H^{as}_α in leading order, cannot be represented as the product of eigenfunctions of $H^{as}_{\rho_\alpha}$ and $H_{\mathbf{r}_\alpha}$, of the type (16). But an alternative splitting of H^{as} into a sum of two operators can be devised such that it can, indeed, be written as a product of eigenfunctions of these new component Hamiltonians. Such a representation serves to elucidate the inherent three-body nature of a system of three charged particles subjected to the long-ranged mutual Coulomb forces. Since the analytical form of our asymptotic wave function is fairly simple it should be well suited for use in practical calculations.

III. ANALYTICALLY SOLVABLE MODEL

In order to explain the basic ideas in a most transparent manner we first discuss the simple model of two particles 1 and 2 which do not interact among themselves but move in the field of an infinitely heavy particle 3. It has the great virtue of being analytically solvable. The solution strategy developed here will be used as guide line for the investigation of the general case in Sec. IV.

Let e_j denote the charge of particle j, and m_j its mass, $j = 1,2$. The charge of particle 3 is e_3. The variables most appropriate are the single-particle coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, with particle 3 being fixed at the origin, and the corresponding momenta $\mathbf{k}_1$ and $\mathbf{k}_2$. Besides we use the relative coordinate $\mathbf{r}_{12}$ between particles 1 and 2, and the coordinate $\boldsymbol{\rho}$ of the center of mass of the pair (1,2), defined as

$$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \qquad \boldsymbol{\rho} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_{12}}. \tag{18}$$

The inverse relations expressing $\mathbf{r}_1$ and $\mathbf{r}_2$ by $\mathbf{r}_{12}$ and $\boldsymbol{\rho}$ are

$$\mathbf{r}_j = \boldsymbol{\rho} + \lambda_j\mathbf{r}_{12}, \quad \lambda_j = -(-1)^j\mu_{12}/m_j, \quad j = 1,2. \tag{19}$$

Here we have introduced the total mass $m_{12} = m_1 + m_2$, and the reduced mass $\mu_{12} = m_1m_2/m_{12}$, of particles 1 and 2. The momenta canonically conjugated to $\mathbf{r}_{12}$ and $\boldsymbol{\rho}$ are the relative momentum $\mathbf{k}_{12}$ between particles 1 and 2, and the total momentum $\mathbf{q}$ of the pair (1,2), respectively,

$$\mathbf{k}_{12} = \frac{m_2\mathbf{k}_1 - m_1\mathbf{k}_2}{m_{12}}, \qquad \mathbf{q} = \mathbf{k}_1 + \mathbf{k}_2. \tag{20}$$

Such a system is described by the Schrödinger equation

$$\{E - H\}\Psi^{(+)}_{\mathbf{k}_1\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2) = \{\,E - T_{\mathbf{r}_1} - T_{\mathbf{r}_2} - V_1(\mathbf{r}_1) - V_2(\mathbf{r}_2)\}\Psi^{(+)}_{\mathbf{k}_1\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2) = 0, \tag{21}$$

where $T_{\mathbf{r}_j} = -\Delta_{\mathbf{r}_j}/2m_j$ is the kinetic-energy operator of particle j, and V_j is the interaction potential between particle j and the heavy particle 3, $j = 1,2$. Since the total Hamiltonian H is the sum of two commuting one-particle Hamiltonians,

$$H = H_1 + H_2, \qquad H_j = T_{\mathbf{r}_j} + V_j(\mathbf{r}_j), \tag{22}$$

the exact solution presents itself as a product of solutions of the corresponding one-particle Schrödinger equations

$$H_j\, \psi^{(+)}_{\mathbf{k}_j}(\mathbf{r}_j) = \frac{\mathbf{k}_j^2}{2m_j}\, \psi^{(+)}_{\mathbf{k}_j}(\mathbf{r}_j) \tag{23}$$

by means of

$$\Psi^{(+)}_{\mathbf{k}_1\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2) = \psi^{(+)}_{\mathbf{k}_1}(\mathbf{r}_1)\, \psi^{(+)}_{\mathbf{k}_2}(\mathbf{r}_2), \tag{24}$$

belonging to the energy $E = \mathbf{k}_1^2/2m_1 + \mathbf{k}_2^2/2m_2$.

Since the exact three-body wave function $\Psi^{(+)}_{\mathbf{k}_1\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2)$ for our system is explicitly known we can, of course, verify that its leading term in

$$\Omega_0 : \quad r_1 \longrightarrow \infty, \quad r_2 \longrightarrow \infty, \quad r_{12} \longrightarrow \infty, \tag{25}$$

is, indeed, given by the specialization of the general result (6), respectively (5), to the present case. In fact, in Ω_0 the nuclear potentials $V_j^N(\mathbf{r}_j)$ have died out so that we can approximate V_j by its Coulombic part

$$V_j(\mathbf{r}_j) \underset{r_j\to\infty}{\widetilde{\quad}} V_j^C(\mathbf{r}_j) = \frac{e_j e_3}{r_j}, \quad j = 1,2. \tag{26}$$

Consequently, the solutions of Eq. (23) reduce to the well-known Coulomb scattering wave functions

$$\begin{aligned}\psi^{(+)}_{\mathbf{k}_j}(\mathbf{r}_j) &\underset{r_j\to\infty}{\widetilde{\quad}} \psi^{(+)}_{C,\mathbf{k}_j}(\mathbf{r}_j)\\ &= e^{i\mathbf{k}_j\cdot\mathbf{r}_j} N_j F(-i\eta_j, 1; i(k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j)),\end{aligned} \tag{27}$$

with

$$\eta_j = \frac{e_j e_3 m_j}{k_j}, \qquad N_j = e^{-\pi\eta_j/2}\,\Gamma(1 + i\eta_j), \tag{28}$$

η_j being the Sommerfeld parameter of particle j. Keeping in mind the identity $\mathbf{k}_1\cdot\mathbf{r}_1 + \mathbf{k}_2\cdot\mathbf{r}_2 = \mathbf{k}_{12}\cdot\mathbf{r}_{12} + \mathbf{q}\cdot\boldsymbol{\rho}$, the desired result follows immediately [cf. Eq. (6)]:

$$\Psi^{(+)}_{\mathbf{k}_1\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2) \underset{r_1, r_2\to\infty}{\widetilde{\quad}} \Psi_0^{\mathrm{as}(+)'}(\mathbf{r}_1,\mathbf{r}_2) = e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}\, N_1 N_2 F(-i\eta_1, 1; i(k_1 r_1 - \mathbf{k}_1\cdot\mathbf{r}_1)) F(-i\eta_2, 1; i(k_2 r_2 - \mathbf{k}_2\cdot\mathbf{r}_2)). \tag{29}$$

Furthermore, in the nonsingular region, i.e., for $\hat{\mathbf{k}}_j\cdot\hat{\mathbf{r}}_j \neq 1$, $j = 1,2$, the asymptotic expansion of the hypergeometric function can be used,

$$\begin{aligned} N_j F(-i\eta_j, 1; i(k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j)) \underset{r_j\to\infty}{=} & \; e^{i\eta_j \ln(k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j)} \left\{1 + O\left(\frac{1}{k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j}\right)\right\} \\ & + f_j^C\, \frac{e^{i(k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j)}}{r_j} e^{-i\eta_j \ln(2k_j r_j)} \left\{1 + O\left(\frac{1}{(k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j)}\right)\right\}, \end{aligned} \tag{30}$$

where f_j^C is the amplitude for Coulomb scattering of particle j off particle 3. Inspection clearly shows that the leading term is the first term on the right-hand side (rhs) that is we have

$$N_j F(-i\eta_j, 1; i(k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j)) \underset{r_j\to\infty}{=} e^{i\eta_j \ln(k_j r_j - \mathbf{k}_j\cdot\mathbf{r}_j)} + O\left(\frac{1}{r_j}\right). \tag{31}$$

Hence, Eq. (29) reduces to

$$\begin{aligned}\Psi^{(+)}_{\mathbf{k}_1\mathbf{k}_2}(\mathbf{r}_1,\mathbf{r}_2) &\underset{\Omega_0}{\longrightarrow} \Psi_0^{\mathrm{as}(+)}(\mathbf{r}_1,\mathbf{r}_2)\\ &= e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}\, e^{i\eta_1 \ln(k_1 r_1 - \mathbf{k}_1\cdot\mathbf{r}_1)} e^{i\eta_2 \ln(k_2 r_2 - \mathbf{k}_2\cdot\mathbf{r}_2)},\end{aligned} \tag{32}$$

which is, in fact, the specialization of Eq. (5) to the present case.

The Schrödinger equation (21) can be rewritten in terms of the Jacobi variables $\mathbf{r}_{12}$ and $\boldsymbol{\rho}$,

$$\{E - T_{\mathbf{r}_{12}} - T_{\rho} - V_1(\boldsymbol{\rho} + \lambda_1\mathbf{r}_{12},) - V_2(\boldsymbol{\rho} + \lambda_2\mathbf{r}_{12})\}\Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho}) = 0, \tag{33}$$

where

$$T_{\mathbf{r}_{12}} = -\Delta_{\mathbf{r}_{12}}/2\mu_{12}, \qquad T_{\rho} = -\Delta_{\rho}/2m_{12}, \tag{34}$$

and the energy eigenvalue is $E = \mathbf{k}_{12}^2/2\mu_{12} + \mathbf{q}^2/2m_{12}$. Equations (33) and (21) are, of course, completely equivalent, i.e., we have $\Psi^{(+)}_{\mathbf{k}_1\mathbf{k}_2}(\mathbf{r}_1, \mathbf{r}_2) = \Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$.

We are interested in the asymptotic solution of Eqs. (21) or (33) in the domain

$$\Omega_{12}: \quad \rho \longrightarrow \infty, \quad r_{12}/\rho \longrightarrow 0. \tag{35}$$

As already mentioned, the first requirement (35) implies that both $r_1 \to \infty$ and $r_2 \to \infty$. Consequently, the rhs of (29) is the leading term in an asymptotic expansion of $\Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$ also in Ω_{12}, provided we ensure that the additional condition $r_{12}/\rho \to 0$ is taken into account. The simplest possibility consists of approximating, according to Eq. (19), $\mathbf{r}_1$ and $\mathbf{r}_2$ by $\boldsymbol{\rho}$. Hence, the leading term in Ω_{12} of the exact wave function (24) is

$$\begin{aligned}\tilde{\Psi}^{\mathrm{as}(+)}(\mathbf{r}_{12}, \boldsymbol{\rho}) &:= \lim_{\rho\to\infty,\, r_{12}/\rho\to 0} \Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho}) \\ &= e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12} + i\mathbf{q}\cdot\boldsymbol{\rho}} N_1 N_2 F(-i\eta_1, 1; i(k_1\rho - \mathbf{k}_1\cdot\boldsymbol{\rho}))F(-i\eta_2, 1; i(k_2\rho - \mathbf{k}_2\cdot\boldsymbol{\rho})) \\ &=: \varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})\, \chi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}),\end{aligned} \tag{36}$$

with

$$\varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12}) = e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12}} \tag{37}$$

and

$$\begin{aligned}\chi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}) = e^{i\mathbf{q}\cdot\boldsymbol{\rho}} N_1 N_2 F(-i\eta_1, 1; i(k_1\rho - \mathbf{k}_1\cdot\boldsymbol{\rho})) \\ \times F(-i\eta_2, 1; i(k_2\rho - \mathbf{k}_2\cdot\boldsymbol{\rho})).\end{aligned} \tag{38}$$

Here $\mathbf{k}_1$ and $\mathbf{k}_2$ are to be substituted by the appropriate linear combinations of $\mathbf{k}_{12}$ and $\mathbf{q}$. We draw attention to the fact that in order to arrive at the result (36) we have neglected terms of the order $O(r_{12}/\rho)$ only in the hypergeometric functions; the plane wave survives unaltered.

On the other hand, the appropriate asymptotic Schrödinger equation in Ω_{12} and its solution are obtained by specializing Eqs. (8) to (16) to the present case corresponding to $V_{12} \equiv 0$. That is,

$$\{E - H^{\mathrm{as}}\}\Phi^{\mathrm{as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho}) = 0, \tag{39}$$

with

$$H^{\mathrm{as}} = \lim_{\rho\to\infty,\, r_{12}/\rho\to 0} H = T_{\mathbf{r}_{12}} + T_{\rho} + v^C(\boldsymbol{\rho}). \tag{40}$$

The center-of-mass Coulomb potential which acts between the total charge of particles 1 and 2 and the charge of particle 3 is given by

$$v^C(\boldsymbol{\rho}) = \frac{(e_1 + e_2)e_3}{\rho}. \tag{41}$$

The decomposition (11) of H^{as} into a sum of two commuting sub-Hamiltonians becomes simply

$$\begin{aligned}H^{\mathrm{as}} = H^{\mathrm{as}}_{\rho} + H_{\mathbf{r}_{12}}, \qquad H^{\mathrm{as}}_{\rho} = \{T_{\rho} + v^C(\boldsymbol{\rho})\}, \\ H_{\mathbf{r}_{12}} = T_{\mathbf{r}_{12}}.\end{aligned} \tag{42}$$

Consequently,

$$\begin{aligned}\Phi^{\mathrm{as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho}) = e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12} + i\mathbf{q}\cdot\boldsymbol{\rho}} \\ \times \bar{N} F(-i\bar{\eta}, 1; i(q\rho - \mathbf{q}\cdot\boldsymbol{\rho})) \\ =: \varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})\, \bar{\psi}^{(+)}_{C,\,\mathbf{q}}(\boldsymbol{\rho})\end{aligned} \tag{43}$$

is the exact solution of Eq. (39), with the corresponding Sommerfeld parameter $\bar{\eta} = (e_1 + e_2)e_3 m_{12}/q$, and $\bar{N}$ defined in terms of $\bar{\eta}$ in the same way as $\bar{N}_\alpha$ in terms of $\bar{\eta}_\alpha$ [cf. Eq. (15)].

Let us emphasize the following important points. As has been mentioned above the approximation leading from the exact solution (24) of the Schrödinger equation (21) to the approximate wave function (36) is the same as that which leads from the original Schrödinger equation (33) to the asymptotic Schrödinger equation (39). It consists of taking in the wave function (24), respectively in the Schrödinger operator in (33), the limits $\rho \to \infty$, $r_{12}/\rho \to 0$. Nevertheless, by comparing Eqs. (36) with (43) the following conclusions can immediately be drawn.

(i) The solution (43) of the asymptotic Schrödinger equation does *not* coincide with the asymptotic form (36) of the solution of the original Schrödinger equation, although each of them can be written as a product of functions depending either on $\mathbf{r}_{12}$ or on $\boldsymbol{\rho}$ only, and hence is *not the leading term in* Ω_{12} of the solution of the original Schrödinger equation (except for $\rho \to \infty$ for the special cases where the particle velocities $\mathbf{k}_1/m_1$ and $\mathbf{k}_2/m_2$ are equal, or in the singular directions where the three vectors $\boldsymbol{\rho}$, $\mathbf{k}_1$, and $\mathbf{k}_2$ are parallel).

(ii) The solution (43) of the asymptotic Schrödinger equation valid in Ω_{12} *does not smoothly match* with the asymptotic form (32) of the solution of the original Schrödinger equation in Ω_0, although this should be expected because of the fact that $\Omega_{12} \bigcap \Omega_0 \neq 0$.

(iii) The leading term (36) in an expansion in Ω_{12} of the solution of the original Schrödinger equation is *not* a solution of the asymptotic Schrödinger equation, i.e., in our terminology it is *not an asymptotic solution* of Eq. (39).

While the first two assertions can trivially be verified by inspection, let us demonstrate explicitly the last one. That is, we would like to show that the asymptotic expression $\tilde{\Psi}^{\mathrm{as}(+)}(\mathbf{r}_{12}, \boldsymbol{\rho})$, as defined in (36), of the solution of the Schrödinger equation (21) does not satisfy the asymptotic Schrödinger equation (39). In fact, application of $\{E - H^{\mathrm{as}}\}$ onto $\tilde{\Psi}^{\mathrm{as}(+)}(\mathbf{r}_{12}, \boldsymbol{\rho})$ yields

$$\{E-H^{\rm as}\}\tilde{\Psi}^{{\rm as}(+)}(\mathbf{r}_{12},\boldsymbol{\rho}) = e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}N_1N_2\Big\{-v^C(\boldsymbol{\rho})F_1F_2 + F_1\left(\frac{\Delta_\rho}{2m_{12}}\right)F_2 + F_2\left(\frac{\Delta_\rho}{2m_{12}}\right)F_1 + \frac{i}{m_{12}}F_1(\mathbf{q}\cdot\boldsymbol{\nabla}_\rho)F_2 + \frac{i}{m_{12}}F_2(\mathbf{q}\cdot\boldsymbol{\nabla}_\rho)F_1 + \frac{1}{m_{12}}(\boldsymbol{\nabla}_\rho F_1)\cdot(\boldsymbol{\nabla}_\rho F_2)\Big\}, \tag{44}$$

where we have adopted the shorthand notation $F_j \equiv F(-i\eta_j, 1; i(k_j\rho - \mathbf{k}_j\cdot\boldsymbol{\rho}))$. From the Schrödinger equation satisfied by $\psi^{(+)}_{C,\mathbf{k}_j}(\boldsymbol{\rho}) = N_j e^{i\mathbf{k}_j\cdot\boldsymbol{\rho}}F(-i\eta_j,1;i(k_j\rho-\mathbf{k}_j\cdot\boldsymbol{\rho}))$,

$$\left\{\frac{k_j^2}{2m_j} + \frac{\Delta_\rho}{2m_j} - \frac{e_je_3}{\rho}\right\} e^{i\mathbf{k}_j\cdot\boldsymbol{\rho}}F(-i\eta_j,1;i(k_j\rho-\mathbf{k}_j\cdot\boldsymbol{\rho})) = 0, \tag{45}$$

follows

$$\Delta_\rho F_j = \frac{2m_je_je_3}{\rho}F_j - 2i\mathbf{k}_j\cdot\boldsymbol{\nabla}_\rho F_j. \tag{46}$$

Substituting these expressions for $\Delta_\rho F_1$ and $\Delta_\rho F_2$ in the rhs of Eq. (44) we find

$$\{E-H^{\rm as}\}\tilde{\Psi}^{{\rm as}(+)}(\mathbf{r}_{12},\boldsymbol{\rho}) = e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}N_1N_2\Big\{\frac{1}{\rho}\left[\frac{(m_1e_1+m_2e_2)e_3}{m_{12}} - (e_1+e_2)e_3\right]F_1F_2 + \frac{i}{m_{12}}F_1(\mathbf{k}_1\cdot\boldsymbol{\nabla}_\rho)F_2 + \frac{i}{m_{12}}F_2(\mathbf{k}_2\cdot\boldsymbol{\nabla}_\rho)F_1 + \frac{1}{m_{12}}(\boldsymbol{\nabla}_\rho F_1)\cdot(\boldsymbol{\nabla}_\rho F_2)\Big\} \neq 0. \tag{47}$$

Hence we end up with the result that the rhs of (47) does not necessarily vanish. This proves our assertion that $\tilde{\Psi}^{{\rm as}(+)}(\mathbf{r}_{12},\boldsymbol{\rho})$ is not (in fact, not even asymptotic) a solution of the asymptotic Schrödinger equation (39).

The rhs of (47) can be worked out further if we take into account that in the domain Ω_{12}, for $\hat{\mathbf{k}}_j\cdot\hat{\boldsymbol{\rho}} \neq 1$, for $j=1,2$, i.e., in the nonsingular region, the leading term of N_jF_j is given by Eq. (31), with $\mathbf{r}_j$ replaced by $\boldsymbol{\rho}$,

$$N_jF_j \underset{\rho\to\infty}{=} e^{i\eta_j\ln(k_j\rho-\mathbf{k}_j\cdot\boldsymbol{\rho})} + O\left(\frac{1}{\rho}\right). \tag{48}$$

Inserting these asymptotic expressions for F_1 and F_2 in (36) leads to

$$\begin{aligned}\tilde{\Psi}^{{\rm as}(+)}(\mathbf{r}_{12},\boldsymbol{\rho}) &= e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}\, e^{i\eta_1\ln(k_1\rho-\mathbf{k}_1\cdot\boldsymbol{\rho})}\, e^{i\eta_2\ln(k_2\rho-\mathbf{k}_2\cdot\boldsymbol{\rho})} + O\left(\frac{1}{\rho}\right)\\ &= \varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})\,\chi^{{\rm as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}) + O\left(\frac{1}{\rho}\right),\end{aligned} \tag{49}$$

where

$$\chi^{{\rm as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}) = e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\, e^{i\eta_1\ln(k_1\rho-\mathbf{k}_1\cdot\boldsymbol{\rho})}\, e^{i\eta_2\ln(k_2\rho-\mathbf{k}_2\cdot\boldsymbol{\rho})} \tag{50}$$

is the leading term for $\rho\to\infty$ of $\chi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$, Eq. (38). The same expression can, of course, be obtained directly by replacing in Eq. (32) $\mathbf{r}_1$ and $\mathbf{r}_2$ by $\boldsymbol{\rho}$. On using the approximation (48) for N_jF_j in Eq. (47) we can evaluate the right-hand side further to yield

$$\{E-H^{\rm as}\}\tilde{\Psi}^{{\rm as}(+)}(\mathbf{r}_{12},\boldsymbol{\rho}) = \varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})\,\chi^{{\rm as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})\Big\{\frac{1}{\rho}\Big[\frac{(m_1e_1+m_2e_2)e_3}{m_{12}} - (e_1+e_2)e_3 - \frac{1}{m_{12}}k_1\eta_2\frac{(\hat{\boldsymbol{\rho}}-\hat{\mathbf{k}}_2)\cdot\hat{\mathbf{k}}_1}{1-\hat{\boldsymbol{\rho}}\cdot\hat{\mathbf{k}}_2} - \frac{1}{m_{12}}k_2\eta_1\frac{(\hat{\boldsymbol{\rho}}-\hat{\mathbf{k}}_1)\cdot\hat{\mathbf{k}}_2}{1-\hat{\boldsymbol{\rho}}\cdot\hat{\mathbf{k}}_1}\Big]\Big\} + O\left(\frac{1}{\rho^2}\right). \tag{51}$$

We draw attention to the fact that the nonzero terms which are explicitly shown on the rhs of Eq. (51) are of the same order $O(\rho^{-1})$ as the center-of-mass Coulomb potential occurring in $H^{\rm as}$ and, thus, cannot be neglected as compared to the left-hand side (lhs). In contrast, the terms of the order $O(\rho^{-1})$ in Eq. (48) contribute in the order $O(\rho^{-2})$ only. Hence the result (51) shows once more directly for the leading asymptotic term (49) in Ω_{12} of the exact solution of (33) that it does not satisfy the asymptotic Schrödinger equation (39), i.e., *it is not an asymptotic solution.* Incidentally, we note that $\tilde{\Psi}^{\rm as(+)}(\mathbf{r}_{12},\boldsymbol{\rho})$ does not smoothly connect to the asymptotic solution (32) in Ω_0 either.

Consequently, in order that asymptotically in Ω_{12} the solution of the Schrödinger equation (33) be also a solution of the asymptotic Schrödinger equation (39), one must go beyond the leading order in the expansion of $\Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$. In other words, we must find an asymptotic wave function $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$ which, being more accurate than $\tilde{\Psi}^{\rm as(+)}(\mathbf{r}_{12},\boldsymbol{\rho})$, does satisfy the asymptotic Schrödinger equation (39), at least up to terms of the order $O(\rho^{-2})$ and $O(r_{12}/\rho^2)$, i.e.,

$$\{E-H^{\rm as}\}\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho}) = O\left(\frac{1}{\rho^2},\frac{r_{12}}{\rho^2}\right). \tag{52}$$

The development leading to Eq. (51) makes it clear that it cannot suffice to retain in the expansions of the Hamiltonian and of the wave function separately the terms contributing to the desired order. Rather, we must also include in the wave-function expansion such terms which, *after application of* $H^{\rm as}$, yield contributions of the same order. As will be seen this demand necessitates keeping terms linear in r_{12}/ρ [terms $\sim\rho^{-1}$ produce, when retained in $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$, in the asymptotic Schrödinger equation (39) contributions $\sim\rho^{-2}$, which can be neglected].

We point out that in order that the notation be more concise, in the following we will not make a distinction between $O(1/\rho^2)$ and $O(1/\rho^2, r_{12}/\rho^2)$, and henceforth we will use the former symbol everywhere.

To find the improved representation of $\Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$ in Ω_{12}, but staying away from the singular direction, i.e., for $\hat{\mathbf{k}}_j\cdot\hat{\mathbf{r}}_j\neq 1$, $j=1,2$, we start again from the expression (32) on which we still have to impose the condition $r_{12}/\rho\longrightarrow 0$. This is accomplished by substituting there, as before, $\mathbf{r}_1$ and $\mathbf{r}_2$ from Eq. (19). Expanding each of the Coulomb distortion factors in the limit $r_{12}/\rho\to 0$ *but now keeping terms* $\sim r_{12}/\rho$, we find for $j=1,2$,

$$e^{i\eta_j\ln(k_jr_j-\mathbf{k}_j\cdot\mathbf{r}_j)}\approx e^{i\eta_j\ln(k_j\rho-\mathbf{k}_j\cdot\boldsymbol{\rho})}e^{i\mathbf{a}^{(j)}(\hat{\boldsymbol{\rho}})\cdot\mathbf{r}_{12}/\rho}, \tag{53}$$

with

$$\mathbf{a}^{(j)}(\hat{\boldsymbol{\rho}})=\eta_j\lambda_j\frac{(\hat{\boldsymbol{\rho}}-\hat{\mathbf{k}}_j)}{1-\hat{\boldsymbol{\rho}}\cdot\hat{\mathbf{k}}_j}. \tag{54}$$

If, instead of Eq. (48), the result (53) is inserted in (32), the following asymptotic expression for $\Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$ is obtained:

$$\begin{aligned}\Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho}) \underset{\Omega_{12}}{\longrightarrow} \Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho}) &= e^{i[\mathbf{k}_{12}+\mathbf{a}(\hat{\boldsymbol{\rho}})/\rho]\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}\\ &\quad\times e^{i\eta_1\ln(k_1\rho-\mathbf{k}_1\cdot\boldsymbol{\rho})}\\ &\quad\times e^{i\eta_2\ln(k_2\rho-\mathbf{k}_2\cdot\boldsymbol{\rho})},\end{aligned} \tag{55}$$

with

$$\mathbf{a}(\hat{\boldsymbol{\rho}})=\sum_{j=1}^{2}\mathbf{a}^{(j)}(\hat{\boldsymbol{\rho}})=\sum_{j=1}^{2}\eta_j\lambda_j\frac{(\hat{\boldsymbol{\rho}}-\hat{\mathbf{k}}_j)}{1-\hat{\boldsymbol{\rho}}\cdot\hat{\mathbf{k}}_j}, \tag{56}$$

provided also $\hat{\mathbf{k}}_j\cdot\hat{\boldsymbol{\rho}}\neq 1$, $j=1,2$. That is, an additional phase factor has appeared in Eq. (55) as compared to the expression (49). It will turn out to be crucial in attaining an improved asymptotic behavior. Other terms in the expansion in Eq. (53) will contribute in next to leading order only and are, therefore, omitted. Introducing a *local relative momentum*

$$\mathbf{k}_{12}(\boldsymbol{\rho}):=\mathbf{k}_{12}+\mathbf{a}(\hat{\boldsymbol{\rho}})/\rho, \tag{57}$$

Eq. (55) can be written as the product of a plane wave $\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})$, with this $\boldsymbol{\rho}$-dependent momentum,

$$\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})=e^{i\mathbf{k}_{12}(\rho)\cdot\mathbf{r}_{12}}, \tag{58}$$

and $\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$,

$$\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})=\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}). \tag{59}$$

The reason why we have to retain in Eq. (55) the additional phase factor $\exp\{i\mathbf{a}(\hat{\boldsymbol{\rho}})\cdot\mathbf{r}_{12}/\rho\}$ becomes clear when we will act on $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$ by $\{E-H^{\rm as}\}$: T_ρ operating on it produces terms at least of the order $O(\rho^{-2})$ which can be neglected; but application of $T_{\mathbf{r}_{12}}$ onto this phase factor yields a term proportional to ρ^{-1} which is *of the same order* as those kept in the procedure leading from the original Schrödinger equation (21) to its asymptotic form (39) and, thus, must not be omitted in a consistent treatment. Its effect is to just cancel the nonvanishing terms on the rhs of Eq. (51). In fact,

$$\begin{aligned}\{E-H^{\rm as}\}\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho}) = \varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})\bigg\{\frac{1}{\rho}\bigg[&\left(\frac{(m_1e_1+m_2e_2)e_3}{m_{12}}-(e_1+e_2)e_3\right)\\ &-\frac{1}{m_{12}}k_1\eta_2\frac{(\hat{\boldsymbol{\rho}}-\hat{\mathbf{k}}_2)\cdot\hat{\mathbf{k}}_1}{1-\hat{\boldsymbol{\rho}}\cdot\hat{\mathbf{k}}_2}-\frac{1}{m_{12}}k_2\eta_1\frac{(\hat{\boldsymbol{\rho}}-\hat{\mathbf{k}}_1)\cdot\hat{\mathbf{k}}_2}{1-\hat{\boldsymbol{\rho}}\cdot\hat{\mathbf{k}}_1}\\ &-\frac{\mathbf{a}(\hat{\boldsymbol{\rho}})\cdot\mathbf{k}_{12}}{\mu_{12}}\bigg]+O\left(\frac{1}{\rho^2}\right)\bigg\}\end{aligned}$$

$$= \varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})\chi^{\mathrm{as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})\left\{\frac{1}{\rho}\left[\left(\frac{(m_1e_1+m_2e_2)e_3}{m_{12}}-(e_1+e_2)e_3\right)+\frac{(m_2e_1+m_1e_2)e_3}{m_{12}}\right]+O\left(\frac{1}{\rho^2}\right)\right\}$$
$$= O\left(\frac{1}{\rho^2}\right). \tag{60}$$

To arrive at the second equality use has been made of the relations $\mathbf{k}_1\cdot\mathbf{a}_1(\hat{\boldsymbol{\rho}}) = -e_1e_3\mu_{12}$ and $\mathbf{k}_2\cdot\mathbf{a}_2(\hat{\boldsymbol{\rho}}) = e_2e_3\mu_{12}$, which follow directly from definition (54).

Thus we have proven that, up to order $O(\rho^{-2})$, $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$ as given by Eq. (55) is simultaneously the generalized leading term in the expansion of the solution of the original Schrödinger equation (21) as well as an asymptotic solution of the asymptotic Schrödinger equation (39), in the domain Ω_{12}. But inspection clearly reveals that $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12},\boldsymbol{\rho})$ cannot be represented as a product of eigenfunctions of the type (43) of the sub-Hamiltonians H^{as}_{ρ} and $H_{\mathbf{r}_{12}}$, of H^{as} [cf. Eq. (42)].

Here we face a rather unfamiliar situation: the asymptotic Schrödinger equation (39) has at least two types of solutions. The first one is exact, and can be written as

$$\Phi^{\mathrm{as}(+)}_1(\mathbf{r}_{12},\boldsymbol{\rho}) = \varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})\,\bar{\psi}^{(+)}_{C,\,\mathbf{q}}(\boldsymbol{\rho}) = e^{i\mathbf{k}_{12}\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}\bar{N}\times F(-i\bar{\eta},1;i(q\rho-\mathbf{q}\cdot\boldsymbol{\rho})), \tag{61}$$

where $\varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})$ and $\bar{\psi}^{(+)}_{C,\,\mathbf{q}}(\boldsymbol{\rho})$ are the exact (two-body) eigenfunctions of the (commuting) two-body Hamiltonians $H_{\mathbf{r}_{12}} = T_{\mathbf{r}_{12}}$ and $H^{\mathrm{as}}_{\rho} = \{T_\rho + v^C(\boldsymbol{\rho})\}$, respectively. But wave functions of this type differ completely from the asymptotic form in Ω_{12} of the exact solution of the original Schrödinger equation (21). On the other hand, an alternative but now only asymptotic solution of the asymptotic Schrödinger equation (39) is provided by

$$\Phi^{\mathrm{as}(+)}_2(\mathbf{r}_{12},\boldsymbol{\rho}) = \varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})\,\chi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}) = e^{i\mathbf{k}_{12}(\rho)\cdot\mathbf{r}_{12}+i\mathbf{q}\cdot\boldsymbol{\rho}}N_1N_2F(-i\eta_1,1;i(k_1\rho-\mathbf{k}_1\cdot\boldsymbol{\rho}))F(-i\eta_2,1;i(k_2\rho-\mathbf{k}_2\cdot\boldsymbol{\rho})), \tag{62}$$

which is simultaneously, up to the same order $O(\rho^{-2})$, also the generalized leading term of the solution of the original Schrödinger equation (33). But it has to be kept in mind that each of the functions $\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})$ and $\chi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$ which $\Phi^{\mathrm{as}(+)}_2$ is composed of is, in contrast to those appearing in $\Phi^{\mathrm{as}(+)}_1$, essentially a three-body wave function. Actually, the modified plane wave $\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})$ is seen to be effectively a two-body wave function. This follows also from the (free) Schrödinger equation satisfied by it, namely

$$\left\{\frac{\mathbf{k}^2_{12}(\boldsymbol{\rho})}{2\mu_{12}} - H_{\mathbf{r}_{12}}\right\}\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12}) = \left\{\frac{\mathbf{k}^2_{12}(\boldsymbol{\rho})}{2\mu_{12}} - T_{\mathbf{r}_{12}}\right\}\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12}) = 0, \tag{63}$$

with the $\boldsymbol{\rho}$-dependent energy $\mathbf{k}^2_{12}(\rho)/2\mu_{12}$. Thus, in Eq. (63) $\boldsymbol{\rho}$ appears as a parameter only. This will become important in Sec. IV when a nonvanishing interaction between particles 1 and 2 will be admitted.

We emphasize that such a situation can occur only for Coulomb-type interactions. For potentials decreasing faster than the Coulomb potential the asymptotic solution of Eq. (21) assumes indeed the typical form of the solution of the asymptotic Schrödinger equation, similar to Eq. (61), as a product of eigenfunctions of $H_{\mathbf{r}_{12}}$ and H^{as}_{ρ}, because in this case $H^{\mathrm{as}}_{\rho} = T_\rho$ to leading order and its eigenfunction is the undistorted plane wave $\exp\{i\mathbf{q}\cdot\boldsymbol{\rho}\}$. But the Coulomb potential decreases so slowly that it modifies the wave function even at asymptotic distances. Hence, in order to satisfy the asymptotic Schrödinger equation one must retain in the asymptotic expansion of the exact wave function all terms which, when acted upon by $\{E - H^{\mathrm{as}}\}$, give contributions of the same order $O(\rho^{-1})$ as the center-of-mass Coulomb potential $v^C(\rho)$ occurring in H^{as}. But these terms definitively prevent the asymptotic solution to assume the factorized form (61).

The representation (59) of $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}$ as a product of two three-body wave functions is non-unique. However, we will demonstrate that a decomposition of H^{as} can be found such that both $\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})$ and $\chi^{\mathrm{as}(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$ are, in fact, eigenfunctions of the corresponding component Hamiltonians, up to terms of the order $O(\rho^{-2})$.

Recalling that we are interested in the asymptotic solution only we can rewrite Eq. (63) as

$$\left\{\frac{\mathbf{k}^2_{12}}{2\mu_{12}} + \frac{\mathbf{a}(\hat{\boldsymbol{\rho}})\cdot\mathbf{k}_{12}}{\mu_{12}}\frac{1}{\rho} - H_{\mathbf{r}_{12}}\right\}\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12}) = O\left(\frac{1}{\rho^2}\right). \tag{64}$$

Let us define a quantity $\tilde{V}(\boldsymbol{\rho})$ as

$$\tilde{V}(\boldsymbol{\rho}) = -\frac{\mathbf{a}(\hat{\boldsymbol{\rho}})\cdot\mathbf{k}_{12}}{\mu_{12}}\frac{1}{\rho}. \tag{65}$$

Note that $\tilde{V}(\boldsymbol{\rho})$ can be interpreted as a noncentral potential acting between the center of mass of particles 1 and 2, and particle 3. It possesses a Coulomb-type radial behavior and is, in addition, proportional to the relative velocity $\mathbf{k}_{12}/\mu_{12} = \mathbf{v}_1 - \mathbf{v}_2$ of the particles 1 and 2. Thus, $\tilde{V}(\boldsymbol{\rho})$ describes the action of a three-body force.

Instead of the decomposition (42) we now introduce a new splitting of $H^{\rm as}$ by adding and subtracting $\tilde{V}(\boldsymbol{\rho})$,

$$H^{\rm as} = \tilde{H}^{\rm as}_{\boldsymbol{\rho}} + \tilde{H}_{\mathbf{r}_{12}}(\boldsymbol{\rho}), \tag{66}$$

with

$$\tilde{H}^{\rm as}_{\boldsymbol{\rho}} = H^{\rm as}_{\boldsymbol{\rho}} - \tilde{V}(\boldsymbol{\rho}) = T_{\boldsymbol{\rho}} + v^C(\boldsymbol{\rho}) - \tilde{V}(\boldsymbol{\rho}), \tag{67}$$

$$\tilde{H}_{\mathbf{r}_{12}}(\boldsymbol{\rho}) = H_{\mathbf{r}_{12}} + \tilde{V}(\boldsymbol{\rho}) = T_{\mathbf{r}_{12}} + \tilde{V}(\boldsymbol{\rho}). \tag{68}$$

Equation (64) then shows that $\varphi_{\mathbf{k}_{12}(\boldsymbol{\rho})}(\mathbf{r}_{12})$ is the eigenfunction of $\tilde{H}_{\mathbf{r}_{12}}(\boldsymbol{\rho})$ up to terms of the order $O(\rho^{-2})$. Furthermore, by reshuffling the terms in Eqs. (51) or (60) we deduce that

$$\left\{\frac{\mathbf{q}^2}{2m_{12}} - \tilde{H}^{\rm as}_{\boldsymbol{\rho}}\right\}\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}) = O\left(\frac{1}{\rho^2}\right), \tag{69}$$

that is, $\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$ is an asymptotic eigenfunction of $\tilde{H}^{\rm as}_{\boldsymbol{\rho}}$.

Herewith, the asymptotic Schrödinger equation for $\Psi^{as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}, \mathbf{r}_{12})$ can be manipulated to yield

$$\begin{aligned}\{E - H^{\rm as}\}\varphi_{\mathbf{k}_{12}(\boldsymbol{\rho})}(\mathbf{r}_{12})\,\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}) &= \varphi_{\mathbf{k}_{12}(\boldsymbol{\rho})}(\mathbf{r}_{12})\left\{\frac{\mathbf{q}^2}{2m_{12}} - \tilde{H}^{\rm as}_{\boldsymbol{\rho}}\right\}\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}) \\ &\quad + \chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})\left\{\frac{\mathbf{k}_{12}^2}{2\mu_{12}} - \tilde{H}_{\mathbf{r}_{12}}(\boldsymbol{\rho})\right\}\varphi_{\mathbf{k}_{12}(\boldsymbol{\rho})}(\mathbf{r}_{12}) + O\left(\frac{1}{\rho^2}\right) \\ &= O\left(\frac{1}{\rho^2}\right).\end{aligned} \tag{70}$$

In the first equality we have restricted the action of $T_{\boldsymbol{\rho}}$ onto the wave function $\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$ since its application on $\varphi_{\mathbf{k}_{12}(\boldsymbol{\rho})}(\mathbf{r}_{12})$, cf. (58), gives contributions proportional to ρ^{-2}. This proves our assertion that Eq. (66) indeed provides a splitting of $H^{\rm as}$ into two components $\tilde{H}^{\rm as}_{\boldsymbol{\rho}}$ and $\tilde{H}_{\mathbf{r}_{12}}(\boldsymbol{\rho})$ such that $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$ can be represented as a product of eigenfunctions of these Hamiltonians up to terms of the order $O(\rho^{-2})$. We note in parentheses that in Eq. (66) the three-body Hamiltonian $H^{\rm as}$ is written as a sum of operators which are themselves three-body quantities, in contrast to the decomposition (42). It is, therefore, *a priori* to be expected that their eigenfunctions will, in general, be three-body wave functions.

Summarizing the results obtained in this section we have found that the generalized leading term $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$ in an asymptotic expansion in Ω_{12} of the solution of the original Schrödinger equation (21) is, indeed, also an asymptotic solution of the asymptotic Schrödinger equation (39), satisfying it up to terms of the order $O(\rho^{-2})$. The part $\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$, as given by Eq. (50), can be interpreted as an effective wave function for the motion of the center of mass of the unbound system of particles 1 and 2 and coincides, up to terms of the order $O(\rho^{-2})$, with $\chi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$, Eq. (38). We stress that $\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$, as well as $\chi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$, depends not only on the momentum $\mathbf{q}$ of the center of mass of the pair (1,2) but on the particle momenta $\mathbf{k}_1$ and $\mathbf{k}_2$ separately. This is a manifestation of the fact that particles 1 and 2 are unbound and, thus, can be influenced individually by the long-ranged Coulomb force exerted by particle 3. Correspondingly, $\varphi_{\mathbf{k}_{12}(\boldsymbol{\rho})}(\mathbf{r}_{12})$ which, because of our assumption $V_{12} \equiv 0$, satisfies the free Schrödinger equation (63) in which $\boldsymbol{\rho}$ acts as a parameter, can be considered the wave function of the relative motion of particles 1 and 2. The presence of the third particle results in changing the internal relative momentum: instead of $\mathbf{k}_{12}$ the local momentum $\mathbf{k}_{12}(\boldsymbol{\rho})$ occurs which only for $\rho \to \infty$ coincides with the former. This constitutes another effect of the infinite range of the Coulomb forces present.

It is to be noted that in the energy eigenvalue $\mathbf{k}^2_{12}(\boldsymbol{\rho})/2\mu_{12}$ in the Schrödinger equation (63) which determines $\varphi_{\mathbf{k}_{12}(\boldsymbol{\rho})}(\mathbf{r}_{12})$ there exists no other parameter compared to which terms $\sim \rho^{-1}$ could *a priori* be considered small. Even for such large values of ρ that all terms which are of the order $O(\rho^{-1})$ and $O(r_{12}/\rho)$ as compared to those kept in the derivation of the asymptotic three-particle wave function could be neglected, there exist relative momenta $\mathbf{k}_{12}$ the magnitude of which are comparable to $|\mathbf{a}(\hat{\boldsymbol{\rho}})/\rho|$. Consequently, the most noticeable effects from the use of the local instead of the asymptotic relative momentum can be expected to show up for small k_{12}. In fact, the "strength" of this modification of the relative momentum k_{12} is determined by $|\mathbf{a}(\hat{\boldsymbol{\rho}})|$. For $k_{12} \to 0$, i.e., when the velocities of particles 1 and 2 become approximately equal, and therefore also approximately equal to the velocity $\mathbf{v}$ of the center of mass of the pair (1,2), $\mathbf{v}_1 \approx \mathbf{v}_2 \approx \mathbf{v}$, we find $|\mathbf{a}(\hat{\boldsymbol{\rho}})| \sim |e_1/m_1 - e_2/m_2|/v$. Hence, the strongest long-ranged influence of particle 3 onto the motion of particles 1 and 2, for $k_{12} \to 0$, as represented by the occurrence of the local momentum in their relative-motion wave function, is proportional to the charge-over-mass ratio difference, and inversely proportional to the velocity, of particles 1 and 2. As will be shown in Sec. IV these conclusions remain valid even in the general case of interacting particles 1 and 2.

The results obtained above have important consequences also for the spectral decomposition of the resolvent $G^{\rm as(+)}(E) = \{E + i0 - H^{\rm as}\}^{-1}$ of the asymptotic Hamiltonian $H^{\rm as}$. Formally we can write for its kernel, using the eigenfunctions (43) of $H^{\rm as}$,

$$G^{\rm as(+)}(\mathbf{r}_{12}, \boldsymbol{\rho}; \mathbf{r}'_{12}, \boldsymbol{\rho}'; E) = \int \frac{d^3k_{12}}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{\varphi^*_{\mathbf{k}_{12}}(\mathbf{r}'_{12})\, \bar{\psi}^{(+)*}_{C,\mathbf{q}}(\boldsymbol{\rho}')\, \bar{\psi}^{(+)}_{C,\mathbf{q}}(\boldsymbol{\rho})\, \varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})}{E + i0 - \mathbf{k}^2_{12}/2\mu_{12} - \mathbf{q}^2/2m_{12}} + \cdots. \tag{71}$$

Here and in the following dots indicate contributions from the discrete spectrum of the corresponding Hamiltonian if there is any. Indeed, since $H^{\rm as}$ is the asymptotic form of the original Schrödinger operator H in the region Ω_{12} the same should hold true, of course, for the relation between the spectral decompositions of the resolvents $G^{\rm as(+)}$ and $G^{(+)}(E) = \{E + i0 - H\}^{-1}$. But this is not the case for the spectral decomposition (71) of $G^{\rm as(+)}$ since, as was shown before, the wave functions $\varphi_{\mathbf{k}_{12}}(\mathbf{r}_{12})\, \bar{\psi}^{(+)}_{C,\mathbf{q}}(\boldsymbol{\rho})$ do not represent the leading term in the asymptotic expansion in Ω_{12} of the exact wave function. Hence Eq. (71) is *not valid as asymptotic form in* Ω_{12} of the spectral decomposition of $G^{(+)}(E)$.

Actually, for the kernel of $G^{(+)}(E)$ we have

$$G^{(+)}(\mathbf{r}_{12}, \boldsymbol{\rho}; \mathbf{r}'_{12}, \boldsymbol{\rho}'; E) = \int \frac{d^3k_{12}}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{\Psi^{(+)*}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}'_{12}, \boldsymbol{\rho}')\, \Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})}{E + i0 - \mathbf{k}^2_{12}/2\mu_{12} - \mathbf{q}^2/2m_{12}} + \cdots, \tag{72}$$

where $\Psi^{(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$ is the solution (24) of the Schrödinger equation with Hamiltonian H. In the limit $\rho', \rho \to \infty$, $r'_{12}/\rho' \to 0$ and $r_{12}/\rho \to 0$, the leading term of Eq. (72) is

$$G^{\rm as(+)}(\mathbf{r}_{12}, \boldsymbol{\rho}; \mathbf{r}'_{12}, \boldsymbol{\rho}'; E) = \int \frac{d^3k_{12}}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{\Psi^{\rm as(+)*}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}'_{12}, \boldsymbol{\rho}')\, \Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})}{E + i0 - \mathbf{k}^2_{12}/2\mu_{12} - \mathbf{q}^2/2m_{12}} + \cdots. \tag{73}$$

Here, $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$ is that eigenfunction of $H^{\rm as}$ which is at the same time also the generalized leading term of the eigenfunction of H in Ω_{12}. Hence when $G^{\rm as(+)}$ is considered to be the limit of $G^{(+)}$ in Ω_{12} the form (73) for the spectral decomposition should be used, instead of Eq. (71).

The spectral representation (73) can be rewritten by inserting the explicit form (59) for $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$ as

$$G^{\rm as(+)}(\mathbf{r}_{12}, \boldsymbol{\rho}; \mathbf{r}'_{12}, \boldsymbol{\rho}'; E) = \int \frac{d^3k_{12}}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{\varphi^*_{\mathbf{k}_{12}(\rho')}(\mathbf{r}'_{12})\chi^{\rm as(+)*}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho}')\, \chi^{as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})\varphi_{\mathbf{k}_{12}(\rho)}(\mathbf{r}_{12})}{E + i0 - \mathbf{k}^2_{12}/2\mu_{12} - \mathbf{q}^2/2m_{12}} + \cdots. \tag{74}$$

Since $\chi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\boldsymbol{\rho})$ depends on both momenta $\mathbf{k}_{12}$ and $\mathbf{q}$, which is a manifestation of the three-body nature of the underlying problem, it is obvious that $G^{\rm as(+)}$ in the form (74) cannot be represented as a folding integral of the resolvents corresponding to the component Hamiltonians $\tilde{H}_{\mathbf{r}_{12}}(\boldsymbol{\rho})$ and $\tilde{H}^{\rm as}_{\rho}$ in the conventional manner.

We finally remark that when the integration is performed in Eq. (73) over $\mathbf{k}_{12}$ and $\mathbf{q}$ in the neighborhood of the singular directions ($\hat{\mathbf{k}}_j \cdot \hat{\mathbf{r}}_j \to 1$, or $k_j \to 0$, $j = 1, 2$) the expression (59) for $\Psi^{\rm as(+)}_{\mathbf{k}_{12}\,\mathbf{q}}(\mathbf{r}_{12}, \boldsymbol{\rho})$ is not applicable and, hence, the wave function should be modified there. Of course, this induces modifications also in the representation (74). To study this problem, e.g., the general prescription proposed in [7] could be employed. An alternative proposal is discussed in the Appendix.

IV. GENERAL CASE OF THREE INTERACTING CHARGED PARTICLES

We now generalize the results obtained in Sec. III to the case of three charged particles, all of which interact via Coulomb-type pair potentials. As mentioned in Sec. II Jacobi variables (cf. Fig. 1) are now most appropriate.

Our goal is to find the leading term of the solution of the Schrödinger equation (2) in the region Ω_α,

$$\Omega_\alpha: \quad \rho_\alpha \longrightarrow \infty, \quad r_\alpha/\rho_\alpha \longrightarrow 0. \tag{75}$$

Such a function (i) must satisfy the asymptotic Schrödinger equation (10), valid in this region, at least asymptotically; (ii) should simultaneously match smoothly to the known asymptotic wave function (5) in Ω_0, since the regions Ω_α and Ω_0 have nonzero overlap; and (iii) if the interaction between particles β and γ is switched off it should reduce to the generalized leading term (55) of the exact solution, as derived in Sec. III.

The well-known class $\Phi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ of solutions of Eq. (10), already mentioned in Sec. II [cf. Eq. (16)], is certainly not a suitable candidate. Because, as pointed out there, it does not possess the matching property with (5). In addition, in the model problem discussed in Sec. III it has been proven to differ completely from the known generalized leading term in Ω_α of the exact solution.

A wave function with the above-mentioned properties is not available at present. In order to construct it we proceed through a generalization of the results derived in Sec. III. For the time being the problem will be somewhat simplified by restricting all three pair potentials to be purely Coulombic, i.e.,

$$V_\alpha(\boldsymbol{\rho}_\alpha) \equiv V_\alpha^C(\boldsymbol{\rho}_\alpha) = \frac{e_\beta e_\gamma}{\rho_\alpha}, \qquad \alpha \neq \beta \neq \gamma, \tag{76}$$

since this will enable us to write down explicit analytic expressions. Later on this restriction will be lifted.

Let us look back at the development in Sec. III leading to Eqs. (55), respectively (59). There we had taken advantage of the fact that the kinematic conditions in Ω_{12} allowed us to start from the asymptotic wave function valid in Ω_0, Eq. (32). Imposing on it the restriction $r_{12}/\rho \longrightarrow 0$ led to the desired wave function (55). The same kinematic situation prevails also in the present general case. In fact, the condition $\rho_\alpha \to \infty$ implies $r_\beta \to \infty$ and $r_\gamma \to \infty$ [cf. Eq. (1)]. Consequently, with respect to the relative motion of the particles α and γ, and α and β, the situation in Ω_α is identical to the one in Ω_0. Therefore, the asymptotic wave function for the relative motion within these two subsystems is described by the same Coulomb-distortion factors as for the asymptotic solution (5) in Ω_0, provided we stay away from the singular directions. Of course, in Ω_α the relative coordinate $\mathbf{r}_\alpha$ between the particles β and γ is constrained to satisfy the requirement $r_\alpha/\rho_\alpha \longrightarrow 0$, which necessitates a completely different description of their relative motion as compared to Ω_0. This is accounted for by introducing, instead of the third Coulomb-distortion factor of Eq. (5), an open function $F_\alpha(\mathbf{r}_\alpha; \boldsymbol{\rho}_\alpha)$. Thus we are led to make the following ansatz for the asymptotic solution of Eq. (2) in Ω_α:

$$\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} F_\alpha(\mathbf{r}_\alpha; \boldsymbol{\rho}_\alpha) \times e^{i\eta_\beta \ln(k_\beta r_\beta - \mathbf{k}_\beta\cdot\mathbf{r}_\beta)} \times e^{i\eta_\gamma \ln(k_\gamma r_\gamma - \mathbf{k}_\gamma\cdot\mathbf{r}_\gamma)}. \tag{77}$$

As indicated by the notation we cannot *a priori* exclude that $F_\alpha(\mathbf{r}_\alpha; \boldsymbol{\rho}_\alpha)$ may depend in some way on the variable $\boldsymbol{\rho}_\alpha$, in addition to its expected dependence on the appropriate coordinate $\mathbf{r}_\alpha$. However, we will show that we can construct F_α within the class of functions for which the $\boldsymbol{\rho}_\alpha$ dependence is such that

$$\boldsymbol{\nabla}_{\rho_\alpha} F_\alpha(\mathbf{r}_\alpha; \boldsymbol{\rho}_\alpha) = O\left(\frac{1}{\rho_\alpha^2}\right). \tag{78}$$

Let us now proceed in complete analogy to Sec. III. If we substitute in the first Coulomb-distortion factor for the coordinate $\mathbf{r}_\beta$ the linear combination of $\mathbf{r}_\alpha$ and $\boldsymbol{\rho}_\alpha$ according to Eq. (1) we find, for $\epsilon_{\alpha\beta}\hat{\boldsymbol{\rho}}_\alpha \cdot \hat{\mathbf{k}}_\beta \neq 1$, in the limit $r_\alpha/\rho_\alpha \to 0$, but including terms of the order $O(r_\alpha/\rho_\alpha)$ [cf. Eq. (53)],

$$e^{i\eta_\beta \ln(k_\beta r_\beta - \mathbf{k}_\beta\cdot\mathbf{r}_\beta)} \approx e^{i\eta_\beta \ln(k_\beta \rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha)} \times e^{i\mathbf{a}_\alpha^{(\beta)}(\hat{\boldsymbol{\rho}}_\alpha)\cdot\mathbf{r}_\alpha/\rho_\alpha}, \tag{79}$$

with

$$\mathbf{a}_\alpha^{(\beta)}(\hat{\boldsymbol{\rho}}_\alpha) = -\eta_\beta \frac{\mu_\alpha}{m_\gamma} \frac{(\epsilon_{\alpha\beta}\hat{\boldsymbol{\rho}}_\alpha - \hat{\mathbf{k}}_\beta)}{(1 - \epsilon_{\alpha\beta}\hat{\boldsymbol{\rho}}_\alpha \cdot \hat{\mathbf{k}}_\beta)}. \tag{80}$$

A similar result, with β interchanged with γ, is obtained for the second Coulomb-distortion term. Inserting these asymptotic forms into Eq. (77) we get

$$\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha} F_\alpha(\mathbf{r}_\alpha; \boldsymbol{\rho}_\alpha) e^{i\eta_\beta \ln(k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha)} e^{i\eta_\gamma \ln(k_\gamma\rho_\alpha - \epsilon_{\alpha\gamma}\mathbf{k}_\gamma\cdot\boldsymbol{\rho}_\alpha)} + O\left(\frac{1}{\rho_\alpha^2}\right). \tag{81}$$

Here again we have introduced a *local momentum* $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)$ as

$$\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha + \frac{\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)}{\rho_\alpha} \tag{82}$$

with

$$\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha) = \sum_{\nu\ (\neq\alpha)} \mathbf{a}_\alpha^{(\nu)}(\hat{\boldsymbol{\rho}}_\alpha). \tag{83}$$

As indicated by the notation $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)$ depends also on the orientation of $\boldsymbol{\rho}_\alpha$. Furthermore, we mention that the same conventions as in Sec. III are adhered to, namely to include collectively in the symbol $O(\rho_\alpha^{-2})$ also terms of the order $O(r_\alpha/\rho_\alpha^2)$.

In the above we demanded that if the interaction between particles β and γ is switched off, the ansatz $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ should, of course, coincide with the asymptotic wave function (55). This is, indeed, the case for $F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)\equiv 1$. Hence, a nontrivial function $F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)\not\equiv 1$ summarizes all the effects of a nonzero interaction in subsystem α, the influence of which has, in general, not yet died out due to the condition $r_\alpha/\rho_\alpha \longrightarrow 0$ in Ω_α.

The as yet undetermined function $F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)$ is to be chosen such that $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ satisfies the Schrödinger equation in Ω_α. Let us introduce the auxiliary potential

$$\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)=-\frac{\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)\cdot\mathbf{k}_\alpha}{\mu_\alpha}\frac{1}{\rho_\alpha}=-\frac{\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)\cdot\mathbf{v}_\alpha}{\rho_\alpha},\quad (84)$$

which has a Coulomb-type dependence on the distance ρ_α between particle α and the center of mass of the pair (β,γ), but is noncentral and depends on the relative velocity $\mathbf{v}_\alpha=\mathbf{k}_\alpha/\mu_\alpha$ of the particles within this pair. Hence it is really a special type of three-body potential.

Furthermore, we define the function $\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ as

$$\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)=e^{i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}e^{i\eta_\beta\ln(k_\beta\rho_\alpha-\epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha)}\times e^{i\eta_\gamma\ln(k_\gamma\rho_\alpha-\epsilon_{\alpha\gamma}\mathbf{k}_\gamma\cdot\boldsymbol{\rho}_\alpha)},\quad (85)$$

generalizing Eq. (50). Here it is understood that $\mathbf{k}_\beta$ and $\mathbf{k}_\gamma$ are to be expressed as linear combinations of $\mathbf{k}_\alpha$ and $\mathbf{q}_\alpha$ according to (1).

First one shows that $\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ is an asymptotic solution of the equation [cf. Eq. (69)]

$$\left\{\frac{\mathbf{q}_\alpha^2}{2M_\alpha}-H^{\mathrm{as}}_{\rho_\alpha}+\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)\right\}\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)=O\left(\frac{1}{\rho_\alpha^2}\right).\quad (86)$$

In fact, using Eqs. (11) and (84) we derive

$$\begin{aligned}
&\left\{\frac{\mathbf{q}_\alpha^2}{2M_\alpha}-H^{\mathrm{as}}_{\rho_\alpha}+\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)\right\}\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\\
&=e^{i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\left\{\frac{i\mathbf{q}_\alpha\cdot\boldsymbol{\nabla}_{\rho_\alpha}}{M_\alpha}-\frac{e_\alpha(e_\beta+e_\gamma)}{\rho_\alpha}+\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)+O\left(\frac{1}{\rho_\alpha^2}\right)\right\}e^{i\eta_\beta\ln(k_\beta\rho_\alpha-\epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha)}e^{i\eta_\gamma\ln(k_\gamma\rho_\alpha-\epsilon_{\alpha\gamma}\mathbf{k}_\gamma\cdot\boldsymbol{\rho}_\alpha)}\\
&=\left\{-\frac{1}{\rho_\alpha}\frac{\mathbf{q}_\alpha}{M_\alpha}\cdot\left[\epsilon_{\beta\alpha}\frac{m_\gamma}{\mu_\alpha}\mathbf{a}^{(\beta)}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)+\epsilon_{\gamma\alpha}\frac{m_\beta}{\mu_\alpha}\mathbf{a}^{(\gamma)}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)\right]-\frac{e_\alpha(e_\beta+e_\gamma)}{\rho_\alpha}+\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)+O\left(\frac{1}{\rho_\alpha^2}\right)\right\}\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\\
&=O\left(\frac{1}{\rho_\alpha^2}\right),
\end{aligned}\quad (87)$$

where use has been made of the definition (80). Thus $\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ is the eigenfunction of the modified Hamiltonian

$$\tilde H^{\mathrm{as}}_{\rho_\alpha}=H^{\mathrm{as}}_{\rho_\alpha}-\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)=T_{\rho_\alpha}+v^C_\alpha(\boldsymbol{\rho}_\alpha)-\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)\quad (88)$$

up to terms of the order $O(\rho_\alpha^{-2})$. Note that since $\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha)$ is a three-body potential, $\tilde H^{\mathrm{as}}_{\rho_\alpha}$ is a three-body Hamiltonian, and $\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ a three-body wave function.

This result suggests splitting the asymptotic Hamiltonian H^{as} according to

$$H^{\mathrm{as}}=\tilde H^{\mathrm{as}}_{\rho_\alpha}+\tilde H^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha),\quad (89)$$

with

$$\tilde H^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)=H^C_{\mathbf{r}_\alpha}+\tilde V^C_\alpha(\boldsymbol{\rho}_\alpha),\quad H^C_{\mathbf{r}_\alpha}=T_{\mathbf{r}_\alpha}+V^C_\alpha(\mathbf{r}_\alpha).\quad (90)$$

Taking into account Eq. (87), the application of the asymptotic Schrödinger operator onto $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ yields

$$\begin{aligned}
\{E-H^{\mathrm{as}}\}e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)\,\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)&=e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)\left\{\frac{\mathbf{q}_\alpha^2}{2M_\alpha}-\tilde H^{\mathrm{as}}_{\rho_\alpha}\right\}\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\\
&\quad+\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\left\{\frac{\mathbf{k}_\alpha^2}{2\mu_\alpha}-\tilde H^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)\right\}e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)+O\left(\frac{1}{\rho_\alpha^2}\right)\\
&=\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\left\{\frac{\mathbf{k}_\alpha^2}{2\mu_\alpha}-\tilde H^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)\right\}e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)+O\left(\frac{1}{\rho_\alpha^2}\right).
\end{aligned}\quad (91)$$

In the first equality the operator T_{ρ_α} could be shifted through the first two terms because when acting on them it would yield terms of the order $O(\rho_\alpha^{-2})$, due to the definition (82) of the local momentum and condition (78). Thus, in order that $\Psi^{as(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)$ be a solution of the asymptotic Schrödinger equation (10) up to terms of the order $O(\rho_\alpha^{-2})$ the function $F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)$ has to satisfy the equation

$$\left\{\frac{\mathbf{k}_\alpha^2}{2\mu_\alpha} - \tilde{H}^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)\right\} e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha} F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha) = O\left(\frac{1}{\rho_\alpha^2}\right). \tag{92}$$

Since

$$\left\{\frac{\mathbf{k}_\alpha^2}{2\mu_\alpha} - \tilde{H}^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)\right\} = \left\{\frac{\mathbf{k}_\alpha^2}{2\mu_\alpha} - H^C_{\mathbf{r}_\alpha} + \frac{\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)\cdot\mathbf{k}_\alpha}{\mu_\alpha}\frac{1}{\rho_\alpha}\right\} = \left\{\frac{\mathbf{k}_\alpha^2(\boldsymbol{\rho}_\alpha)}{2\mu_\alpha} - H^C_{\mathbf{r}_\alpha} + O\left(\frac{1}{\rho_\alpha^2}\right)\right\} \tag{93}$$

it is apparent that the dependence on $\boldsymbol{\rho}_\alpha$, up to terms of the order $O(\rho_\alpha^{-2})$, of the operator acting in Eq. (92) on $e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)$ can be completely absorbed by replacing the two-body energy $E_\alpha = \mathbf{k}_\alpha^2/2\mu_\alpha$ by a local energy

$$E_\alpha(\boldsymbol{\rho}_\alpha) = \frac{\mathbf{k}_\alpha^2(\boldsymbol{\rho}_\alpha)}{2\mu_\alpha}, \tag{94}$$

calculated from the local subsystem momentum $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)$.

Hence if $\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ is the continuum solution of the two-body Schrödinger equation for the subsystem α for a local energy $E_\alpha(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha^2(\boldsymbol{\rho}_\alpha)/2\mu_\alpha$,

$$\{E_\alpha(\boldsymbol{\rho}_\alpha) - H^C_{\mathbf{r}_\alpha}\}\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) = \left\{\frac{\mathbf{k}_\alpha^2(\boldsymbol{\rho}_\alpha)}{2\mu_\alpha} - T_{\mathbf{r}_\alpha} - V^C_\alpha(\mathbf{r}_\alpha)\right\}\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) = 0, \tag{95}$$

we have the simple result that for $r_\alpha/\rho_\alpha \to 0$,

$$\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) = e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha) + O\left(\frac{1}{\rho_\alpha^2}\right). \tag{96}$$

Equation (95) generalizes the free effective Schrödinger equation (63) for noninteracting particles β and γ in a natural way. It is to be noted that in the Schrödinger equation (95), and hence also in its solution $\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$, the vector $\boldsymbol{\rho}_\alpha$ enters only parametrically through the local momentum $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha) = \mathbf{k}_\alpha + \mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)/\rho_\alpha$. Consequently, $F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)$, defined via Eq. (96), belongs indeed to the class (78) of functions. We point to the interesting result that, although $\tilde{H}^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)$ is a three-body operator, the leading term $e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)$ of its (three-body) eigenfunction is, in fact, given by the effective two-body wave function $\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$. In other words, all genuine three-body contributions in the eigenfunctions of $\tilde{H}^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)$ have the intuitively appealing property to die out at least as fast as the inverse square of the distance ρ_α between particle α and the center of mass of the pair (β,γ).

As a matter of fact, since we have assumed for the present discussion the interaction V_α between the particles β and γ to be purely Coulombic the exact solution of the Schrödinger equation (95) can immediately be written down,

$$\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) = e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha}\,N_\alpha(\boldsymbol{\rho}_\alpha)F(-i\eta_\alpha(\boldsymbol{\rho}_\alpha),1;i[k_\alpha(\boldsymbol{\rho}_\alpha)r_\alpha - \mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha]), \tag{97}$$

with

$$\eta_\alpha(\boldsymbol{\rho}_\alpha) = \frac{e_\beta e_\gamma \mu_\alpha}{k_\alpha(\boldsymbol{\rho}_\alpha)}, \qquad N_\alpha(\boldsymbol{\rho}_\alpha) = e^{-\pi\eta_\alpha(\boldsymbol{\rho}_\alpha)/2}\,\Gamma(1+i\eta_\alpha(\boldsymbol{\rho}_\alpha)). \tag{98}$$

That is, $\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ is an ordinary two-particle Coulomb scattering wave function, except that the momentum $\mathbf{k}_\alpha$ has been replaced by the corresponding local momentum $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)$.

To summarize, we have found the remarkably simple result that the wave function

$$\begin{aligned}\Psi^{as(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) &= \psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)\,\chi^{as(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\\ &= e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha + i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\,N_\alpha(\boldsymbol{\rho}_\alpha)F(-i\eta_\alpha(\boldsymbol{\rho}_\alpha),1;i[k_\alpha(\boldsymbol{\rho}_\alpha)r_\alpha - \mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha])\\ &\quad\times e^{i\eta_\beta\ln(k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha)}e^{i\eta_\gamma\ln(k_\gamma\rho_\alpha - \epsilon_{\alpha\gamma}\mathbf{k}_\gamma\cdot\boldsymbol{\rho}_\alpha)},\end{aligned} \tag{99}$$

where $\chi^{as(+)}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ is an asymptotic solution of Eq. (86) and $\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ satisfies the ordinary two-particle equation

(95) but for a local energy $E_\alpha(\boldsymbol{\rho}_\alpha)$, is a solution, up to terms of the order $O(\rho_\alpha^{-2})$, of the asymptotic Schrödinger equation (10), and hence also of the original Schrödinger equation (2) in Ω_α. Furthermore, if the interaction between particles β and γ is switched off it reduces to the explicitly derived generalized leading term (59) in the asymptotic expansion of the exact solution of the three-body Schrödinger equation discussed in Sec. III. For these reasons we can conclude that $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ is the leading term of the total three-charged-particle wave function in Ω_α.

For applications it is important to keep in mind that $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ as given by Eq. (99) cannot yet be continued into the region Ω_0. Such a generalized representation can, however, be written down without difficulties. In fact, starting from Eq. (77) it is easily verified that

$$\Psi^{\mathrm{as}(+)\,\prime}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) = e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha+i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}N_\alpha(\boldsymbol{\rho}_\alpha)F(-i\eta_\alpha(\boldsymbol{\rho}_\alpha),1;i[k_\alpha(\boldsymbol{\rho}_\alpha)r_\alpha-\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha]) \times e^{i\eta_\beta\ln(k_\beta r_\beta-\mathbf{k}_\beta\cdot\mathbf{r}_\beta)}e^{i\eta_\gamma\ln(k_\gamma r_\gamma-\mathbf{k}_\gamma\cdot\mathbf{r}_\gamma)} \tag{100}$$

coincides, due to Eqs. (79) and (82), in Ω_α with $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ up to terms of the order $O(\rho_\alpha^{-2})$. If, however, all interparticle distances r_α, r_β, and r_γ are allowed to go to infinity arbitrarily (but not into the singular directions), i.e., in Ω_0, also ρ_α grows beyond any limit and, consequently, $\Psi^{\mathrm{as}(+)\,\prime}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ goes over into the leading term $\Psi^{\mathrm{as}(+)}_0(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$, Eq. (5), of the asymptotic expansion of the three-particle wave function suggested in [1]. Hence, $\Psi^{\mathrm{as}(+)\,\prime}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ is the leading term of the three-charged-particle wave function in Ω_α *and* Ω_0.

It is worth emphasizing that $\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ is not of the conventional form of solutions of the asymptotic Schrödinger equation (10). Hence also in the general case the latter has at least two types of solutions. One is of the familiar form [cf. Eq. (16)]

$$\begin{aligned}\Phi^{\mathrm{as}(+)}_1(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) &\equiv \Phi^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)\\ &= \psi^{(+)}_{C,\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\,\bar{\psi}^{(+)}_{C,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\\ &= e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha+i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}N_\alpha\,\bar{N}_\alpha F(-i\eta_\alpha,1;i(k_\alpha r_\alpha-\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha))\,F(-i\bar{\eta}_\alpha,1;i(q_\alpha\rho_\alpha-\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha)),\end{aligned} \tag{101}$$

where $\psi^{(+)}_{C,\mathbf{k}_\alpha}(\mathbf{r}_\alpha)$ and $\bar{\psi}^{(+)}_{C,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ are the exact eigenfunctions of the (commuting) two-body Hamiltonians $H^C_{\mathbf{r}_\alpha}$ and $H^{\mathrm{as}}_{\boldsymbol{\rho}_\alpha}$, respectively. Since we have assumed at present that all particles interact via Coulomb forces only, also $\psi^{(+)}_{C,\mathbf{k}_\alpha}(\mathbf{r}_\alpha)$ is an ordinary Coulomb scattering wave function. Wave functions of the type (101) can, however, not be smoothly joined to the asymptotic solution in Ω_0 of the original Schrödinger equation (2). Also from the physical point of view the product form (101) is unsatisfactory: particle α could not exert any influence onto the internal motion of particles β and γ, in contrast to what has to be expected even for $\rho_\alpha \to \infty$ because of the infinite range of the Coulomb interactions involved.

Another type of asymptotic solutions of Eq. (10), valid in the nonsingular directions, is provided by

$$\begin{aligned}\Phi^{\mathrm{as}(+)}_2(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) &\equiv \Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)\\ &= \psi^{(+)}_{C,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha).\end{aligned} \tag{102}$$

The part $\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ depends, besides on the momentum $\mathbf{q}_\alpha$ canonically conjugated to $\boldsymbol{\rho}_\alpha$, also on $\mathbf{k}_\alpha$. This additional dependence on $\mathbf{k}_\alpha$ is the manifestation of the fact that the system of particles β and γ is unbound. Its occurrence also prevents the interpretation of $\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ as an ordinary two-body wave function describing the motion of the particle α relative to the center of mass of the pair (β,γ). The wave function $\psi^{(+)}_{C,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ depends on $\mathbf{r}_\alpha$, and parametrically also on the center-of-mass coordinate $\boldsymbol{\rho}_\alpha$. It can be considered an effective wave function describing the relative motion of the particles β and γ. The presence of the third particle α results in changing the relative momentum of β and γ, the magnitude of the change depending on $\boldsymbol{\rho}_\alpha$. It manifests itself through the appearance of the local momentum $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)$, instead of the genuine momentum $\mathbf{k}_\alpha$.

These results have again important consequences for the spectral decomposition of the resolvent $G^{\mathrm{as}(+)}(E)$ of H^{as}. Using the wave functions of the type $\Phi^{\mathrm{as}(+)}_1(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ we find for the kernel of $G^{\mathrm{as}(+)}(E)$

$$\begin{aligned}G^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha;\mathbf{r}'_\alpha,\boldsymbol{\rho}'_\alpha;E) &\equiv G^{\mathrm{as}(+)}_1(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha;\mathbf{r}'_\alpha,\boldsymbol{\rho}'_\alpha;E)\\ &= \int\frac{d^3k_\alpha}{(2\pi)^3}\frac{d^3q_\alpha}{(2\pi)^3}\frac{\psi^{(+)*}_{C,\mathbf{k}_\alpha}(\mathbf{r}'_\alpha)\,\bar{\psi}^{(+)*}_{C,\mathbf{q}_\alpha}(\boldsymbol{\rho}'_\alpha)\,\bar{\psi}^{(+)}_{C,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\,\psi^{(+)}_{C,\mathbf{k}_\alpha}(\mathbf{r}_\alpha)}{E+i0-\mathbf{k}^2_\alpha/2\mu_\alpha-\mathbf{q}^2_\alpha/2M_\alpha}+\cdots\end{aligned} \tag{103}$$

(here and in the following the dots indicate contributions from the eventual discrete spectrum of the corresponding Hamiltonian). If, however, $G^{\mathrm{as}(+)}(E)$ is considered to be the limit of the resolvent of the total Hamiltonian H in Ω_α, the representation (103) is not valid; instead the spectral decomposition with wave functions of the type $\Phi_2^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ should be used,

$$G^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha;\mathbf{r}'_\alpha,\boldsymbol{\rho}'_\alpha;E)\equiv G_2^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha;\mathbf{r}'_\alpha,\boldsymbol{\rho}'_\alpha;E)$$
$$=\int\frac{d^3k_\alpha}{(2\pi)^3}\frac{d^3q_\alpha}{(2\pi)^3}\frac{\psi^{(+)*}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}'_\alpha)}(\mathbf{r}'_\alpha)\,\chi^{\mathrm{as}(+)*}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\boldsymbol{\rho}'_\alpha)\,\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)}{E+i0-\mathbf{k}_\alpha^2/2\mu_\alpha-\mathbf{q}_\alpha^2/2M_\alpha}+\cdots. \tag{104}$$

As mentioned before wave functions of the type $\Phi_2^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ are asymptotic solutions in Ω_α only. A suitable generalization of (99) which is then an asymptotic solution [up to terms of the order $O(\rho_\nu^{-2})$] of the Schrödinger equation (2) in all three regions Ω_ν, $\nu=1,2,\text{and}\,3$, except for the singular directions, is provided by

$$\tilde{\Phi}_2^{(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)=e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha+i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\prod_{\nu=1}^{3}N_\nu(\boldsymbol{\rho}_\nu)F(-i\eta_\nu(\boldsymbol{\rho}_\nu),1;i[k_\nu(\boldsymbol{\rho}_\nu)r_\nu-\mathbf{k}_\nu(\boldsymbol{\rho}_\nu)\cdot\mathbf{r}_\nu]), \tag{105}$$

where each function $F(-i\eta_\nu(\boldsymbol{\rho}_\nu),1;i[k_\nu(\boldsymbol{\rho}_\nu)r_\nu-\mathbf{k}_\nu(\boldsymbol{\rho}_\nu)\cdot\mathbf{r}_\nu])$ is the solution of the corresponding two-particle Coulomb Schrödinger equation [cf. Eq. (95)]

$$\left\{\frac{\mathbf{k}_\nu^2(\boldsymbol{\rho}_\nu)}{2\mu_\nu}-T_{\mathbf{r}_\nu}-V_\nu^C(\mathbf{r}_\nu)\right\}e^{i\mathbf{k}_\nu(\boldsymbol{\rho}_\nu)\cdot\mathbf{r}_\nu}F(-i\eta_\nu(\boldsymbol{\rho}_\nu),1;i[k_\nu(\boldsymbol{\rho}_\nu)r_\nu-\mathbf{k}_\nu(\boldsymbol{\rho}_\nu)\cdot\mathbf{r}_\nu])=0 \tag{106}$$

with local momentum $\mathbf{k}_\nu(\boldsymbol{\rho}_\nu)$. It is somewhat tedious but straightforward to show that in the domain Ω_α the wave functions $\tilde{\Phi}_2^{(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ and $\Phi_2^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$, Eq. (102), are equivalent in the sense that both satisfy the Schrödinger equation (10) to the same order $O(\rho_\alpha^{-2})$.

Similarly to Eq. (100) we can generalize also the wave function (105) even further so that it is valid, in addition, in the region Ω_0. To this end we introduce a new local momentum

$$\mathbf{k}_\alpha(R,\hat{\boldsymbol{\rho}}_\alpha)=\mathbf{k}_\alpha+\frac{2\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)}{R}\qquad\text{with}\quad R=\sum_{\nu=1}^{3}r_\nu. \tag{107}$$

The motivation for this choice, which is nonunique but highly symmetric in all particle coordinates, instead of Eq. (82), rests upon the fact that, as mentioned in Sec. II, in Ω_0 directions exist such that when all interparticle distances tend to infinity, i.e., if $r_\nu\to\infty$, for $\nu=1,2,\text{and}\,3$, nevertheless one of the center-of-mass variables ρ_α can remain finite. This would imply that we no longer are in Ω_α. Such a situation is excluded, e.g., by the choice (107). However, in any of the domains Ω_α this new definition of $\mathbf{k}_\alpha(R,\hat{\boldsymbol{\rho}}_\alpha)$ coincides in the leading order [up to terms of the order $O(\rho_\alpha^{-2})$] with the previously given one, for $\alpha=1,2,\text{and}\,3$. Hence the most general wave function which is an asymptotic solution of the three-body Schrödinger equation (2) with purely Coulombic interactions in Ω_α, for $\alpha=0,1,2,\text{and}\,3$, except for the singular directions, is

$$\tilde{\Phi}_2^{(+)\prime}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)=e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha+i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\prod_{\nu=1}^{3}N_\nu(R,\hat{\boldsymbol{\rho}}_\nu)F(-i\eta_\nu(R,\hat{\boldsymbol{\rho}}_\nu),1;i[k_\nu(R,\hat{\boldsymbol{\rho}}_\nu)r_\nu-\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)\cdot\mathbf{r}_\nu]), \tag{108}$$

where the hypergeometric functions $F(-i\eta_\nu(R,\hat{\boldsymbol{\rho}}_\nu),1;i[k_\nu(R,\hat{\boldsymbol{\rho}}_\nu)r_\nu-\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)\cdot\mathbf{r}_\nu])$ satisfy the equation

$$\left\{\frac{\mathbf{k}_\nu^2(R,\hat{\boldsymbol{\rho}}_\nu)}{2\mu_\nu}-T_{\mathbf{r}_\nu}-V_\nu^C(\mathbf{r}_\nu)\right\}e^{i\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)\cdot\mathbf{r}_\nu}F(-i\eta_\nu(R,\hat{\boldsymbol{\rho}}_\nu),1;i[k_\nu(R,\hat{\boldsymbol{\rho}}_\nu)r_\nu-\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)\cdot\mathbf{r}_\nu])=0. \tag{109}$$

The quantities $\eta_\nu(R,\hat{\boldsymbol{\rho}}_\nu)$ and $N_\nu(R,\hat{\boldsymbol{\rho}}_\nu)$ follow from the expressions (98) by the substitution $\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)$ for $\mathbf{k}_\nu(\boldsymbol{\rho}_\nu)$. It is easily verified that in Ω_α the wave function $\tilde{\Phi}_2^{(+)'}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ coincides in the leading order with $\Psi^{\mathrm{as}(+)'}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$, Eq. (100). In fact, this is true even in Ω_0 except for regions where all three interparticle distances go to infinity but ρ_α remains finite. In Ω_0, as was the case for $\Psi^{\mathrm{as}(+)'}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$, also $\tilde{\Phi}_2^{(+)'}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ coincides in the leading order with the asymptotic wave function (5), of a three-particle Coulomb-distorted plane wave, i.e., a product of plane waves times the leading terms of three hypergeometric functions.

The results obtained up to now can easily be extended to the case when, in addition to Coulomb, also short-range interactions are present. Of course, since in Ω_α the center-of-mass variable ρ_α, and hence also r_β and r_γ, tend to infinity the terms in the ansatz (81) which describe the relative motion of particles α and γ, and α and β, respectively, remain unchanged: the short-range part of the interactions V_β and V_γ has died out. Hence the sole modifications will concern the description of the relative motion of particles β and γ. But these are easy to accomplish. In order that the ansatz (81) be the leading term of the solution of the asymptotic Schrödinger equation (10) in Ω_α, $F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha)$ has to satisfy the equation (92), but with $\tilde{H}^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)$ now being replaced by $\tilde{H}_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha)$,

$$\begin{aligned}\tilde{H}_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha) &= \tilde{H}^C_{\mathbf{r}_\alpha}(\boldsymbol{\rho}_\alpha) + V^N_\alpha(\mathbf{r}_\alpha)\\ &= T_{\mathbf{r}_\alpha} + V^C_\alpha(\mathbf{r}_\alpha) + V^N_\alpha(\mathbf{r}_\alpha) + \tilde{V}^C_\alpha(\boldsymbol{\rho}_\alpha),\end{aligned} \qquad (110)$$

which includes the nuclear interaction in channel α. Equivalently, if we introduce the solution $\psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ of the Schrödinger equation with potential $V_\alpha = V^N_\alpha + V^C_\alpha$ for a local energy $E_\alpha(\boldsymbol{\rho}_\alpha) = \mathbf{k}^2_\alpha(\boldsymbol{\rho}_\alpha)/2\mu_\alpha$,

$$\{E_\alpha(\boldsymbol{\rho}_\alpha) - T_{\mathbf{r}_\alpha} - V_\alpha(\mathbf{r}_\alpha)\}\psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) = 0, \qquad (111)$$

we have again for $r_\alpha/\rho_\alpha \to 0$

$$\psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) = e^{i\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)\cdot\mathbf{r}_\alpha} F_\alpha(\mathbf{r}_\alpha;\boldsymbol{\rho}_\alpha) + O\left(\frac{1}{\rho^2_\alpha}\right). \qquad (112)$$

Of course, in general for the solution of Eq. (111) one must take resort to numerical techniques.

Hence for general two-particle interactions we conclude that the wave function

$$\begin{aligned}\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) &= \psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)\,\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)\\ &= \psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)\,e^{i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}\\ &\quad\times e^{i\eta_\beta\ln(k_\beta\rho_\alpha-\epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha)}\\ &\quad\times e^{i\eta_\gamma\ln(k_\gamma\rho_\alpha-\epsilon_{\alpha\gamma}\mathbf{k}_\gamma\cdot\boldsymbol{\rho}_\alpha)},\end{aligned} \qquad (113)$$

where $\chi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\boldsymbol{\rho}_\alpha)$ is an asymptotic solution of Eq. (86), and $\psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ is the solution of the Schrödinger equation (111), satisfies [up to terms of the order $O(\rho_\alpha^{-2})$] the asymptotic [Eq. (10)], and hence also the original Schrödinger equation (2), in the region Ω_α. Furthermore, for $V_\alpha \equiv 0$ it coincides with the generalized leading term (55) in the asymptotic expansion of the exact wave function derived analytically in Sec. III. This proves that $\Psi^{(+)}_{\mathbf{k}_\alpha\,\mathbf{q}_\alpha}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ is the leading term in Ω_α of the three-charged-particle wave function, thereby generalizing expression (99).

Consequently, our discussion of the applicability of the two possible spectral decompositions of the resolvent of H^{as} remain generally valid, provided everywhere $\psi^{(+)}_{C,\,\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$ is replaced by $\psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha)$.

In an analogous manner the wave function (108) can be generalized to yield

$$\begin{aligned}\tilde{\Phi}_2^{(+)'}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha) = e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_\alpha+i\mathbf{q}_\alpha\cdot\boldsymbol{\rho}_\alpha}&\\ \times\prod_{\nu=1}^{3} e^{-i\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)\cdot\mathbf{r}_\nu}&\\ \times\psi^{(+)}_{\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)}(\mathbf{r}_\nu),&\end{aligned} \qquad (114)$$

where $\psi^{(+)}_{\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)}(\mathbf{r}_\nu)$ is the solution of the Schrödinger equation

$$\left\{\frac{\mathbf{k}^2_\nu(R,\hat{\boldsymbol{\rho}}_\nu)}{2\mu_\nu} - T_{\mathbf{r}_\nu} - V_\nu(\mathbf{r}_\nu)\right\}\psi^{(+)}_{\mathbf{k}_\nu(R,\hat{\boldsymbol{\rho}}_\nu)}(\mathbf{r}_\nu) = 0, \qquad (115)$$

with the full interaction in channel ν. This wave function, which is the asymptotic solution of the Schrödinger equation (2) with general Coulomb-type pair interactions in all regions Ω_α, $\alpha = 0,1,2,\text{and}\,3$, is therefore the leading term of an asymptotic expansion of the three-charged-particle wave function in all these domains.

V. DISCUSSION AND CONCLUSIONS

In this paper we have presented the asymptotic wave function $\tilde{\Phi}_2^{(+)'}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ for three charged particles in the continuum which is valid not only when all three interparticle distances tend to infinity, but also when the distance between any two particles is small compared to the distance between the center of mass of this pair and the third particle. This wave function has been shown to be an asymptotic solution of the asymptotic Schrödinger equation in all the asymptotic regions Ω_α, $\alpha = 0,1,2,\text{and}\,3$, except for the singular directions. Its explicit form is given by Eq. (114) for general Coulomb plus nuclear interactions. In Ω_0 it coincides in the leading order with the standard asymptotic solution $\Psi_0^{\mathrm{as}(+)}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$, Eq. (5), i.e., it is equivalent there to $\Psi_0^{(+)'}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$, Eq. (6). In Ω_α, for $\alpha = 1,2,\text{or}\,3$, the wave function $\tilde{\Phi}_2^{(+)'}(\mathbf{r}_\alpha,\boldsymbol{\rho}_\alpha)$ coincides in leading order with (113), for general potentials V_α, and with (99), respectively (105), for purely Coulombic interactions. Note that although we have always discussed the wave function with prescribed outgoing boundary conditions only, the corresponding one with prescribed incoming boundary conditions follows from it in the conventional manner.

From the physical point of view our main results are the following. First, in Ω_α, $\alpha = 1,2,\text{or}\,3$, the asymptotic three-charged-particle wave function cannot be decomposed into a product of the internal relative-motion wave function of the pair of particles β and γ, times an independent wave function describing the relative motion of the third particle α with respect to the center of mass of this pair, as is the case if the latter is in a bound state. The physically intuitive reason being that if the two particles of the pair are in the continuum such a splitting would imply a complete decoupling of the motion of the third particle from the individual movement of the other two particles, at least asymptotically, despite the infinite range of the Coulomb interactions present. In contrast, the requirements to be an asymptotic solution in Ω_α *and* in Ω_0 of the three-body Schrödinger equation quite naturally exclude such a structure as a product of the two independent wave functions. To be sure, also our asymptotic wave function in Ω_α, $\alpha = 1, 2, \text{or } 3$, can be represented as a product of eigenfunctions of two suitably chosen component Hamiltonians in an evident way, but both of them are three-body wave functions. This has the consequence that a continuing modification of the internal motion of the considered pair by the third particle cannot even asymptotically be avoided. Formally, this manifests itself in the result that the corresponding internal relative-motion wave function of the pair depends on a local momentum which contains the distance between its center of mass and the third particle as a parameter. And the other wave function of the product which essentially describes the motion of the third particle relative to the center of mass of this pair depends not only on the corresponding canonically conjugated relative momentum, but also on the relative momentum of the particles within the pair through the individual particle momenta. This is, of course, nothing but a reflection of the genuine three-body nature of the system under consideration: even in the asymptotic region Ω_α the long-range three-particle correlations arising from the Coulomb interaction between each of the three pairs of particles affect their individual motion.

Second, it is obvious that the wave functions obtained are valid also if only two of the particles are charged, the third one being neutral. However, because of its practical importance let us explicitly write down the corresponding formulas. To be specific assume particle α to be the neutral one, i.e., $e_\alpha = 0$, but $e_\beta, e_\gamma \neq 0$. Then $\eta_\beta = \eta_\gamma = 0$, and hence also $\mathbf{a}_\alpha^{(\beta)}(\hat{\boldsymbol{\rho}}_\alpha) = \mathbf{a}_\alpha^{(\gamma)}(\hat{\boldsymbol{\rho}}_\alpha) = 0$. This implies that for the subsystems of particles β and γ the local relative momentum $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)$ coincides with the physical momentum, $\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha) \equiv \mathbf{k}_\alpha$. Consequently, when the relative distance between the two charged particles β and γ is small compared to the separation of their center of mass from the neutral particle α, i.e., in the region Ω_α, the asymptotic wave function (113) reduces to

$$\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = \psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)\, e^{i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha} \quad \text{in} \quad \Omega_\alpha. \tag{116}$$

This is just its conventional form since $\psi^{(+)}_{\mathbf{k}_\alpha}(\mathbf{r}_\alpha)$ is the solution of the Schrödinger equation (111) but to the asymptotic energy $E_\alpha = \mathbf{k}_\alpha^2/2\mu_\alpha$. In the domain Ω_β, for $\beta \neq \alpha$, which characterizes a situation in which the charged particle β is far separated from the center of mass of the pair (α, γ) while the neutral particle α and the charged particle γ can be close to each other, we find

$$\Psi^{\mathrm{as}(+)}_{\mathbf{k}_\beta \mathbf{q}_\beta}(\mathbf{r}_\beta, \boldsymbol{\rho}_\beta) = \psi^{(+)}_{\mathbf{k}_\beta(\boldsymbol{\rho}_\beta)}(\mathbf{r}_\beta) \times e^{i\mathbf{q}_\beta \cdot \boldsymbol{\rho}_\beta} e^{i\eta_\alpha \ln(k_\alpha \rho_\beta - \epsilon_{\beta\alpha} \mathbf{k}_\alpha \cdot \boldsymbol{\rho}_\beta)} \quad (\text{in} \quad \Omega_\beta), \tag{117}$$

with $\mathbf{k}_\beta(\boldsymbol{\rho}_\beta) = \mathbf{k}_\beta + \mathbf{a}_\beta^{(\alpha)}(\hat{\boldsymbol{\rho}}_\beta)/\rho_\beta$. The wave function $\psi^{(+)}_{\mathbf{k}_\beta(\boldsymbol{\rho}_\beta)}(\mathbf{r}_\beta)$ is the solution of the subsystem-β analog of Eq. (111) for the local energy $E_\beta(\boldsymbol{\rho}_\beta)$, where it has to be kept in mind that the interaction between particles α and γ consists of the short-range part $V_\beta^N(\mathbf{r}_\beta)$ only. In Ω_0, of course, the specialization of Eq. (5) results.

A third, more technical point concerns the fact that our asymptotic wave function has been shown to be the asymptotic solution of the Schrödinger equation only away from the singular directions. However, for practical purposes it is desirable to have expressions which can also be used there and in the immediate neighborhood. This problem has not yet been solved from a fundamental point of view. However, in the Appendix we suggest one practical possibility to improve our wave function in the singular directions. This is achieved by replacing $\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)$, which enters the definition of the local momentum and becomes singular there, by a quantity which remains well behaved everywhere and, in the nonsingular regions, coincides in the main order with $\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)$. With such a modification our wave function is, however, not a solution of the Schrödinger equation in the singular directions, a deficiency shared by the extension [4,5] to $\Psi_0^{\mathrm{as}(+)\,\prime}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, Eq. (6), of $\Psi_0^{\mathrm{as}(+)}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$, Eq. (5). But, nevertheless, as is the case for $\Psi_0^{\mathrm{as}(+)\,\prime}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha)$ (see, e.g., Ref. [5]) such a generalized wave function might be useful for practical calculations.

Among the physical applications of our wave function we point specifically to the approximate calculation of ionization processes in atomic physics, and break-up reactions in nuclear physics, with charged particles in the three-body final state. In the prior form the corresponding amplitude contains the overlap of the initial state, which consists of a two-body bound-state wave function for the subsystem α times a plane wave for particle α, multiplied by the channel interaction, with the final three-body scattering state. When evaluating the contribution from large impact parameters the wave function (113), or its asymptotically equivalent form

$$\Psi^{(+)\,\prime}_{\mathbf{k}_\alpha \mathbf{q}_\alpha}(\mathbf{r}_\alpha, \boldsymbol{\rho}_\alpha) = e^{i\mathbf{q}_\alpha \cdot \boldsymbol{\rho}_\alpha - i\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha) \cdot \mathbf{r}_\alpha/\rho_\alpha}\, \psi^{(+)}_{\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)}(\mathbf{r}_\alpha) \prod_{\nu\ (\neq\alpha)} N_\nu F(-i\eta_\nu, 1; i(k_\nu r_\nu - \mathbf{k}_\nu \cdot \mathbf{r}_\nu)), \tag{118}$$

should be used. In the singular directions it can be modified according to the prescription discussed in the Appendix.

Under what circumstances might one expect an appreciable influence on ionization cross sections from our modified wave functions? When terminating the expansion of the Coulomb distortion factors as in Eq. (79) we had to assume $r_\alpha/\rho_\alpha \ll 1$. But this does not preclude a significant change of the local momentum $|\mathbf{k}_\alpha(\boldsymbol{\rho}_\alpha)| = |\mathbf{k}_\alpha + \mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)/\rho_\alpha|$ as compared to its asymptotic value k_α when the latter is small. In fact, for $k_\alpha \to 0$ we derive from Eq. (83) with (80) that the "strength" $|\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)|$ of this modification is given by

$$| \mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha) | \underset{k_\alpha \to 0}{\sim} \frac{M_\alpha}{q_\alpha} \left| \left[\frac{e_\beta}{m_\beta} - \frac{e_\gamma}{m_\gamma} \right] \right|. \tag{119}$$

That is, we have found in our quantum-mechanical treatment that the famous charge-over-mass ratio difference is the crucial parameter for such processes. Furthermore, the change of $k_\alpha(\boldsymbol{\rho}_\alpha)$ due to $|\mathbf{a}_\alpha(\hat{\boldsymbol{\rho}}_\alpha)|$ becomes the more pronounced the smaller the relative velocity q_α/M_α between particle α and the center of mass of the pair (β,γ) is.

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APPENDIX

In the preceding sections we have pointed out that the expressions for the various asymptotic wave functions presented in this paper are not valid in the singular directions where at least one of the $\mathbf{a}_\alpha^{(\nu)}(\hat{\boldsymbol{\rho}}_\alpha)$, $\nu \neq \alpha$, becomes singular. One possible remedy is provided by the following procedure.

Let us start from the asymptotic representation

$$N_\beta F(-i\eta_\beta, 1; i(k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta \cdot \boldsymbol{\rho}_\alpha)) \underset{\rho_\alpha \to \infty}{\approx} e^{i\eta_\beta \ln(k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha)}, \tag{A1}$$

which is valid in the nonsingular region characterized by $\epsilon_{\alpha\beta}\hat{\mathbf{k}}_\beta \cdot \hat{\boldsymbol{\rho}}_\alpha \neq 1$. We introduce the shorthand notation $\xi_{\alpha\beta} = k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta \cdot \boldsymbol{\rho}_\alpha$. From Eq. (A1) we derive

$$\frac{d \ln F(-i\eta_\beta, 1; i\xi_{\alpha\beta})}{d\xi_{\alpha\beta}} \approx \frac{i\eta_\beta}{\xi_{\alpha\beta}} \tag{A2}$$

which can be used to write

$$\begin{aligned}\frac{\mathbf{a}_\alpha^{(\beta)}(\hat{\boldsymbol{\rho}}_\alpha)}{\rho_\alpha} &\approx ik_\beta \frac{\mu_\alpha}{m_\gamma}(\epsilon_{\alpha\beta}\hat{\boldsymbol{\rho}}_\alpha - \hat{\mathbf{k}}_\beta) \\ &\quad\times \frac{d \ln F(-i\eta_\beta, 1; i(k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha))}{d\xi_{\alpha\beta}} \\ &= \eta_\beta k_\beta \frac{\mu_\alpha}{m_\gamma}(\epsilon_{\alpha\beta}\hat{\boldsymbol{\rho}}_\alpha - \hat{\mathbf{k}}_\beta) \\ &\quad\times \frac{F(1-i\eta_\beta, 2; i(k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha))}{F(-i\eta_\beta, 1; i(k_\beta\rho_\alpha - \epsilon_{\alpha\beta}\mathbf{k}_\beta\cdot\boldsymbol{\rho}_\alpha))}.\end{aligned} \tag{A3}$$

Here we have made use of the relation $F'(a,b;x) = a\,F(1+a,1+b;x)/b$. The rhs of Eq. (A3) coincides in the nonsingular direction to leading order in ρ_α^{-1} with the lhs, but it is well-behaved everywhere, including the singular direction where it goes to zero. Hence substitution of $\mathbf{a}_\alpha^{(\beta)}(\hat{\boldsymbol{\rho}}_\alpha)/\rho_\alpha$ by the rhs of Eq. (A3), and a similar expression for $\mathbf{a}_\alpha^{(\gamma)}(\hat{\boldsymbol{\rho}}_\alpha)/\rho_\alpha$ in all equations provides us with wave functions which can be used in practical calculations everywhere. [It is obvious that near the singular directions the ratio of the two hypergeometric functions occurring in Eq. (A3) is easily calculable as a sum of few terms in the series expansion of the latter.] In the nonsingular directions the wave functions modified in such a way coincide with those obtained before; but, of course, they are not asymptotic solutions of the Schrödinger equation (2) in the singular directions.

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* Permanent address: Institute for Nuclear Physics, Tashkent, Usbekistan.

[1] P. J. Redmond (unpublished).
[2] L. Rosenberg, Phys. Rev. D **8**, 1833 (1972).
[3] R. J. Peterkop, *Theory of Ionisation of Atoms by Electron Impact* (University of Colorado Press, Boulder, 1977).
[4] S. P. Merkuriev, Theor. Math. Phys. **32**, 680 (1977).
[5] M. Brauner, J. S. Briggs, and H. J. Klar, J. Phys. B **22**, 2265 (1989).
[6] P. L. Altik, J. Phys. B **16**, 3543 (1983).
[7] S. P. Merkuriev and L. D. Faddeev, *Kvantovaya Teoria Rasseyaniya dlya Sistem Neskol'kich Tschastits* (Nauka, Moscow, 1985) (in Russian).
[8] M. R. H. Rudge and M. J. Seaton, Proc. R. Soc. London Ser. A **283**, 262 (1965).