Asymptotic expansions for three-body Coulomb scattering state



1999 J. Phys. A: Math. Gen. 32 677

(http://iopscience.iop.org/0305-4470/32/4/011)

J. Phys. A: Math. Gen. **32** (1999) 677–692. Printed in the UK PII: S0305-4470(99)94589-4

# Asymptotic expansions for three-body Coulomb scattering state

Sh D Kunikeev†

Skobeltsyn Institute of Nuclear Physics, Moscow State University, 119899 Moscow, Russia

Received 26 May 1998 , in final form 28 September 1998

**Abstract.** A wavefunction possessing the correct asymptotic behaviour in the region of configuration space where two particles are only slightly separated and a third particle is located far away is constructed within the quasiclassical eikonal, WKB and quantum-mechanical approach. This function cannot be represented as a product of independent two-particle distortion functions and in the limiting cases it passes into the continuum-distorted-wave (CDW) function and the asymptotic state of Kunikeev and Senashenko (1996 *Sov. Phys.–JETP* **82** 839). The derived function gives a better account of the interaction zone and is used to investigate a fragmentation process. As an application, the ionization process of an atom by ion impact is considered. The amplitude and the double-differential cross section (DDCS) for the ionization process are developed. The problem to calculate the DDCS is reduced to a three-dimensional integration.

## 1. Introduction

The description of the complicated quantum-mechanical dynamics of few charged particles is one of the fundamental unsolved problems in atomic, molecular and nuclear physics. For example, an adequate description of resonant or direct fragmentation processes involving charged particles requires the knowledge of the final many-body scattering state both at finite and infinite interparticle distances. However, our knowledge of the fragmentation dynamics at finite interparticle distances is still scarce, in particular, if the strength of the different interactions involved is of the same order and a perturbative approach is inappropriate. Moreover, the behaviour in the inner or reaction zone, $\Omega_{int}$, where all particles are nearby, depends on the asymptotic behaviour of the continuum state.

Asymptotic Coulombic states for the three-body scattering problem have been reported in the region $\Omega_0$ where all interparticle distances are large (Rosenberg 1973, Peterkop 1977, Merkuriev 1977, Belkić 1978, Brauner *et al* 1989). In this region particles can be regarded as almost independent ones so that the wavefunction can be represented in factorized form as the product of Coulomb two-particle distortion factors. On the contrary, in the asymptotic region $\Omega_{ij}$ where two particles $(i, j)$ are close to one another and a third particle $(k)$ is located far away from the pair $(i \neq j \neq k \neq i = 1, 2, 3)$ this wavefunction has the wrong asymptotic behaviour. Only recently (Alt and Mukhamedzhanov 1992, 1993, Kunikeev and Senashenko (KS) 1996, Mukhamedzhanov and Lieber 1996, Kunikeev 1997, Kim and Zubarev 1997) have asymptotic three-body scattering states been derived in the asymptotic regions $\Omega_{ij}$. Thus, Alt and Mukhamedzhanov (1992, 1993) have obtained a zeroth-order wavefunction satisfying the Schrödinger equation in $\Omega_{ij}$ up to terms of $O(1/R_k^2)$ where $R_k$ is the distance between particle

† E-mail address: kunikeev@anna19.npi.msu.su

0305-4470/99/040677+16$19.50  

$k$ and the centre-of-mass of pair $(i, j)$. Later, the asymptotic wavefunction in $\Omega_{ij}$ that satisfies the Schrödinger equation up to terms of $O(1/R_k^2)$ and contains the zeroth-order term and all of the first-order $O(1/R_k)$ terms, was suggested in Kunikeev and Senashenko (1996). Similar results were also obtained by Mukhamedzhanov and Lieber (1996) and further developed by Kim and Zubarev (1997).

In this work we derive approximate analytical expressions for the solution of the non-relativistic Schrödinger equation of three charged particles that generalize the KS asymptotic states. The study is restricted to a description of a light particle moving in the field of two heavy particles. This enables us to separate out the interaction between heavy particles into an individual factor with good accuracy. The derived wavefunction gives a better account of the reaction zone and may be used in describing the ionization process. As an application, we develop the amplitude and the double-differential cross section (DDCS) for the direct ionization of an atom by ion impact. The atomic system of units is used throughout.

## 2. The three-body Coulomb continuum state

We consider the system of three charged particles: the ejected electron (particle 2) moving in the combined field of the scattered ion (1) and the residual target ion (3). The Hamiltonian of such a system has the form

$$\hat{H} = \hat{K} + \sum_{i<j=1}^{3} V_{ij} = -\frac{1}{2m_{23}}\boldsymbol{\nabla}^2_{\boldsymbol{r}_{23}} - \frac{1}{2\mu_1}\boldsymbol{\nabla}^2_{\boldsymbol{R}_1} + \sum_{i<j=1}^{3}\frac{Z_i Z_j}{r_{ij}} \tag{1}$$

where $\boldsymbol{r}_{ij}$ are the relative coordinates of the particle pair $(i, j)$, $\boldsymbol{R}_k$ are the coordinates of particle $k$ in respect to the centre of mass of the particle pair $(i, j)$; $Z_i$, $m_i$ ($Z_2 = -1, m_2 = 1, i = 1, 2, 3$) are charge and mass of the $i$th particle, $m_{ij} = m_i m_j/(m_i + m_j)$, $\mu_k = m_k(m_i + m_j)/(m_i + m_j + m_k)$ $(i \neq j \neq k \neq i)$ are the reduced masses.

Within the continuum-distorted-wave (CDW) approach, a solution of the three-body Schrödinger equation is sought in the form

$$\Psi^-_{as} = \exp(\mathrm{i}\boldsymbol{k}_{23}\boldsymbol{r}_{23} + \mathrm{i}\boldsymbol{K}_1\boldsymbol{R}_1)F_q(\nu_{12}, \zeta_{12})F_{e0}(\nu_{13}, \zeta_{13})F(\boldsymbol{r}_{23}, \boldsymbol{R}_1) \tag{2}$$

where

$$F_q(\nu, \zeta) = \exp(-\pi\nu/2)\Gamma(1 - \mathrm{i}\nu)\,{}_1F_1(\mathrm{i}\nu, 1, -\mathrm{i}\zeta) \tag{3}$$

$$F_{e0}(\nu, \zeta) = \exp(-\mathrm{i}\nu\ln\zeta)$$
$$\nu_{ij} = \frac{Z_i Z_j m_{ij}}{k_{ij}} \qquad \zeta_{ij} = k_{ij}\xi_{ij} = k_{ij}r_{ij} + \boldsymbol{k}_{ij}\boldsymbol{r}_{ij} \tag{4}$$

are the quantum-mechanical and eikonal continuum distortion functions which are due to interaction of the particle pairs $(1, 2)$ and $(1, 3)$ respectively; $(\boldsymbol{k}_{ij}, \boldsymbol{K}_k)$ are the momenta which are canonically conjugate to the Jakobi coordinates $(\boldsymbol{r}_{ij}, \boldsymbol{R}_k)$. The distortion function $F$ satisfies the equation

$$(-\tfrac{1}{2}\boldsymbol{\nabla}^2_{\boldsymbol{r}_{23}} - \mathrm{i}\boldsymbol{k}_{23}(\boldsymbol{r}_{12})\cdot\boldsymbol{\nabla}_{\boldsymbol{r}_{23}} + V_{23} - \mathrm{i}\boldsymbol{v}\cdot\boldsymbol{\nabla}_{\boldsymbol{R}_1})F(\boldsymbol{r}_{23}, \boldsymbol{R}_1) = 0 \tag{5}$$

where

$$\boldsymbol{k}_{23}(\boldsymbol{r}_{12}) = \boldsymbol{k}_{23} + \boldsymbol{u}_{12}(\boldsymbol{r}_{12}) = \boldsymbol{k}_{23} - \mathrm{i}\boldsymbol{\nabla}_{\boldsymbol{r}_{12}}\ln F_q(\nu_{12}, \zeta_{12}) \tag{6}$$

is the local relative momentum of the particle pair $(2, 3)$ which is modified by interaction of the particle pair $(1, 2)$; $\boldsymbol{v}$ is the velocity of particle 1 (scattered ion) relative to the centre of mass of the particle pair $(2, 3)$. Hereafter, we neglect terms of order $1/m_{1,3} \ll 1$.

Within the CDW method, the influence of interaction of the particle pair $(1, 2)$ on the motion of the particle pair $(2, 3)$ is usually disregarded, i.e. one makes the so-called basic approximation of the CDW method and puts $\boldsymbol{k}_{23}(\boldsymbol{r}_{12}) \equiv \boldsymbol{k}_{23}$ in equation (5). Then the equation (5) has an explicit solution satisfying incoming boundary conditions, $F(\boldsymbol{r}_{23}, \boldsymbol{R}_1) = F_q(\nu_{23}, \zeta_{23})$, and the wavefunction (2) can be written in the form factorized in interaction of the particle pairs. Such a representation of the CDW function proves to be valid in the asymptotic region $\Omega_0$ where all three particle pairs are well separated ($r_{12} \sim r_{23} \sim r_{13} \gg 1$) and the influence of a third particle on the relative motion of a particle pair can be neglected. On the contrary, in the asymptotic region $\Omega_{23}$ where $r_{23} \ll r_{12}$, the three-body operator $-\mathrm{i}\boldsymbol{u}_{12}(\boldsymbol{r}_{12}) \cdot \boldsymbol{\nabla}_{r_{23}}$ in equation (5), which establishes a correlation between the relative motion of the particle pairs $(1, 2)$ and $(2, 3)$, essentially modifies the distortion function $F$ and it should be taken into account in constructing the wavefunction that satisfies proper boundary conditions.

### 2.1. *The eikonal approximation*

Let us first examine the effects introduced by this three-body operator within the eikonal approximation for which explicit formulae can be derived. Using the substitution $F_e = \exp(\mathrm{i}\Phi_e)$ and neglecting the quadratic kinetic energy operator in equation (5), we write the equation for the phase function $\Phi_e$ as

$$(\boldsymbol{k}_{12}(\boldsymbol{r}_{12}) \cdot \boldsymbol{\nabla}_{r_{12}} + \boldsymbol{v} \cdot \boldsymbol{\nabla}_{R_1})\Phi_e(\boldsymbol{r}_{12}, \boldsymbol{R}_1) = -V_{23}(r_{23}) \tag{7}$$

where $\boldsymbol{k}_{12}(\boldsymbol{r}_{12}) = \boldsymbol{k}_{23}(\boldsymbol{r}_{12}) - \boldsymbol{v} = \boldsymbol{k}_{12} + \boldsymbol{u}_{12}(\boldsymbol{r}_{12})$.

Note that the momentum (6) is, in general, a complex vector. Hereafter, we will neglect the imaginary part of the local momentum, $\boldsymbol{k}_{12}(\boldsymbol{r}_{12}) \equiv \mathrm{Re}\, \boldsymbol{k}_{12}(\boldsymbol{r}_{12})$, which is proposed to be an infinitesimal of second order. We write equations that define the characteristic trajectories of motion in the form

$$\begin{aligned} &\dot{\boldsymbol{r}}_{12}(t) = \boldsymbol{k}_{12}(\boldsymbol{r}_{12}(t)) \\ &\dot{\boldsymbol{R}}_1(t) = \boldsymbol{v}. \end{aligned} \tag{8}$$

Integrating equation (7) along the trajectory, we obtain

$$\Phi_e(\boldsymbol{r}_{12}, \boldsymbol{R}_1) = \Phi_{e0} - \int_{t_0}^{t} \mathrm{d}\tau\, V_{23}(\boldsymbol{r}_{23}(\tau)) \tag{9}$$

where $\Phi_{e0} = \Phi_e(\boldsymbol{r}_{12}(t_0), \boldsymbol{R}_1(t_0))$ is a value of the phase at an initial moment of time $t_0$. The integral in (9) determines a shift of the phase in the Coulomb field $V_{23}$ calculated along the trajectory which is curved by the interaction of the particle pair $(1, 2)$. In calculating it is assumed that the trajectory starts in a point $(\boldsymbol{r}_{12}(t_0), \boldsymbol{R}_1(t_0))$ at an initial moment $t_0$, so that it ends in the point $(\boldsymbol{r}_{12}(t) = \boldsymbol{r}_{12}, \boldsymbol{R}_1(t) = \boldsymbol{R}_1)$ at time $t$. Let us divide the time interval $(t_0, t)$ into $N$ subintervals: $(t_0, t_1)$, $(t_1, t_2), \ldots,$ $(t_{N-1}, t_N = t)$ such that on an each time interval $(t_{i-1}, t_i)$, $i = 1, \ldots, N$ the changes of the relative momentum of the particle pair $(2, 3)$ can be neglected, i.e. $\boldsymbol{k}_{23}(\tau) \simeq \boldsymbol{k}_{23}(t_i) = \mathrm{const}$ at $\tau \in (t_{i-1}, t_i)$. The curved part of the trajectory on the interval $(t_{i-1}, t_i)$ can then be approximated by a rectilinear segment of the form: $\boldsymbol{r}_{23}(\tau) = \boldsymbol{r}_{23}(t_{i-1}) + \boldsymbol{k}_{23}(t_i)(\tau - t_{i-1})$ and the total phase shift summed over all the rectilinear parts of the trajectory reads as

$$\Phi_e(\boldsymbol{r}_{12}, \boldsymbol{R}_1) = \Phi_{e0} + \sum_{i=1}^{N}(\varphi_c(\boldsymbol{k}_{23}(t_i), \boldsymbol{r}_{23}(t_i)) - \varphi_c(\boldsymbol{k}_{23}(t_i), \boldsymbol{r}_{23}(t_{i-1}))) \tag{10}$$

where

$$\varphi_c(\boldsymbol{k}, \boldsymbol{r}) = -\frac{Z_2 Z_3}{k} \ln(kr + \boldsymbol{k}\boldsymbol{r})$$

is the Coulomb logarithmic phase. If we put the initial phase $\Phi_{e0} = \varphi_c(\boldsymbol{k}_{23}(t_0), \boldsymbol{r}_{23}(t_0))$ and consider that $\boldsymbol{r}_{23}(t_N) = \boldsymbol{r}_{23}$, $\boldsymbol{k}_{23}(t_N) = \boldsymbol{k}_{23}(\boldsymbol{r}_{12})$, equation (10) can be rewritten in the form

$$\Phi_e(\boldsymbol{r}_{12}, \boldsymbol{R}_1) = \varphi_c(\boldsymbol{k}_{23}(\boldsymbol{r}_{12}), \boldsymbol{r}_{23}) - \Delta\varphi_c \tag{11}$$

where

$$\Delta\varphi_c = \sum_{i=1}^{N} (\varphi_c(\boldsymbol{k}_{23}(t_i), \boldsymbol{r}_{23}(t_{i-1})) - \varphi_c(\boldsymbol{k}_{23}(t_{i-1}), \boldsymbol{r}_{23}(t_{i-1}))) \tag{12}$$

represents an additional phase shift which is due to the momentum changes during the motion along the broken trajectory consisting of straight-line segment paths. In the limit $N \to \infty$, the broken trajectory passes into a continuous one, and the summation in equation (12)—into an integration along the trajectory:

$$\Delta\varphi_c = \int_{t_0}^{t} \mathrm{d}\tau \, \dot{\boldsymbol{k}}_{23}(\tau) \cdot \nabla_{k_{23}} \varphi_c(\boldsymbol{k}_{23}(\tau), \boldsymbol{r}_{23}(\tau)) \tag{13}$$

where the derivative with respect to time is

$$\dot{\boldsymbol{k}}_{23}(\tau) = (\boldsymbol{k}_{12}(\boldsymbol{r}_{12}(\tau)) \cdot \nabla_{r_{12}}) \boldsymbol{k}_{23}(\boldsymbol{r}_{12}(\tau)).$$

On the other hand, the function $\varphi_c(\boldsymbol{k}_{23}(\boldsymbol{r}_{12}), \boldsymbol{r}_{23})$ satisfies the equation (7) up to a remainder term of the form

$$\delta\varphi_c = ((\boldsymbol{k}_{12}(\boldsymbol{r}_{12}) \cdot \nabla_{r_{12}}) \boldsymbol{k}_{23}(\boldsymbol{r}_{12}) \cdot \nabla_{k_{23}}) \varphi_c(\boldsymbol{k}_{23}(\boldsymbol{r}_{12}), \boldsymbol{r}_{23}). \tag{14}$$

It follows from (13), (14) that $\Delta\varphi_c = \int_{t_0}^{t} \delta\varphi_c \, \mathrm{d}\tau$. Thus, we can conclude that a requirement imposed on the remainder (14) to be locally small is a necessary condition and not a sufficient one for that the function $\varphi_c$ would be close to an exact solution of equation (7). In the general case, for this it is necessary to require that the summed (12) or integral (13) contribution from $\delta\varphi_c$ would be small. As follows from (14), $\delta\varphi_c$ is small if $(\boldsymbol{k}_{12}(\boldsymbol{r}_{12}) \cdot \nabla_{r_{12}}) \boldsymbol{k}_{23}(\boldsymbol{r}_{12})$ is small. In the limit $\xi_{12} \to \infty$, the real part of the local momentum (6) takes the asymptotic form

$$\boldsymbol{k}_{23}(\boldsymbol{r}_{12}) \simeq \boldsymbol{k}_{23} - \nu_{12} \frac{\hat{\boldsymbol{r}}_{12} + \hat{\boldsymbol{k}}_{12}}{\xi_{12}} (1 + \cos(-\zeta_{12} + 2\nu_{12} \ln \zeta_{12} - 2\delta_c(\nu_{12}))) \tag{15}$$

where $\delta_c(\nu) = \arg \Gamma(\mathrm{i}\nu)$, $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$. In view of (14), (15), both $\boldsymbol{u}_{12}(\boldsymbol{r}_{12})$ and $\delta\varphi_c$ are infinitesimals of the same order: $\boldsymbol{u}_{12}(\boldsymbol{r}_{12}) = \mathrm{O}(\xi_{12}^{-1})$, $\delta\varphi_c = \mathrm{O}(\xi_{12}^{-1})$. Therefore, we can not neglect a contribution from the integral term in (11). In order to obtain a correct asymptotic solution, $\delta\varphi_c$ should be an infinitesimal of second order at least.

To this end, following Kunikeev and Senashenko (1996) we separate the contributions from the waves that are and are not scattered in the wavefunction (2), namely we employ the following expansion of the quantum-mechanical distortion function

$$F_q(\nu, \zeta) = F_{q0}(\nu, \zeta) + F_{q1}(\nu, \zeta) \tag{16}$$

where

$$F_{q0}(\nu, \zeta) = \exp(\pi\nu/2) G(\mathrm{i}\nu, 1, -\mathrm{i}\zeta) \tag{17}$$

$$F_{q1}(\nu, \zeta) = \mathrm{i}\nu \exp(\pi\nu/2 - 2\mathrm{i}\delta_c(\nu)) \exp(-\mathrm{i}\zeta) G(1 - \mathrm{i}\nu, 1, \mathrm{i}\zeta). \tag{18}$$

Here, $G(a, c, z)$ is the confluent hypergeometric function that is irregular at the origin. The term $F_{q0}(\nu, \zeta)$, which makes the main contribution to the asymptotic behaviour of $F_q(\nu, \zeta)$ at $\zeta \to \infty$, represents particles which have not been rescattered, and the term $F_{q1}(\nu, \zeta)$, which is asymptotically proportional to the Coulomb two-particle scattering amplitude, describes single collisions of a pair of particles. We note that all three functions in expansion (16) are solutions of the same confluent hypergeometric equation, two of the three solutions being linearly independent. Therefore, we require that the unknown distortion functions $F_j(\boldsymbol{r}_{23}, \boldsymbol{R}_1)$ corresponding to the unscattered and scattered waves at $j = 0, 1$ satisfy equations of the form (5) where one should replace

$$\boldsymbol{k}_{23}(\boldsymbol{r}_{12}) \to \boldsymbol{k}_{23}^{(j)}(\boldsymbol{r}_{12}) = \boldsymbol{k}_{23} + \boldsymbol{u}_{12}^{(j)}(\boldsymbol{r}_{12}) = \boldsymbol{k}_{23} + \nabla_{r_{12}}\Phi_{qj}(\nu_{12}, \zeta_{12}). \tag{19}$$

where $\Phi_{qj}$ is the phase of the complex function $F_{qj}$.

All the formulae obtained above in the eikonal approximation can directly be generalized in the case of a separate contribution from the waves that are scattered and are not scattered. Thus, in the limit $\xi \to \infty$, the local momenta (19) possess different asymptotic behaviour

$$\begin{aligned}\boldsymbol{k}_{23}^{(0)}(\boldsymbol{r}_{12}) &= \boldsymbol{k}_{23} - \nu_{12}(\hat{\boldsymbol{r}}_{12} + \hat{\boldsymbol{k}}_{12})/\xi_{12}\\ \boldsymbol{k}_{23}^{(1)}(\boldsymbol{r}_{12}) &= \boldsymbol{v} - k_{12}\hat{\boldsymbol{r}}_{12} + \nu_{12}(\hat{\boldsymbol{r}}_{12} + \hat{\boldsymbol{k}}_{12})/\xi_{12}.\end{aligned} \tag{20}$$

Then, as follows from (14), (20), $\delta\varphi_{cj} = \mathrm{O}(\xi_{12}^{-2})$ at $j = 0, 1$. For $\delta\varphi_{c1}$, for example, we have

$$\begin{aligned}\delta\varphi_{c1} &\sim (\boldsymbol{k}_{12}^{(1)}(\boldsymbol{r}_{12}) \cdot \nabla_{r_{12}})\boldsymbol{k}_{23}^{(1)}(\boldsymbol{r}_{12})\\ &= (-k_{12}\hat{\boldsymbol{r}}_{12} \cdot \nabla_{r_{12}})(\boldsymbol{v} - k_{12}\hat{\boldsymbol{r}}_{12}) + \mathrm{O}(\xi_{12}^{-2}) = \mathrm{O}(\xi_{12}^{-2}).\end{aligned}$$

Thus, the function $\varphi_{cj} = \varphi_c(\boldsymbol{k}_{23}^{(j)}(\boldsymbol{r}_{12}), \boldsymbol{r}_{23})$ satisfies equation (7) with the local momentum (19) neglecting infinitesimals of second order in the limit $\xi_{12} \to \infty$, i.e. it is an asymptotic solution. If the variable $\xi_{12}$ is bounded or does not approach infinity rapidly enough, it is necessary to regard an additional correction $\Delta\varphi_{cj}$ arising in summing (12) or integration (13) of $\delta\varphi_{cj}$ along the curved trajectory.

### 2.2. *Quasiclassical trajectories*

Let us define the integral trajectories or rays corresponding to the waves that are and are not scattered. If the second vector equation in a set of independent equations (8) gives straight-line trajectories of the form: $\boldsymbol{R}_1(t) = \boldsymbol{v}t + \boldsymbol{b}$ where $\boldsymbol{b}$ is the vector impact parameter, the first one defines trajectories of relative motion of the particles pair (1,2) distorted by the Coulomb interaction between them and can be integrated in the parabolic coordinates: $\xi_{12} = r_{12} + \hat{\boldsymbol{k}}_{12} \cdot \boldsymbol{r}_{12}$, $\eta_{12} = r_{12} - \hat{\boldsymbol{k}}_{12} \cdot \boldsymbol{r}_{12}$ and $\varphi_{12}$ (azimuthal angle). These equations in parabolic coordinates take the form

$$\begin{aligned}\dot{\xi} &= \frac{2k\xi}{\xi + \eta}p_{qj}(\xi)\\ \dot{\eta} &= -\frac{2k\eta}{\xi + \eta}\\ \dot{\varphi} &= 0\end{aligned} \tag{21}$$

where

$$p_{qj}(\xi) = 1 + 2\frac{\mathrm{d}}{\mathrm{d}\zeta}\Phi_{qj}(\nu, \zeta) \qquad \zeta = k\xi \qquad j = 0, 1.$$

Hereafter, for convenience we omit subindexes 1, 2.

It follows from equation (21) that the trajectories lie in a half-plane: $\varphi = \varphi_0 = \mathrm{const}$, and the trajectory equation has the form

$$\eta = C \exp(-\Pi_{qj}(\xi)) \tag{22}$$

where

$$\Pi_{qj} = \int \frac{\mathrm{d}\xi}{\xi p_{qj}(\xi)}.$$

Equation (22) at different values of integration constant $C$ specifies a set of trajectories. The constant $C$ and the azimuthal angle $\varphi_0$ are chosen so that an integral curve passes through a given point $\boldsymbol{r} = (\xi, \eta, \varphi)$.

In the quasiclassical WKB approximation, the quantum-mechanical distortion functions, $F_{qj}(\nu, \zeta)$, should be replaced by corresponding quasiclassical counterparts,

$$F_{qj}(\nu,\zeta) \to F_{cj}(\nu,\zeta) = a_{cj}(\nu,\zeta)\exp(\mathrm{i}\Phi_{cj}(\nu,\zeta))$$

which explicit forms in terms of elementary functions can be written as (Kunikeev and Senashenko 1996)

$$\Phi_{c0,1}(\nu,\zeta) = \frac{\zeta}{2}\left(\pm\sqrt{1-4\nu/\zeta} - 1\right) \pm \nu \ln \frac{\sqrt{1-4\nu/\zeta} - 1}{\sqrt{1-4\nu/\zeta} + 1} \tag{23}$$

and

$$a_{c0}(\nu,\zeta) = C_0(\nu)\sqrt{1 + \frac{1-2\nu/\zeta}{\sqrt{1-4\nu/\zeta}}} \tag{24}$$

$$a_{c1}(\nu,\zeta) = C_1(\nu)\frac{1}{\zeta\sqrt{1-4\nu/\zeta + (1-2\nu/\zeta)\sqrt{1-4\nu/\zeta}}} \tag{25}$$

where the integration constants

$$C_0(\nu) = \frac{1}{\sqrt{2}}\exp(\mathrm{i}\nu(1-\ln(-\nu)))$$

$$C_1(\nu) = \sqrt{2}\nu\frac{\Gamma(-\mathrm{i}\nu)}{\Gamma(\mathrm{i}\nu)}\exp(\mathrm{i}\nu(-1+\ln(-\nu)))$$

are chosen such that the WKB functions go over into the corresponding eikonal representations $F_{e0,1}(\nu,\zeta)$ at $\zeta \to \infty$.

Substituting the functions (23), we obtain the following quasiclassical expressions

$$\Pi_{cj}(\xi) = \pm 2\int \frac{\mathrm{d}w}{1-w^2} \qquad w = \sqrt{1-\frac{4\nu}{\zeta}}. \tag{26}$$

Here, the upper (lower) sign on the right-hand side of the equation corresponds to $j = 0(1)$ on the left-hand side of the equation. In view of (22), (26), the following equation for quasiclassical trajectories can be derived

$$\eta = C\left|\frac{w-1}{w+1}\right|^{\pm 1}. \tag{27}$$

For the unscattered (distorted plane) wave, equation (27) (upper sign) in the polar coordinates $(r, \theta)$ takes the form

$$r = \frac{p}{\pm 1 + \sin(\theta \mp \theta_0)/\sin\theta_0} \tag{28}$$

where

$$p = \frac{k\rho_0^2}{|\nu|} \qquad \sin\theta_0 = \frac{|\nu|/(k\rho_0)}{\sqrt{1+(\frac{\nu}{k\rho_0})^2}} \qquad \cos\theta_0 = \frac{1}{\sqrt{1+(\frac{\nu}{k\rho_0})^2}} \qquad 0 < \theta_0 < \frac{\pi}{2}.$$

Here, the upper (lower) sign corresponds to $\nu < 0$ $(\nu > 0)$. The constant $C(\rho_0)$ in (27) is defined so that $r\sin\theta = \sqrt{\xi\eta} = \rho \to \rho_0 = \text{const} > 0$ at $\xi \to \infty$ or $\theta \to 0$, where $\rho_0$ is an

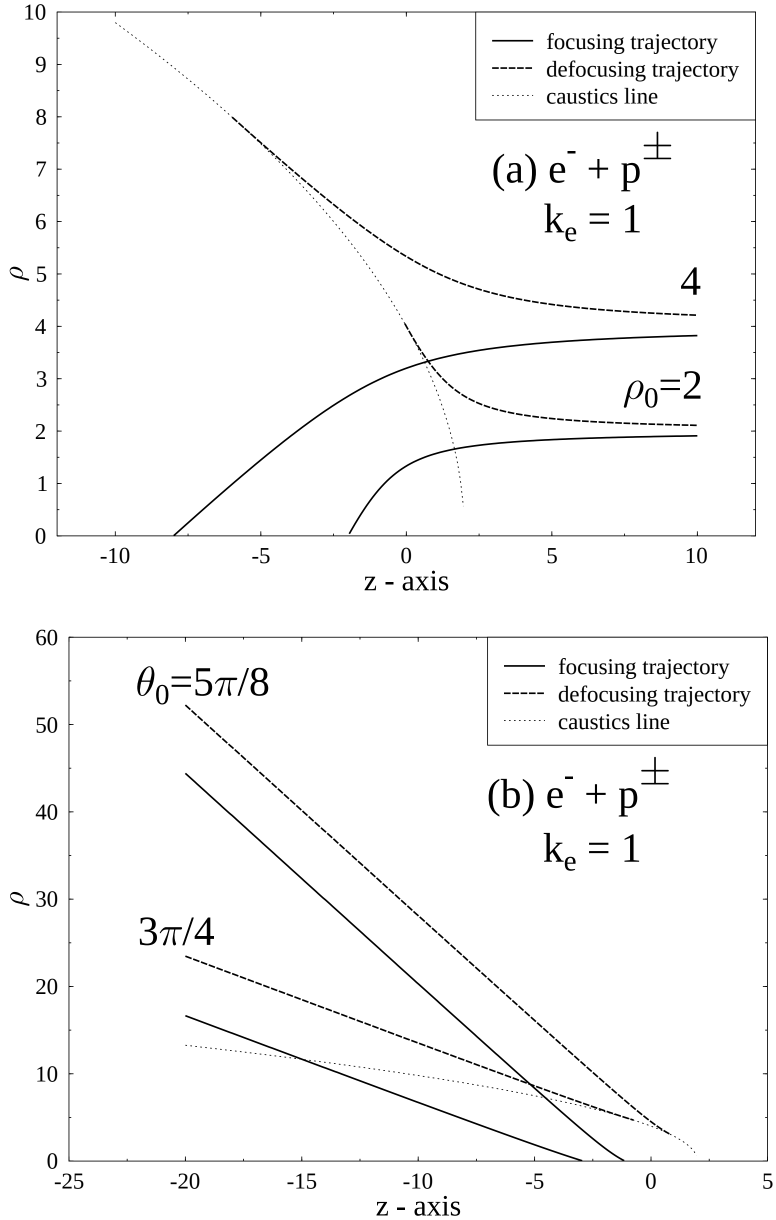


**Figure 1.** Coulomb trajectories corresponding to the distorted plane wave (*a*) at asymptotic momentum $k = 1$ and impact parameters $\rho_0 = 2$ and 4 au, calculated for the $e^- - p^\pm$ collisions in the WKB approximation, and the distorted spherical wave (*b*) at asymptotic momentum $k = 1$ and angles $\theta_0 = 3\pi/4$ and $5\pi/8$ specifying a direction of the trajectory asymptote.

impact parameter. Equation (28) at different $\rho_0$ describes a set of hyperbolic trajectories $r(\theta)$ with one of the asymptotes: $\rho = \rho_0$ at $\theta = 0$. Depending on the sign of $\nu$, the arrangement of the hyperboles relative to the Coulomb centre at the origin is qualitatively different (see figure 1(*a*)).

In the attractive field ($\nu < 0$), the trajectories with an impact parameter $\rho_0$ and different azimuthal angles at the range $0 \leqslant \varphi_0 < 2\pi$ converge to the focussing point, $z_{f0} = -p/2$, located on the negative $z$-axis $l_- = \{(z, \rho) : z < 0, \rho = 0\}$. This axis, $l_-$, is a set of singular points in which a uniqueness condition for a solution of a set of equations (21) is not fulfilled. In the focusing points, the quasiclassical amplitudes (24), (25) of both the scattered and unscattered wave are singular: $a_{c0,1} \sim \xi^{-1/4}$. Continuously changing the parameters $\rho_0$ and $\varphi_0$, we obtain a three-dimensional space in which one and only one trajectory passes through an each point $\boldsymbol{r} \notin l_-$ (at $\rho_0 = 0$ the hyperbolic trajectory reduces to a straight line $l_+ = \{(z, \rho) : z > 0, \rho = 0\}$). At $\rho_0 \to \infty$ and/or $k \to \infty$, a deflection of the trajectory from a rectilinear line decreases because the focusing point $z_{f0} = -(k\rho_0)^2/(2Z_1) \to -\infty$.

In contrast, in the repulsive field ($\nu > 0$) the trajectories with an impact parameter $\rho_0$ and different azimuthal angles $\varphi_0$ diverge, i.e. an effect of defocussing of particles occurs. A particle moving from infinity along the hyperbolic divergent trajectory comes to the caustics point (or the turning point) where the WKB approximation is inappropriate. The equation that defines the points of caustics reads as

$$r = \frac{4\nu}{k(1 + \cos\theta)}.$$

It follows that the trajectory with an impact parameter $\rho_0$ is tangent to the caustics line at point $(r_{c0}, \theta_{c0})$ defined by

$$\begin{aligned} r_{c0} &= \frac{2\nu}{k}\left[1 + \left(\frac{k\rho_0}{2\nu}\right)^2\right] \\ \theta_{c0} &= \arccos\left(\frac{1 - (\frac{k\rho_0}{2\nu})^2}{1 + (\frac{k\rho_0}{2\nu})^2}\right). \end{aligned} \qquad (29)$$

We note that equation (29) defines a turning point in respect to $\xi$ rather than to a radial coordinate, i.e. $r_{c0} \neq r_{\min}$, $\theta_{c0} \neq \theta_{\min}$ where $r_{\min} = p/(-1 + 1/\sin\theta_0)$ is the distance of the closest approach to the Coulomb centre at the origin and $\theta_{\min} = \pi/2 - \theta_0$. As a consequence, at that point, the $\xi$-coordinate takes a minimum value, $\xi_{\min} = 4\nu/k$. Moreover, the region of the coordinate space where $\xi < \xi_{\min}$ is classically inaccessible. In that region, the quasiclassical local momentum and the corresponding trajectories become complex. In the points of caustics, the quasiclassical amplitudes are singular: $a_{c0,1} \sim (\xi - \xi_{\min})^{-1/4}$. Thus, in both the focusing points and turning points, the WKB approximation is not valid and the quantum-mechanical approximation should be used near these points.

Substituting equation (28) into the second one of (21) and integrating it, we obtain an equation that establishes a one-to-one dependence of the polar angle $\theta(t)$ upon time in moving a particle along the trajectory

$$f_\pm(\theta) = -\frac{\nu^2}{k\rho_0^3}(t - t_0) \qquad (30)$$

$$\begin{aligned} f_\pm(\theta) = &\int \mathrm{d}\theta\, [\mp 1 + \sin(\theta \pm \theta_0)/\sin\theta_0]^{-2} \\ = &-2(\tan(\theta \pm \theta_0)/2 \mp \sin\theta_0)/[\cos^2\theta_0(\tan(\theta \pm \theta_0)/2 \\ &\mp (1 + \cos\theta_0)/\sin\theta_0)(\tan(\theta \pm \theta_0)/2 \mp (1 - \cos\theta_0)/\sin_0)] \\ &\pm \tan^3\theta_0 \ln\left|\frac{\sin\theta_0 \tan(\theta \pm \theta_0)/2 \mp (1 - \cos\theta_0)}{\sin\theta_0 \tan(\theta \pm \theta_0)/2 \mp (1 + \cos\theta_0)}\right|. \end{aligned}$$

Here, the $\pm$-signs in the functions $f_+(\theta)$, $f_-(\theta)$ correspond to $\nu > 0$, $\nu < 0$, respectively; $t_0$ is an initial moment of time (integration constant). Note the limiting cases: (i) $f_\pm(\theta) \to -\infty$,

$t \to \infty$ as $\theta \to 0$; (ii) in the attractive field, the angle varies in the range $0 < \theta \leqslant \pi$ and $f_-(\theta)$ takes a finite value at $\theta = \pi$; (iii) in the repulsive field, $0 < \theta < \theta_{c0}$ and $f_+(\theta)$ is finite at $\theta \to \theta_{c0}$.

Similarly, for the scattered (distorted spherical) wave, equation (27) (lower sign) in the polar coordinates has the form

$$r = \frac{p}{1 - \cos(\theta - \theta_0/2)/\cos(\theta_0/2)} \qquad p = -\frac{\nu}{k}\tan^2(\theta_0/2). \tag{31}$$

Here, $\theta_0 \in (0, \pi)$ is a polar angle that specifies a direction of the hyperbolic trajectory asymptote: $r(\theta) \to \infty$ at $\theta \to \theta_0$. Depending on the sign of $\nu$, the trajectory is arranged in different sides from the asymptote line (see figure 1(*b*)). Thus, in the attractive field the polar angle changes in the range from $\theta_0$ to $\pi$. In addition, it appears that the trajectories with a polar angle $\theta_0$ and different azimuthal angles $\varphi_0$ converge to the focussing point, $z_{f1} = p/2 = \frac{\nu}{2k}\tan^2(\theta_0/2) \in l_-$. In contrast, in the repulsive field the polar angle changes in the interval $\theta_{c1} < \theta < \theta_0$ and the hyperbolic trajectory is tangent to the caustics line at point

$$r_{c1} = (2\nu/k)(1 + 0.25\tan^2(\theta_0/2)) \qquad \theta_{c1} = 2\arctan(0.5\tan(\theta_0/2)). \tag{32}$$

The dependence of the polar angle upon time can be established from the equation

$$f_{sc}(\theta) = -\frac{k^2}{\nu\tan^3(\theta_0/2)}(t - t_0) \tag{33}$$

$$\begin{aligned} f_{sc}(\theta) &= \int \mathrm{d}\theta\,[1 - \cos(\theta - \theta_0/2)/\cos(\theta_0/2)]^{-2} \\ &= -\frac{\cot^2(\theta_0/2)}{\cos^2(\theta_0/4)}\left(\frac{\tan((\theta - \theta_0/2)/2)}{\tan^2((\theta - \theta_0/2)/2) - \tan^2(\theta_0/4)}\right. \\ &\quad \left. + \frac{\cos(\theta_0/2)}{2\tan(\theta_0/4)}\ln\left|\frac{\tan((\theta - \theta_0/2)/2) - \tan(\theta_0/4)}{\tan((\theta - \theta_0/2)/2) + \tan(\theta_0/4)}\right|\right). \end{aligned}$$

Note the limiting cases. In the attractive field $\theta$ varies in the range $(\theta_0, \pi]$ and we obtain the following behaviour in passing to the boundary points: (i) at $\theta \to \theta_0 + 0$, when a particle goes to infinity along the trajectory asymptote, $f_{sc}(\theta) \to -\infty$, $t \to \infty$ and (ii) in the focusing point, $f_{sc}(\pi)$ is finite. In the repulsive field $\theta$ varies in the range $(\theta_{c1}, \theta_0)$ and we have the following asymptotic behaviour near the boundaries: (i) in the turning point, $f_{sc}(\theta)$ is finite and (ii) $f_{sc}(\theta) \to \infty$, $t \to -\infty$ at $\theta \to \theta_0 - 0$ (on the asymptote).

### 2.3. *Quantum-mechanical generalization*

Let us generalize now the results obtained in the eikonal approximation in order to take into consideration the effects related to the kinetic energy operator in equation (5). Formally replacing the eikonal distorting factors by the corresponding quantum-mechanical factors

$$F_{ej} = \exp(\mathrm{i}\varphi_c(\boldsymbol{k}_{23}^{(j)}(\boldsymbol{r}_{12}), \boldsymbol{r}_{23})) \to F_q(\nu_{23}^{(j)}, \zeta_{23}^{(j)})$$

gives the following generalization:

$$\Psi_{as}^- = \Psi_0^- + \Psi_1^- \tag{34}$$

$$\Psi_j^- = \exp(\mathrm{i}\boldsymbol{k}_{23}\boldsymbol{r}_{23} + \mathrm{i}\boldsymbol{K}_1\boldsymbol{R}_1)F_{qj}(\nu_{12}, \zeta_{12})F_e(\nu_{13}, \zeta_{13})F_q(\nu_{23}^{(j)}, \zeta_{23}^{(j)}) \tag{35}$$

where

$$\nu_{23}^{(j)} = \frac{Z_2 Z_3 m_{23}}{k_{23}^{(j)}(\boldsymbol{r}_{12})} \qquad \zeta_{23}^{(j)} = k_{23}^{(j)}(\boldsymbol{r}_{12}) r_{23} + \boldsymbol{k}_{23}^{(j)}(\boldsymbol{r}_{12}) \boldsymbol{r}_{23} \qquad j = 0, 1.$$

The quantum-mechanical distortion factor $F_q(\nu_{23}^{(j)}, \zeta_{23}^{(j)})$ is seen to satisfy equation (5) with the local momentum $\boldsymbol{k}_{23}^{(j)}$ up to the remainder

$$\delta F_q(\nu_{23}^{(j)}, \zeta_{23}^{(j)}) = \hat{h}_{12}^{(j)} F_q(\nu_{23}^{(j)}, \zeta_{23}^{(j)})$$

where

$$\hat{h}_{12}^{(j)} = -\tfrac{1}{2}\nabla_{r_{12}}^2 - \nabla_{r_{23}} \cdot \nabla_{r_{12}} - \mathrm{i}\boldsymbol{k}_{12}^{(j)}(\boldsymbol{r}_{12}) \cdot \nabla_{r_{12}}.$$

It follows in the limit $\xi_{12} \to \infty$ that $\delta F_q(\nu_{23}^{(0)}, \zeta_{23}^{(0)}) = \mathrm{O}(\xi_{12}^{-2})$ and $\delta F_q((\nu_{23}^{(1)}, \zeta_{23}^{(1)}) = \mathrm{O}(\xi_{12}^{-1})$. Besides, considering that $F_{q0}(\nu_{12}, \zeta_{12}) = \mathrm{O}(1)$, $F_{q1}(\nu_{12}, \zeta_{12}) = \mathrm{O}(\xi_{12}^{-1})$ at $\xi_{12} \to \infty$, as a result we obtain that the function (35) is an asymptotic solution of the Schrödinger equation in the region $\Omega_{23}$ up to the remainder term $\delta\Psi_j^- = \mathrm{O}(\xi_{12}^{-2})$.

If we set $\boldsymbol{k}_{23}^{(j)}(\boldsymbol{r}_{12}) \equiv \boldsymbol{k}_{23}$ in (35), then equations (34), (35) determine the CDW function. Note that in the limit $r_{12} \to \infty$ the unscattered part of the wavefunction, $\Psi_0^-$, goes over into the corresponding part of the CDW function, while the scattered part, $\Psi_1^-$, does not do the same since $\boldsymbol{k}_{23}^{(1)}(\boldsymbol{r}_{12})|_{r_{12}\to\infty} \neq \boldsymbol{k}_{23}$. Thus, the main feature that distinguishes the function (35), (36) from the CDW one consists in a modification of the electron momentum by the field of the scattered ion. As follows from the asymptotic behaviour of $\boldsymbol{k}_{23}^{(0)}(\boldsymbol{r}_{12})$, one can expect that the most strong deviation from the CDW description will be exhibited in the kinematic region where $k_{23} \leqslant |\nu_{12}|$. Moreover, the departure is expected to become more prominent as the projectile charge increases. At the same time, for the scattered part of the wavefunction the difference between the local and asymptotic momentum is seen to be proportional to $k_{12}$ to leading order and, hence, this part of the wavefunction will differ greater from the CDW one with increasing $k_{12}$.

Neglecting the second-order terms in the asymptotic region $\Omega_{23}$ where $r_{23} \ll r_{12}, R_1$, we can also reduce the function (35) to the form given earlier by Kunikeev and Senashenko (1996)

$$\begin{aligned} &\Psi_j^- = \psi_{\boldsymbol{k}_j(\boldsymbol{R}_1)}^-(\boldsymbol{r}_{23}) \exp(\mathrm{i}\boldsymbol{K}_1\boldsymbol{R}_1) F_{qj}(\nu_{12}, \zeta_{12}(\boldsymbol{R}_1)) F_e(\nu_{13}, \zeta_{13}(\boldsymbol{R}_1)) \\ &\zeta_{12}(\boldsymbol{R}_1) = k_{12}R_1 - \boldsymbol{k}_{12}\boldsymbol{R}_1 \qquad \zeta_{13}(\boldsymbol{R}_1) = k_{13}R_1 + \boldsymbol{k}_{13}\boldsymbol{R}_1 \end{aligned} \tag{36}$$

where $\psi_{\boldsymbol{k}_j(\boldsymbol{R}_1)}^-(\boldsymbol{r}_{23})$ is the Coulomb wavefunction of an electron moving in the Coulomb field of the residual ion with the local momentum $\boldsymbol{k}_j(\boldsymbol{R}_1) = \boldsymbol{k}_{23} + \mathrm{Re}\, \boldsymbol{u}_{12}^{(j)}(-\boldsymbol{R}_1)$.

Both the function (35) and (36) are correct asymptotic solutions in the region $\Omega_{23}$ with the exception of the singular direction where $\xi_{12} \leqslant r_{23}$, i.e. where $\hat{\boldsymbol{r}}_{12} \simeq -\hat{\boldsymbol{k}}_{12}$ or $\hat{\boldsymbol{R}}_1 \simeq \hat{\boldsymbol{k}}_{12}$. However, the function (35) seems to be more preferable because, in contrast to the representation (36), it passes into the well known exact expression for the wavefunction of the system of three particles, in which two particles are charged and a third one is neutral, when the charge of one of the particles $Z_1$ or $Z_3 \to 0$.

Near the singular direction, the corresponding asymptotic wavefunction containing the summed (12) or integral (13) correction terms to the phase can be used within the eikonal approximation. To go beyond the eikonal approximation, it is desirable to make an extension of the integration procedure along the broken quasiclassical trajectories which was used in section 2.1. To facilitate the task, we suppose that the local momentum in (5) depends only on time, i.e. we make an approximation, $\boldsymbol{k}_j(\boldsymbol{r}_{12}) \simeq \boldsymbol{k}_j(-\boldsymbol{R}_1(t)) = \boldsymbol{k}_j(t)$, up to terms of $\mathrm{O}(R_1^{-2})$. Then, the equation (5) can be rewritten in the form

$$(\hat{h}_{23} - \mathrm{i}\boldsymbol{k}_j(t) \cdot \nabla_{\boldsymbol{r}} - \mathrm{i}\partial_t) F_j(\boldsymbol{r}, t) = 0 \tag{37}$$

where

$$\hat{h}_{23} = -\tfrac{1}{2}\nabla_{\boldsymbol{r}}^2 + V_{23}$$

denotes the two-body Hamiltonian. We choose a large enough moment of time $t_0$ at which the momentum $\boldsymbol{k}_j(t)$ takes its asymptotic value and define the initial condition at that point:

$$F_j(\boldsymbol{r}, t_0) = F_{\boldsymbol{k}_j(t_0)}(\boldsymbol{r}) \tag{38}$$

where the two-body Coulomb distortion function $F_{\boldsymbol{k}}(\boldsymbol{r})$ with momentum $\boldsymbol{k}$ is defined by (16). Further, divide the time interval $(t_0, t)$ into $N$ subintervals such that $\boldsymbol{k}_j(t) \approx \boldsymbol{k}_j(t_i)$ on the $i$th interval $(t_{i-1}, t_i)$, $i = 1, \ldots, N$. Then, an approximate solution for (37) takes the form

$$F_j^{(N)}(\boldsymbol{r}, t) = \hat{U}^{(N)}(t, t_0)\, F_{\boldsymbol{k}_j(t_0)}(\boldsymbol{r}) \tag{39}$$

where the time-evolution operator

$$\hat{U}^{(N)}(t, t_0) = \hat{U}_N(t_N, t_{N-1}) \ldots \hat{U}_i(t_i, t_{i-1}) \ldots \hat{U}_1(t_1, t_0) \tag{40}$$

$$\hat{U}_i(t_i, t_{i-1}) = \exp(-\mathrm{i}\boldsymbol{k}_j(t_i)\boldsymbol{r}) \exp(-\mathrm{i}(\hat{h}_{23} - k_j^2(t_i)/2)(t_i - t_{i-1})) \exp(\mathrm{i}\boldsymbol{k}_j(t_i)\boldsymbol{r}) \tag{41}$$

describes evolution of the system in moving along the broken trajectory provided that $\hat{U}_i(t_i, t_{i-1})$ is a propagator on the time interval $(t_{i-1}, t_i)$. One can see that the propagator (41) is related to the two-body time-dependent Coulomb propagator for which an analytic, although involved, formula is found by Blinder (1991). In principle the formulae (39)–(41) give an analytic solution for the problem that generalizes the corresponding eikonal expressions. However, their direct calculation is a formidable task since the determination of (39) requires a $3N$-dimensional integration. Using the spectral representation of the propagator in terms of the complete set of eigenstates $\psi_\alpha$ of $\hat{h}_{23}$, we can rewrite equation (39) as

$$F_j^{(N)}(\boldsymbol{r}, t) = \exp\left( - \mathrm{i}\boldsymbol{k}_j(t) \cdot \boldsymbol{r} + \int_{t_0}^{t} \mathrm{d}\tau\, k_j^2(\tau)/2\right) \sum_{\alpha_N \ldots \alpha_1} \left( \prod_{i=1}^{N} a_{\alpha_i \alpha_{i-1}}(t_i, t_{i-1})\right) \psi_{\alpha_N}(\boldsymbol{r}) \tag{42}$$

where

$$a_{\alpha_i \alpha_{i-1}}(t_i, t_{i-1}) = \langle \psi_{\alpha_i} | \exp(\mathrm{i}(\boldsymbol{k}_j(t_i) - \boldsymbol{k}_j(t_{i-1}))\boldsymbol{r}) | \psi_{\alpha_{i-1}} \rangle \exp(-\mathrm{i}\epsilon_{\alpha_i}(t_i - t_{i-1})). \tag{43}$$

In deriving equation (42) the relation $\int_{t_0}^{t} \mathrm{d}\tau\, k_j^2(\tau)/2 \approx \sum_{i=1}^{N} (\frac{1}{2}) k_j^2(t_i)(t_i - t_{i-1})$ was used. The first factor in (42) represents the Volkov–Keldysh state (Keldysh 1965) which describes the motion of the unbound electron with definite value of momentum $-\boldsymbol{k}_{23}$ in the time-dependent field $\boldsymbol{E}_j(t) = \dot{\boldsymbol{k}}_j(t)$ produced by the projectile ion, while the second one is due to virtual transitions of the active electron in a superposition of the target and projectile fields. Summing in (42) is performed over discrete and continuum intermediate target states $\psi_{\alpha_1}, \ldots, \psi_{\alpha_N}$ ($\epsilon_{\alpha_i}$ is the eigenenergy of the state $\psi_{\alpha_i}$, $\psi_{\alpha_0} = \exp(\mathrm{i}\boldsymbol{k}_j(t_0)\boldsymbol{r}) F_{\boldsymbol{k}_j(t_0)}(\boldsymbol{r})$) and these intermediate contributions are induced by the stepped changes, $\Delta\boldsymbol{k}_j(t_i) = \boldsymbol{k}_j(t_i) - \boldsymbol{k}_j(t_{i-1})$, of the effective momentum $\boldsymbol{k}_j(t)$ when the state evolves from the initial moment of time $t_0$ up to $t$. The representation (42) can be referred to as an $N$-step (or $N$-order) asymptotic expansion of the distortion function $F_j$ into powers of small parameters $|\Delta\boldsymbol{k}_j(t_i)| \approx |\dot{\boldsymbol{k}}_j(t_i)| \cdot |t_i - t_{i-1}| \sim |\boldsymbol{E}_j(t_i)|$. The bound-state contributions, $F_{Bj}^{(N)}$, to the $N$-step distortion function (42) can be readily calculated since the transition matrix elements in the weighted coefficients (43) are evaluated analytically for hydrogen-like bound states.

Within the one-step approximation of (42) the continuum-state contribution writes as

$$F_{Cj}^{(1)}(\boldsymbol{r}, t_1) = \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi)^3} \exp(\mathrm{i}(p^2/2 - k_j^2(t_1)/2)(t_1 - t_0)) \exp(-\mathrm{i}\boldsymbol{k}_j(t_1)\boldsymbol{r}) |\psi_{\boldsymbol{p}}^-\rangle \times \langle \psi_{\boldsymbol{p}}^- | \exp(\mathrm{i}\boldsymbol{k}_j(t_1)\boldsymbol{r}') | F_{\boldsymbol{k}_j(t_0)}(\boldsymbol{r}') \rangle. \tag{44}$$

One can estimate a contribution from intermediate Coulomb continuum states $\psi_{\boldsymbol{p}}^-$ in the following way. If $\boldsymbol{k}_j(t_1) = \boldsymbol{k}_j(t_0)$, the matrix element in (44) is seen to be a $\delta$-function $\delta(\boldsymbol{p}-\boldsymbol{k}_j(t_1))$ and the operator $\hat{U}_1(t_1, t_0)$ does not change the initial function. At $\boldsymbol{k}_j(t_1) \neq \boldsymbol{k}_j(t_0)$, the matrix element has a $\delta$-like singularity $\sim \delta(\boldsymbol{p} - \boldsymbol{k}_j(t_1))$ and near the singularity we can approximate $\psi_{\boldsymbol{p}}^-(\boldsymbol{r}') \approx \exp(\mathrm{i}\boldsymbol{p}\boldsymbol{r}')F_{\boldsymbol{k}_j(t_1)}(\boldsymbol{r}')$ and $\epsilon_{\boldsymbol{p}} \approx k_j^2(t_1)/2 + (\boldsymbol{p} - \boldsymbol{k}_j(t_1)) \cdot \boldsymbol{k}_j(t_1)$ up to terms of second order. Then, integration over $\boldsymbol{p}$ gives a $\delta$-function $\delta(\boldsymbol{r} - \boldsymbol{r}' - \boldsymbol{k}_j(t_1)(t_1 - t_0))$ and (44) takes the form

$$F_{Cj}^{(1)}(\boldsymbol{r}, t_1) \approx F_{\boldsymbol{k}_j(t_1)}(\boldsymbol{r})F^*_{\boldsymbol{k}_j(t_1)}(\boldsymbol{r}')F_{\boldsymbol{k}_j(t_0)}(\boldsymbol{r}')|_{r'=r-\boldsymbol{k}_j(t_1)(t_1-t_0)}. \tag{45}$$

Similarly, using the approximation (45) on the subsequent segments of path, we obtain

$$\begin{aligned} F_{Cj}^{(N)}(\boldsymbol{r}, t) &\approx \prod_{i=1}^{N}(F_{\boldsymbol{k}_j(t_i)}(\boldsymbol{r}(t_i))F^*_{\boldsymbol{k}_j(t_i)}(\boldsymbol{r}(t_{i-1})))F_{\boldsymbol{k}_j(t_0)}(\boldsymbol{r}(t_0)) \\ &= F_{\boldsymbol{k}_j(t)}(\boldsymbol{r})\prod_{i=1}^{N}(F_{\boldsymbol{k}_j(t_{i-1})}(\boldsymbol{r}(t_{i-1}))F^*_{\boldsymbol{k}_j(t_i)}(\boldsymbol{r}(t_{i-1}))) \end{aligned} \tag{46}$$

where $\boldsymbol{r}(t_N = t) = \boldsymbol{r}$ and $\boldsymbol{r}(t_i) = \boldsymbol{r}(t_{i-1}) + \boldsymbol{k}_j(t_i)(t_i - t_{i-1})$ at $i = 1, \ldots, N$. If we replace $F_{\boldsymbol{k}}$ by the corresponding eikonal distortion function, $F_{\boldsymbol{k}}^{(e)}$, equation (46) reduces to a phase factor where the phase function is determined by equation (10) with local momentum $\boldsymbol{k}_j(t)$. Neglecting an additional phase shift which is due to the momentum changes during the motion along the broken trajectory consisting of straight-line segments and replacing again $F_{\boldsymbol{k}}^{(e)} \to F_{\boldsymbol{k}}$, we arrive at the scattering state (Kunikeev and Senashenko 1996).

## 3. The ionization DDCS

We consider now the single ionization process

$$I^{Z_1} + A(i) \to I^{Z_1} + A^+(f) + \mathrm{e}^-(E_e, \theta_e) \tag{47}$$

where a heavy ion $I^{Z_1}$ of charge $Z_1$ hits an atom $A(i)$, as a result of which one electron $\mathrm{e}^-$ (called active) is ionized while the other electrons (called passives) remain in the same state during the collision.

In the entry channel, the initial state is proposed to be the boundary-corrected Born (B1B, Dewangan and Eichler 1994) wavefunction. As an exact final state, we take the three-body asymptotic wavefunction in the form (36). Then, the ionization DDCS as a function of the active electron ejection angle $\theta_e$ and energy $E_e$ results in

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E_e\mathrm{d}\Omega_e} = v_e \int \mathrm{d}^2\boldsymbol{b}\, P(\boldsymbol{b}) \tag{48}$$

where the ionization probability, $P(\boldsymbol{b})$, as a function of impact parameter vector is defined as

$$P(\boldsymbol{b}) = \left| \int_{-\infty}^{\infty} \mathrm{d}t\, A_{fi}(t, \boldsymbol{b}) \right|^2 \tag{49}$$

$$A_{fi}(t, \boldsymbol{b}) = A_0(t, \boldsymbol{b}) + A_1(t, \boldsymbol{b}) \tag{50}$$

$$A_j(t, \boldsymbol{b}) = a_j(\boldsymbol{R})F^*_{qj}(\nu_{12}, \zeta_{12}(\boldsymbol{R}))F^*_{e0}(\nu_{13}, \zeta_{13}(\boldsymbol{R}))\exp(\mathrm{i}(E_e - \epsilon_i)t) \tag{51}$$

$$a_j(\boldsymbol{R}) = \left\langle \psi^-_{\boldsymbol{k}_j(\boldsymbol{R})}(\boldsymbol{r}) \left| \frac{-Z_1}{|\boldsymbol{r} - \boldsymbol{R}|} \right| \varphi_i(\boldsymbol{r}) \right\rangle. \tag{52}$$

Here, $A_j(t, \boldsymbol{b})$ at $j = 0, 1$ determines a separate contribution to the total ionization amplitude from the waves that are not and are rescattered by projectile ion, respectively; $a_j(\boldsymbol{R})$ is the matrix element of ionization transition as a result of which an electron with momentum $\boldsymbol{k}_j(\boldsymbol{R})$ is in the continuum; $\epsilon_i$ is the binding energy of the initial bound state $\varphi_i$, $v_e = \sqrt{2E_e}$, $\boldsymbol{R} = \boldsymbol{b}+\boldsymbol{v}t$. Note that we could also substitute a more general form of the final-state wavefunction including contributions due to changing of the local momentum in moving along the broken trajectories. In this case, the general structure of the amplitudes (50), (51) was the same, but the ionization matrix element (52) should be altered, namely, $\psi^-_{\boldsymbol{k}_j(\boldsymbol{R})}(\boldsymbol{r}) \to \exp(\mathrm{i}\boldsymbol{k}_j(\boldsymbol{R})r)F_j^{(N)}(\boldsymbol{r}, t)$ where $F_j^{(N)}(\boldsymbol{r}, t)$ is defined by (42).

Expanding the Coulomb wavefunction and interaction potential in (52) into a partial wave series and integrating over angular coordinates, we obtain the following partial wave expansion of the matrix element

$$a_j(\boldsymbol{R}) = \sum_{l=0}^{\infty}(-\mathrm{i})^l \exp(\mathrm{i}\delta_{cl}(k_j))\, f_l(k_j, R) P_l(\hat{\boldsymbol{k}}_j \cdot \hat{\boldsymbol{R}}). \tag{53}$$

Here, $\delta_{cl}(k)$ is the Coulomb partial wave phase; $f_l(k, R)$ is the radial matrix element:

$$f_l(k, R) = -4\pi Z_1 \int_0^{\infty} r^2 \mathrm{d}r\, R_{kl}(r) \frac{r_<^l}{r_>^{l+1}} \varphi_i(r) \tag{54}$$

where $R_{kl}(r)$ is the radial wavefunction of an electron moving in the Coulomb field of the residual ion of charge $Z_3 = 1$ with momentum $k$ and orbital momentum $l$; $r_< = r$ $(r_> = R)$ if $r < R$ or $r_< = R$ $(r_> = r)$ if $r > R$.

The radial integral (54) with the bound state wavefunction $\varphi_i(r) = N_\alpha \exp(-\alpha r)$, where $N_\alpha$ is the normalization constant, can conveniently be represented as a sum of two terms

$$f_l(k, R) = f_l^{as}(k, R) + f_l^{\exp}(k, R) \tag{55}$$

where

$$f_l^{as}(k, R) = C_l(k) \frac{2k^l(2l+1)!(\alpha(l+1)+\nu k)}{(k^2+\alpha^2)^{l+2}R^{l+1}} \exp(2\nu \arctan(k/\alpha)) \tag{56}$$

$$f_l^{\exp}(k, R) = -C_l(k)(kR)^l \left( (2l+1)I_{2l}(k, R) + \sum_{n=2}^{2l+2} \frac{(2l+2)!}{(2l+2-n)!R^{n-1}} I_{(n+1)l}(k, R) \right) \tag{57}$$

$$\begin{aligned} I_{nl}(k, R) &= \frac{(2l+1)!}{|\Gamma(l+1-\mathrm{i}\nu)|^2} \int_0^1 \mathrm{d}t\, t^{l-\mathrm{i}\nu}(1-t)^{l+\mathrm{i}\nu} \frac{\exp(-(\alpha+\mathrm{i}k-2\mathrm{i}kt)R)}{(\alpha+\mathrm{i}k-2\mathrm{i}kt)^n} \\ C_l(k) &= -4\pi Z_1 N_\alpha \frac{2^l \exp(-\pi\nu/2)|\Gamma(l+1+\mathrm{i}\nu)|}{(2l+1)!} \qquad \nu = -Z_3/k. \end{aligned} \tag{58}$$

The first term in expansion (55) determines an asymptotic behaviour of $f_l(k, R)$ as $R \to \infty$ since the second one decays as $\exp(-\alpha R)/R$. Thus, we can neglect a contribution of the exponentially small integral term (57) at large enough values of $R > R_{\max}$ where $R_{\max}$ is some internuclear separation, whereas in the range $0 \leqslant R < R_{\max}$, both terms are values of the same order and their contributions should be taken into account simultaneously. However, an expansion of the form (55) turns out to be inconvenient for making a direct calculation of the radial matrix element in the range $0 \leqslant R < R_{\max}$ because both the asymptotic and integral terms are singular as $R \to 0$ while their sum remains finite in the same limit. In order to obtain an appropriate expression, we develop an exponential in the integrand of (58) as a series in powers of $R$. Then the integral over $t$ can readily be evaluated and after collecting like terms an expression for $f_l(k, R)$ can be derived in the closed form

$$\begin{aligned} f_l(k, R) = C_l(k)(kR)^l \Bigg[ &(\alpha+\mathrm{i}k)^{-2}{}_2F_1\left(l+1-\mathrm{i}\nu, 2, 2l+2, \frac{2\mathrm{i}k}{\alpha+\mathrm{i}k}\right) \\ &-(2l+1)R^2 \sum_{m=0}^{\infty} \frac{(-R)^m}{m!} \frac{(\alpha+\mathrm{i}k)^m}{(m+2)(m+2l+3)} \end{aligned}$$

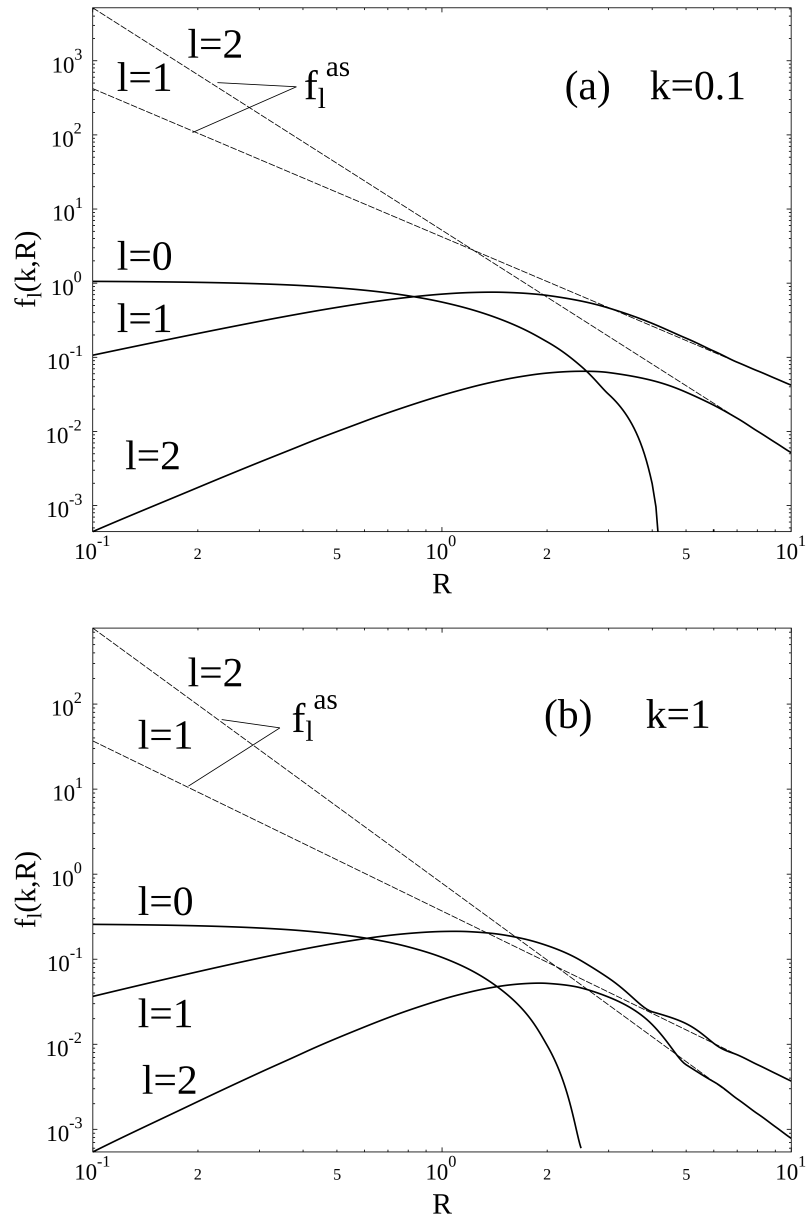


**Figure 2.** The radial matrix element, $f_l(k, R)$, at $k = 0.1$ ($a$) and $k = 1$ ($b$) and different values of $l = 0, 1, 2$ as a function of $R$.

$$\times\, {}_2F_1\left(l + 1 - \mathrm{i}\nu, -m, 2l + 2, \frac{2\mathrm{i}k}{\alpha + \mathrm{i}k}\right)\Bigg] \qquad (59)$$

where ${}_2F_1(a, b, c, z)$ is the hypergeometric function.

As an example, we plot $f_l(k, R)$ at $k = 0.1$ (figure 2($a$)) and $k = 1$ (figure 2($b$)) and different values of $l = 0, 1, 2$ as a function of $R$. One can see that the main contribution to the asymptotic behaviour at $R \to \infty$ gives the dipole wave ($l = 1$), whereas at $R \to 0$

the monopole wave ($l = 0$) contribution is leading. As momentum $k$ increases, contributions from the higher partial waves become more prominent. Note that $f^{as}_{l=0}(k, R) = 0$ because $\alpha = Z_3 = 1$ is chosen and the functions $R_{kl}(r)$ and $\varphi_i(r)$ are orthogonal. Besides, we cannot approximate $f_l(k, R)$ by $f^{as}_l(k, R)$ in the range $0 \leqslant R < R_{\max}(k, l) \simeq 5$ because of a poor agreement between them in that range.

Thus, we have reduced the problem to calculate the ionization DDCS with the final-state wavefunction (36) to a three-dimensional integration (one integration over the time and two integrations over the impact parameter and the azimuthal angle). Equations (48)–(59) make it possible to investigate in detail the three-body effects due to the momentum modification $\boldsymbol{k}_j(\boldsymbol{R})$ by the projectile field as well as the rescattering effects. Examples of such an investigation can be found in (Kunikeev 1998b).

## 4. Summary and conclusions

The presented analysis of the three-body Coulomb continuum state clearly demonstrates that in the asymptotic region $\Omega_{ij}$ where two particles $(i, j)$ are close to one another while a third one $k$ is far away from the pair the asymptotic state cannot be adequately reproduced in terms of separate two-body subsystems since the momentum of the pair is modified by a long-range Coulomb field of the third particle and thereby the interaction in one pair of particles is transferred to another pair through the field-modified local momenta. The problem is examined within the quasiclassical eikonal, WKB and quantum mechanical formalisms. It should be clear, in particular, that the derived expressions for the eikonal phase factor (10) or for the quantum-mechanical distortion function (42) incorporate intermediate contributions due to changes of the local momentum in moving a particle from the asymptotic region along the curved characteristic trajectories to the inner or reaction zone. Apparently, such an integral information enables one to give a better account of the reaction zone. Moreover, some integral conditions are formulated under which the intermediate contributions can be ignored.

The derived asymptotic scattering states can be used to treat a fragmentation process. We have obtained analytical expressions (48)–(59) for the amplitude and the DDCS for ionization of an atom by ion impact with the final-state wavefunction (36). The remaining three-dimensional integral should be evaluated numerically.

In closing, we note that the above results obtained for the three-body Coulomb continuum states can be extended to the bound-state problem, i.e. to the bound state of a target electron in the field of an incident projectile ion (Kunikeev 1998a).

## Acknowledgment

This research is supported in part by the National Program Russia Universities—Basic Problems grant no 98-1.5247.

## References

Alt E O and Mukhamedzhanov A M 1992 *Sov. Phys.–JETP Lett.* **56** 435
——1993 *Phys. Rev.* A **47** 2004
Belkić Dž 1978 *J. Phys. B: At. Mol. Phys.* **11** 3529
Blinder S M 1991 *Phys. Rev.* A **43** 13
Brauner M, Briggs J S and Klar H 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2265
Dewangan D P and Eichler J 1994 *Phys. Rep.* **247** 59
Keldysh L V 1965 *Sov. Phys.–JETP* **20** 1307
Kim Y E and Zubarev A L 1997 *Phys. Rev.* A **56** 521

Kunikeev Sh D 1998a *J. Phys. B: At. Mol. Opt. Phys.* **31** L849
——1998b *J. Phys. B: At. Mol. Opt. Phys.* **31** 2649
——1997 *Nucl. Instrum. Methods* B **124** 350
Kunikeev Sh D and Senashenko V S 1996 *Sov. Phys.–JETP* **82** 839
Merkuriev S P 1977 *Theor. Math. Phys.* **32** 680
Mukhamedzhanov A M and Lieber M 1996 *Phys. Rev.* A **54** 3078
Peterkop R K 1977 *Theory of Ionization of Atoms by the Electron Impact* (Boulder, CO: Colorado Associated University Press)
Rosenberg L 1973 *Phys. Rev.* D **8** 1833