Three-particle Coulomb effects in autoionization phenomena

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A wave function possessing the correct asymptotic behavior in the region of configuration space where two particles are only slightly separated and a third is located far away is constructed for a system of three nonrelativistic asymptotically free charged particles. It is shown that the effect of the long-range Coulomb field of the third particle on the motion of the weakly separated pair of particles modifies the momentum of their relative motion—the momentum becomes a three-particle momentum which depends on the position and characteristics of the motion of the third particle. In addition, the modification of the momentum is different for terms in the expansion of the wave function which do and do not account for the rescattering of the third particle by the particles in the pair; this is important in order to obtain the correct asymptotic behavior of the wave function. The wave function constructed is used to calculate the profile of the $(2s^2)^1S$ and $(2s2p)^1P$ autoionization resonances excited in the helium atom by protons, $^3He^+$ ions, and antiprotons with energies from 10 to 50 keV. The effect of the three-particle postcollision interaction on the shape of the resonance lines for small angles of ejection of the autoionization electrons is investigated. It is shown that the additional peak observed experimentally in the low-energy wing of the $(2s^2)^1S$ resonance in the spectra of the electrons ejected at an angle of 5° in collisions of 10 keV $^3He^+$ ions with He atoms is due to the interference of waves corresponding to electrons which are and are not rescattered by the $^3He^+$ ion. A new three-particle interference effect was discovered—under certain kinematic conditions an additional structure can also appear in the low-energy wing of the nonisotropic resonance for negatively charged particles (antiprotons). [S1063-7761(96)00605-1]

1. INTRODUCTION

Inelastic collisions of charged particles are often accompanied by the excitation of autoionized states or the formation of vacancies in the inner electronic shells of the atoms. The emission of an autoionization or Auger electron occurs with high probability as a result of nonradiative decay of the highly excited states which are formed. Under certain kinematic conditions the charged particles formed in the final state can interact strongly with one another, which greatly affects their angular and energy distributions. Characteristic manifestations of the interaction are a broadening and shift of the resonance lines in the autoionization-electron spectra, first observed by Barker and Berry in slow collisions of He^+ and Ne^+ ions with He atoms.[1] The diverse manifestations of the interaction of charged particles in the final state for processes proceeding via intermediate resonance states were subsequently investigated intensively both experimentally and theoretically.[2–4] In the literature such studies are known postcollision interaction (PCI) investigations.

Various theoretical models for taking into account the PCI have been proposed to describe the observed postcollisional phenomena. For example, near threshold, when the velocity v of the scattered particle is much lower than the velocity v_e of the autoionization electron ($v \ll v_e$) and the angle of divergence of the particles is large and their interaction with one another can be neglected, the PCI is determined by the interaction of the scattered particle and the residual target ion (the interaction of the autoionization electron with the residual target ion is traditionally not considered to be a PCI, which is determined by the interaction of the scattered particle with the products of the decay of the ionization resonance). For this reason, the theoretical models developed in this field for taking into account the PCI, such as the classical Barker–Berry model,[1] the semiclassical model,[5,6] the quantum-mechanical model,[7] the quasimolecular adiabatic approach,[8] and others, are limited to a description of the two-particle postcollision effects.

As the velocity of the scattered particle increases or for small angles of divergence of the charged particles, their motion is strongly affected by the interaction of the autoionization electron and the scattered particle. This makes it necessary to take into account the three-particle Coulomb dynamics in the final state—three-particle PCI, most strongly manifested when the velocities of the diverging particles are close in magnitude and direction. The key point in the solution of this problem is describing correctly the wave function of the final state of the system.

In Refs. 9–11 an asymptotic wave function consisting of the product of three-particle plane waves and distorting Coulomb factors, expressed in terms of degenerate hypergeometric functions, and describing the relative motion of the interacting pairs of particles in the continuum, was used to describe the final-state scattering dynamics of the three particles formed in the decay of autoionization resonances. The use of such a wave function for describing the final state is justified in the case when all distances between the pairs of particles approach infinity, except in directions for which one or more vectors determining the relative position of the particle pairs are parallel to the corresponding canonically conjugate momenta. In Refs. 12 and 13 an analogous wave function obtained in the continuum distorted wave (CDW) approximation was used to describe the three-particle PCI.

For slow collisions, in which the interaction of an autoionization electron and the scattered particle can be neglected, the analytic expression obtained in Ref. 9 for the amplitude of autoionization decay of atomic resonances simplifies to the form obtained in Ref. 8. For sufficiently large angles of divergence of the charged particles in the final state, when the interaction energy of the receding particles is less than the kinetic energy of their relative motion, the autoionization amplitude obtained in Ref. 9 simplifies to the expression obtained previously in Refs. 14 and 15 in the simplest semiclassical eikonal approximation. When the effect of the three-particle PCI is large (an electron is ejected close to the direction of the receding scattered particle with velocity higher than the projectile velocity), the quantum-mechanical description of the ionization[9–11] predicts large changes, which are absent from the semiclassical eikonal theory of Refs. 14 and 15, in the intensity and shape of the resonance line:[9] The intensity of the resonance increases sharply at small ejection angles as a result of the capture of an autoionization electron in the continuum of the scattered particle and an additional peak appears in the left-hand wing of the resonance for small ejection angles $\theta_c \simeq 1-5°$ as a result of the rescattering of some autoionization electrons by a scattered particle.[10]

Recent experimental investigations of autoionization[16,17] and Auger[18] resonances in ion–atom collisions have confirmed the existence of these three-particle PCI effects. In Ref. 16 the increase in the intensity of electrons in the forward direction is interpreted as being the result of "focusing" of electrons in the Coulomb field of the receding ion and in Ref. 17 the appearance of the additional peak in the left-wing of the resonance is interpreted as resulting from the interference of two coherent amplitudes corresponding to two possible different classical trajectories of the autoionization electron in the field of the receding ion. It should be kept in mind, however, that even though the quantum-mechanical models of Refs. 9–13 predict a sharp increase in the intensity of the resonance at small ejection angles, the increase found in the electron emission in some directions is not accompanied by a decrease in the electron emission in other directions with the integrated yield of the resonance being conserved, i.e. the theoretical models which take into account the PCI[9–13] are substantially nonunitary. A quantum-mechanical model of the PCI that is unitary in the diagonalization approximation and reproduces the "Coulomb focusing" effect was developed in Ref. 19. In addition, to describe the "Coulomb focusing" effect systematically the PCI in the final and intermediate resonance states must be taken into account simultaneously.

Moreover it turns out that the theoretical models developed for taking into account three-particle PCI[9–13] predict the appearance of additional structure on the left-hand wing of the resonance only for positively charged scattered particles. When a negatively charged particle, for example, a scattered electron or antiproton, is present in the final state no additional structure appears in the profile of the resonance. At the same time such structure was observed in an experiment[20] where the shape of the $L_3-M_{2,3}^2(^1D_2)$ line in the spectra of Auger electrons ejected from an argon atom in a collision with electrons was investigated. The authors attributed this effect to the strong interaction between the initially ejected electron (as a result of whose ejection a vacancy is formed in an inner shell of the atom) and the Auger electron, since the energy of the ejected electron ($E_{ej}=207$ eV) was chosen to be close to the energy of the Auger electron ($E_{Aug}=203.4$ eV), and the energy of the scattered electron was much higher ($E_{sc}=750$ eV). In the calculations performed in Ref. 21 on the basis of the approximations used in Refs. 9–13 no structure was found on the low-energy shoulder of the Auger line. This discrepancy between theory and experiment is motivating the further elaboration of our ideas about the dynamics of the PCI of the receding particles.

A serious deficiency, characteristic of all preceding theoretical models which take into account the three-particle PCI, should be noted in this connection: A wave function that has the wrong asymptotic behavior in the region of configuration space where two particles are close to one another and a third particle is located far away from the pair is used to describe the final state. At the same time, in calculating the decay amplitude of the autoionization resonance the integration over the coordinates of the separating receding was performed over the entire configuration space of the system, including the asymptotic region where the particle pair—the autoionization electron and the residual target ion—are close to one another the scattered particle is located far away from their center of mass. It appears that this region make the main contribution to the amplitude is present in the decay matrix element, since the decay matrix element contains the exponentially decaying wave function of the excited bound state of the autoionization electron and the residual target ion. In Refs. 22 and 23 an attempt was made to construct the asymptotic solution of the three-particle Schrödinger equation in the indicated asymptotic region. As will be shown below, however, the wave function obtained in Refs. 22 and 23 taking into account the Coulomb rescattering of the particle pairs has the wrong asymptotic behavior in the region of configuration space which is of interest to us.

Our objective in the present work is to construct the wave function of a system of three asymptotically free charged particles that possesses the correct asymptotic behavior in the region of configuration space where two particles are located close to one another and the third particle is located far away, to calculate, using the wave function obtained, the profile of the lowest autoionization resonances excited in the helium atom by ions, and to investigate the effect of the three-particle PCI on the shape of the resonance lines.

In Sec. 2, first, a more precise formulation of the problem is given and then the correct asymptotic solution of Schrödinger's equation is constructed. It is found that when the effect of the long-range Coulomb field of the distant particle on the motion of the weakly separated pair of particles is taken into account, the "local" momentum of the relative motion of the particles in the pair is different from the asymptotic value. In Sec. 3 the stationary-phase method is used to calculate the decay amplitude of the autoionization resonance. In Sec. 4 the expression obtained for the decay amplitude of an isolated resonance is used to investigate quantitatively the effect of the three-particle PCI on the shape of the $(2s^2)^1S$ and $(2s2p)^1P$ autoionization resonances excited in the helium atom in a collision with 10–50 keV protons, $^3He^+$ ions, and antiprotons for small ejection angles. It is proved directly that the additional peak observed experimentally in Ref. 17 on the left-hand wing of the $(2s^2)^1S$ resonance for small ejection angles and 10 keV $^3He^+$ is associated with the rescattering of some autoionization electrons by the scattered ion. In addition, the effective charge $Z_{\rm eff}$ of the $^3He^+$ ion, determined by the incomplete screening of the nuclear charge of the ion by the bound electron in the process of rescattering of autoionization electrons by the $^3He^+$ ion (if $Z_{\rm eff}=1$, then no additional structure arises in the profile of the resonance), plays a large role in the formation of this structure in the profile of the resonance.

An investigation of the effect of the sign of the charge of the incident particle on the ionization of the atom is a rapidly developing direction of study of the dynamics of different elementary processes in atomic-collision physics.[24–26] The dependence of the profile of the autoionization resonances on the sign of the charge of the exciting particle ($p^{\pm}$) is investigated in Sec. 4. For antiprotons, a new effect due to the three-particle PCI, which does not occur in previous PCI models, has been observed[9–13]: for small angles of ejection of the electron, an additional interference peak appears on the low-energy side of the profile of the nonisotropic resonance. It is shown that this effect arises as a result of the influence of the scattered charged particle on the motion of the autoionization electron at the moment it is transferred into the continuous spectrum.

Some of the results obtained in the present work in application to Auger processes were reported at the 19th International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC).[27] The atomic system of units is used throughout this work, with the exception of some explicitly indicated cases where different units are employed.

2. CONSTRUCTION OF THE WAVE FUNCTION OF THREE ASYMPTOTICALLY FREE CHARGED PARTICLES

Let us consider a system of three nonrelativistic quantum particles with charge Z_i and mass m_i ($i=1,2,3$). The Hamiltonian of the system has the form

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

where $m_{ij}=m_im_j/(m_i+m_j)$ and $\mu_1=m_1(m_2+m_3)/(m_1+m_2+m_3)$ are the reduced masses, $\mathbf{r}_{ij}$ are the relative coordinates of the particle pair (i,j), and $\mathbf{R}_1$ are the coordinates of particle 1 with respect to the center of mass of the particle pair (2,3). In the region Ω_0 where all three particle pairs are well separated ($r_{12}\sim r_{22}\sim r_{13}\gg 1$), the asymptotic wave function Ψ^-_{as} away from the direction of three-particle forward scattering can be determined in factorized form:[28]

$$\Psi^-_{as}=\exp(i\mathbf{k}_{23}\mathbf{r}_{23}+i\mathbf{K}_1\mathbf{R}_1)\prod_{i<j=1}^{3} F_q(\nu_{ij},\xi_{ij}),$$

$$F_q(\nu,\xi)=\exp(-\pi\nu/2)\Gamma(1-i\nu)\,{}_1F_1(i\nu,1,-i\xi),$$

$$\nu_{ij}=\frac{Z_iZ_jm_{ij}}{k_{ij}},\quad \xi_{ij}=k_{ij}r_{ij}+\mathbf{k}_{ij}\mathbf{r}_{ij}, \tag{2}$$

where $\mathbf{k}_{ij}$ and $\mathbf{K}_1$ are the momenta which are canonically conjugate to the coordinates $\mathbf{r}_{ij}$ and $\mathbf{R}_1$; ${}_1F_1(a,c,z)$ is the confluent hypergeometric function that is regular at the origin; and, $\Gamma(z)$ is the gamma function. We operate on the wave function Ψ^-_{as} with the operator $\hat{H}-E$, where $E=k_{23}^2/2m_{23}+K_1^2/2\mu_1$ is the total energy of the system. As a result, we obtain the following expression for $\delta\Psi^-_{as}\equiv(\hat{H}-E)\Psi^-_{as}$ (if the solution is exact, then $\delta\Psi^-_{as}\equiv 0$):

$$\delta\Psi^-_{as}=-\exp(i\mathbf{k}_{23}\mathbf{r}_{23}+i\mathbf{K}_1\mathbf{R}_1)(1+\hat{P}_{231}+\hat{P}_{321})\frac{1}{m_1}F_q \times(\nu_{23},\xi_{23})\nabla_{\mathbf{r}_{12}}F_q(\nu_{12},\xi_{12})\cdot\nabla_{\mathbf{r}_{13}}F_q(\nu_{13},\xi_{13}), \tag{3}$$

where the symbols $\hat{P}_{231}$ and $\hat{P}_{321}$ are cyclic permutation operators in the particle numbers. We represent the quantum-mechanical distortion factor of the continuum states for a pair of particles as the sum

$$F_q(\nu,\xi)=F_{q0}(\nu,\xi)+F_{q1}(\nu,\xi), \tag{4}$$

where

$$F_{q0}(\nu,\xi)=\exp\left(\frac{\pi\nu}{2}\right)G(i\nu,1,-i\xi),$$

$$F_{q1}(\nu,\xi)=i\nu\frac{\Gamma(-i\nu)}{\Gamma(i\nu)}\exp\left(\frac{\pi\nu}{2}\right)\exp(-i\xi)G(1-i\nu,1,i\xi).$$

Here $G(a,c,z)$ is the confluent hypergeometric function that is irregular at the origin. We note that all three functions in the expansion (4) are solutions of the same confluent hypergeometric equation, two of the three solutions being linearly independent. It follows from the asymptotic behavior of the function $G(a,c,z)$ in the limit $|z|\to\infty$ that to terms $\sim\xi^{-1}$

$$F_q(\nu,\xi)=F_{e0}(\nu,\xi)+F_{e1}(\nu,\xi)$$
$$=\exp(-i\nu\ln\xi)(1+i\nu^2/\xi)+\nu\frac{\Gamma(-i\nu)}{\Gamma(i\nu)}\exp(-i\xi+i\nu\ln\xi)/\xi,$$

$$dF_q(\nu,\xi)/d\xi=dF_{e0}(\nu,\xi)/d\xi+dF_{e1}(\nu,\xi)/d\xi$$
$$=-i\nu\exp(-i\nu\ln\xi)/\xi-iF_{e1}(\nu,\xi). \tag{5}$$

The asymptotic expansions (5) give the eikonal representations for the quantum-mechanical functions: $F_{q0(1)}(\nu,\xi)\to F_{e0(1)}(\nu,\xi)$. The term $F_{q0}(\nu,\xi)$, which makes the main contribution to the asymptotic behavior of $F_q(\nu,\xi)$, represents particles which have not been rescattered, and the term $F_{q1}(\nu,\xi)$, which is asymptotically proportional to the Coulomb two-particle rescattering amplitude, describes single collisions of a pair of particles. We underscore the fact that if $F_{e0}(\nu,\xi)=O(1)$ compared to $F_{e1}(\nu,\xi)=O(\xi^{-1})$, then their derivatives $dF_{e0(1)}(\nu,\xi)/d\xi$ are infinitesimals of the same order in ξ^{-1}. Since

$$\nabla_{\mathbf{r}}F_q(\nu,\xi)=\frac{dF_q(\nu,\xi)}{d\xi}\,k(\hat{\mathbf{r}}+\hat{\mathbf{k}}),\quad \hat{\mathbf{k}}=\mathbf{k}/k, \tag{6}$$

we obtain from Eqs. (3) and (5) that $(\hat{H}-E)\Psi_{as}^{-}=O(\xi^{-2})$, if all $\xi_{ij}\sim\xi\to\infty$, i.e. the function (2) is an asymptotic solution of the Schrödinger equation in the region Ω_0 away from the singular directions.

In the region Ω_{23}, where the variable ξ_{23} is bounded or does not approach infinity rapidly enough, $|\nabla_{\mathbf{r}_{23}}F_q(\nu_{23},\xi_{23})|\sim O(1)$ or $\sim O(\xi^{-\varepsilon})$, where $0\leqslant\varepsilon<1$ is sufficiently small, and the function (2) is no longer an asymptotic solution, since $\delta\Psi_{as}^{-}\sim O(\xi^{-1-\varepsilon})$ decreases with distance relatively slowly (for $\varepsilon=0$ as the Coulomb interaction potential). The terms F_{q0} and F_{q1} in the expansion (4) make contributions of the same order of magnitude to the slow decrease of $\delta\Psi_{as}^{-}$. Therefore in constructing the asymptotic wave function Ψ_{as}^{-} in the region Ω_{23} the contribution of the corresponding terms responsible for waves that are and are not rescattered must be taken into account at the same time.

In the region Ω_{23} an asymptotic solution exists in the form

$$\Psi_{as}^{-}=\exp(i\mathbf{k}_{23}\mathbf{r}_{23}+i\mathbf{K}_1\mathbf{R}_1)F_q(\nu_{23},\xi_{23})F_q(\nu_1,\xi_1),$$

$$\nu_1=\frac{Z_1(Z_2+Z_3)\mu_1}{K_1},\quad \xi_1=K_1R_1+\mathbf{K}_1\mathbf{R}_1, \tag{7}$$

which is obtained by expanding the interaction potentials in the Schrödinger equation with respect to the small parameter r_{23}/R_1 in the region Ω_{23}: $V_{12}+V_{13}=Z_1(Z_2+Z_3)/R_1+O(r_{23}/R_1^{-2})$. However, the asymptotic solution (7) does not "match" the asymptotic solution (2) at the boundary of the regions Ω_0 and Ω_{23}. Therefore it must be ensured that the asymptotic wave function in the region Ω_{23} is a direct continuation of the function (2).

Using the expansion (4), we seek an asymptotic solution of the Schrödinger equation in the region Ω_{23} in the following form:

$$\Psi_{as}^{-}=\Psi_0^{-}+\Psi_1^{-}, \tag{8}$$

where

$$\Psi_0^{-}=\psi_{\mathbf{k}_{23}}^{-}(\mathbf{r}_{23})\exp(i\mathbf{K}_1\mathbf{R}_1)F_{q0}(\nu_{12},\xi_{12})F_{q0}(\nu_{13},\xi_{13}), \tag{9}$$

$$\Psi_1^{-}=\psi_{\mathbf{k}_{23}}^{-}(\mathbf{r}_{23})\exp(i\mathbf{K}_1\mathbf{R}_1)(F_{q1}(\nu_{12},\xi_{12})F_{q0}(\nu_{13},\xi_{13})+F_{q0}(\nu_{12},\xi_{12})F_{q1}(\nu_{13},\xi_{13})). \tag{10}$$

Here we have collected terms referring to unscattered Ψ_0^{-1} and scattered Ψ_1^{-} waves. We neglected the term corresponding to double rescattering of the particle pairs (1,2) and (1,3), since in the asymptotic region Ω_{23} (away from the singular directions, where $\hat{\mathbf{r}}_{12}=-\hat{\mathbf{k}}_{12}$ and/or $\hat{\mathbf{r}}_{13}=-\hat{\mathbf{k}}_{13}$), $\xi_{12}\sim\xi_{13}\sim R_1\gg 1$ and, as follows from Eq. (5), $F_{q1}(\nu_{12},\xi_{12})F_{q1}(\nu_{13},\xi_{13})=O(R_1^{-2})$—a second-order infinitesimal, while $F_{q0}(\nu_{12},\xi_{12})F_{q0}(\nu_{13},\xi_{13})=O(1)$ and $F_{q1}(\nu_{12},\xi_{12})F_{q0}(\nu_{13},\xi_{13})=O(R_1^{-1})$—a first-order infinitesimal. The wave function $\psi_{\mathbf{k}_{23}}^{-}(\mathbf{r}_{23})=\exp(i\mathbf{k}_{23}\cdot\mathbf{r}_{23})F_q(v_{23},\xi_{23})$ in Eqs. (9) and (10) satisfies the Schrödinger equation for the particle pair (2,3)

$$\left(-\frac{1}{2m_{23}}\nabla_{\mathbf{r}_{23}}^2+V_{23}-\frac{k_{23}^2}{2m_{23}}\right)\psi_{\mathbf{k}_{23}}^{-}(\mathbf{r}_{23})=0. \tag{11}$$

To simplify the calculations, in what follows, without loss of generality, we shall take into account rescattering only for the particle pair (1,2), dropping the analogous terms corresponding to the rescattering of the particle pair (1,3). Using the asymptotic representation (5), we write the wave functions Ψ_0^{-} and Ψ_1^{-} away from the singular directions up to terms $\sim R_1^{-1}$ in the form

$$\Psi_i^{-}=\psi_{\mathbf{k}_{23}}^{-}(\mathbf{r}_{23})\exp(i\mathbf{K}_1\mathbf{R}_1)F_{ei}(\nu_{12},\xi_{12})\times F_{e0}(\nu_{13},\xi_{13})\quad (i=0,1). \tag{12}$$

Using the relations between the coordinates

$$\mathbf{r}_{12}=-\mathbf{R}_1+m_{23}\mathbf{r}_{23},\quad \mathbf{r}_{13}=\mathbf{R}_1+(1-m_{23})\mathbf{r}_{23},$$

we write variables ξ_{12} and ξ_{13} in the asymptotic region Ω_{23} up to terms $\sim r_{23}/R_1$ as

$$\xi_{12}=\xi_{12}(\mathbf{R}_1)+m_{23}k_{12}(\hat{\mathbf{k}}_{12}-\hat{\mathbf{R}}_1)\mathbf{r}_{23},$$

$$\xi_{13}=\xi_{13}(\mathbf{R}_1)+(1-m_{23})k_{13}(\hat{\mathbf{k}}_{13}+\hat{\mathbf{R}}_1)\mathbf{r}_{23}, \tag{13}$$

where $\xi_{12}(\mathbf{R}_1)=k_{12}R_1-\mathbf{k}_{12}\cdot\mathbf{R}_1$ and $\xi_{13}(\mathbf{R}_1)=k_{13}R_1+\mathbf{k}_{13}\cdot\mathbf{R}_1$. Using the relations (13), we now expand the Coulomb logarithmic phases in Eq. (12) up to terms $\sim r_{23}/R_1$. The result is

$$\Psi_i^{-}=\psi_{\mathbf{k}_{ei}(\mathbf{R}_1)}^{-}(\mathbf{r}_{23})\exp(i\mathbf{K}_1\mathbf{R}_1)F_{ei}(\nu_{12},\xi_{12}(\mathbf{R}_1))\times F_{e0}(\nu_{13},\xi_{13}(\mathbf{R}_1))\quad (i=0,1), \tag{14}$$

where

$$\mathbf{k}_{e0}(\mathbf{R}_1)=\mathbf{k}_{23}+\Delta\mathbf{k}_{e0}(\mathbf{R}_1)=\mathbf{k}_{23}-\left(m_{23}\nu_{12}\frac{\hat{\mathbf{k}}_{12}-\hat{\mathbf{R}}_1}{1-\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{R}}_1}+(1-m_{23})\nu_{13}\frac{\hat{\mathbf{k}}_{13}+\hat{\mathbf{R}}_1}{1+\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{R}}_1}\right)\frac{1}{R_1},$$

$$\mathbf{k}_{e1}(\mathbf{R}_1)=\mathbf{k}_{23}+\Delta\mathbf{k}_{e1}(\mathbf{R}_1)=\mathbf{k}_{23}-m_{23}k_{12}(\hat{\mathbf{k}}_{12}-\hat{\mathbf{R}}_1)+\left(m_{23}\nu_{12}\frac{\hat{\mathbf{k}}_{12}-\hat{\mathbf{R}}_1}{1-\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{R}}_1}-(1-m_{23})\nu_{13}\frac{\hat{\mathbf{k}}_{13}+\hat{\mathbf{R}}_1}{1+\hat{\mathbf{k}}_{13}\cdot\hat{\mathbf{R}}_1}\right)\frac{1}{R_1}. \tag{15}$$

In deriving the expression (14), following Refs. 22 and 23 we redefined the product of the wave function of the particle pair (2,3) and the additional phase factor arising in the expansion of the expressions for the phases in the distorting factors $F_{ei}(\nu_{12},\xi_{12})$ and $F_{e0}(\nu_{13},\xi_{13})$ up to terms $\sim r_{23}/R_1$:

$$\psi^-_{\mathbf{k}_{23}}(\mathbf{r}_{23})\exp(i\Delta\mathbf{k}_{ei}(\mathbf{R}_1)\mathbf{r}_{23})\to\psi^-_{\mathbf{k}_{23}+\Delta\mathbf{k}_{ei}(\mathbf{R}_1)}(\mathbf{r}_{23}). \qquad (16)$$

In Refs. 22 and 23 it is shown that $\delta\Psi_0^-=O(R_1^{-2})$. We shall now show that $\delta\Psi_1^-=O(R_1^{-2})$. We note first that $(V_{13}+V_{12})\Psi_1^-=O(R_1^{-2})$ and that the operator $\nabla_{\mathbf{R}_1}$ acting on the functions $\psi^-_{\mathbf{k}_{e1}(\mathbf{R}_1)}(\mathbf{r}_{23})$ and $\exp(\pm\nu_{ij}\ln\xi_{ij}(\mathbf{R}_1))$ gives quantities $\sim O(R_1^{-1})$, and therefore the contribution of these terms to $\delta\Psi_1^-$ will be $\sim O(R_1^{-2})$. Accordingly, we have

$$(\hat{H}-E)\Psi_1^-=(E_1(\hat{\mathbf{R}}_1)-E)\Psi_1^-+O(R_1^{-2}), \qquad (17)$$

where

$$E_1(\hat{\mathbf{R}}_1)=\frac{k_{e1}^2(\hat{\mathbf{R}}_1)}{2m_{23}}+\frac{(\mathbf{K}_1-\Delta\mathbf{k}_{e1}(\hat{\mathbf{R}}_1)/m_{23})^2}{2\mu_1}.$$

In Eq. (17) we dropped the part of the "local" momentum $\mathbf{k}_{e1}(\mathbf{R}_1)$ that is proportional to R_1^-, since its contribution to $\delta\Psi_1^-$ is $\sim O(R_1^{-2})$. It can be shown by direct calculation that for any direction of the unit vector $\hat{\mathbf{R}}_1$

$$E_1(\hat{\mathbf{R}}_1)=\frac{k_{23}^2}{2m_{23}}+\frac{K_1^2}{2\mu_1},$$

i.e. $E_1(\hat{\mathbf{R}}_1)\equiv E$. Therefore we have constructed an asymptotic wave function, taking into account the scattered waves away from the singular directions of the region Ω_{23}, which by construction "matches" to leading order the asymptotic wave function (2) in the region Ω_0.

The present results differ from those of Refs. 22 and 23 mainly by the fact that the "local" momentum is defined differently for the unscattered $\mathbf{k}_{e0}(\mathbf{R}_1)$ and scattered $\mathbf{k}_{e1}(\mathbf{R}_1)$ waves. In addition, this difference is important for determining correctly the asymptotic wave function in the region Ω_{23}. For example, a serious error can result if the overall "local" momentum $\mathbf{k}_{e0}(\mathbf{R}_1)=k_{e1}(\mathbf{R}_1)\equiv\mathbf{k}_{23}(\mathbf{R}_1)$ in Eq. (14) is defined as in Refs. 22 and 23. For example, if $\mathbf{k}_{23}(\mathbf{R}_1)=\mathbf{k}_{e0}(\mathbf{R}_1)$, then $(\hat{H}-E)\Psi_1^-=O(R_1^{-1})$ in the region Ω_{23} and the wave function (8) has the wrong asymptotic behavior. We note that the "local" momenta $\mathbf{k}_{e0}(\mathbf{R}_1)$ and $\mathbf{k}_{e1}(\mathbf{R}_1)$ are no longer two-particle momenta, but rather they become three-particle momenta, since they depend on the position and the kinematic and dynamic characteristics of the third particle. The asymptotic values of the three-particle momenta $\mathbf{k}_{e0}(\mathbf{R}_1)$ and $\mathbf{k}_{e1}(\mathbf{R}_1)$ are different in the limit $R_1\to\infty$: $\mathbf{k}_{e0}(\mathbf{R}_1)=\mathbf{k}_{23}$—the asymptotic momentum of the particle pair (2,3) and $\mathbf{k}_{e1}(\mathbf{R}_1)=\mathbf{k}_1(\hat{\mathbf{R}}_1)\equiv\mathbf{k}_{23}-m_{23}k_{12}(\hat{\mathbf{k}}_{12}-\hat{\mathbf{R}}_1)$. If the particles 1 and 3 are heavy (for example, the scattered ion and the residual target ion, respectively) and the particle 2 is light (electron), then $m_{23}\simeq m_{12}\simeq 1$ and the asymptotic local momentum $\mathbf{k}_1(\hat{\mathbf{R}}_1)=\mathbf{v}+|\mathbf{v}_e'|\hat{\mathbf{R}}_1$, where $\mathbf{v}$ is the velocity of the scattered ion and $\mathbf{v}_e'=\mathbf{v}_e-\mathbf{v}$ is the velocity of the electron relative to the scattered ion, i.e. in the coordinate system tied to the scattered ion, and the "local" asymptotic momentum of the electron $\mathbf{k}_1'(\hat{\mathbf{R}}_1)=v_e'\hat{\mathbf{R}}_1$. Then the presence of the scattered wave in Ψ_1^- can be interpreted as follows: an electron moving in the direction $\hat{\mathbf{R}}_1$ with velocity v_e' in the coordinate system of the scattered particle is elastically rescattered by it in the direction $\hat{\mathbf{v}}_e'$ and acquires as a result the asymptotic momentum $\mathbf{k}_{23}=\mathbf{v}_e$ in the laboratory coordinate system.

In the singular directions, the eikonal asymptotic solutions (14) are invalid. As a result, the Coulomb logarithmic phases in the solutions (14) and the "local" momenta $\mathbf{k}_{e1}(\mathbf{R}_1)$ become singular for $\hat{\mathbf{R}}_1=\hat{\mathbf{k}}_{12}$ and $\hat{\mathbf{R}}_1=\hat{\mathbf{k}}_{13}$. Near a singular direction, for example, $\hat{\mathbf{R}}_1\simeq\hat{\mathbf{k}}_{12}$, the singular part of the "local" momentum is

$$\mathbf{k}_{ei}(\mathbf{R}_1)\sim\frac{\hat{\mathbf{k}}_{12}-\hat{\mathbf{R}}_1}{1-\hat{\mathbf{k}}_{12}\hat{\mathbf{R}}_1}\frac{1}{R_1}.$$

Let $\cos\theta=\hat{\mathbf{k}}_{12}\cdot\hat{\mathbf{R}}_1$ and let $\mathbf{n}$ be an arbitrary unit vector. Then

$$\mathbf{k}_{ei}(\mathbf{R}_1)\mathbf{n}\sim\frac{1}{R_1\theta}\quad\text{for }\theta\ll 1,\quad \mathbf{n}\neq\hat{\mathbf{k}}_{12}\quad(\mathbf{k}_{ei}(\mathbf{R}_1)\hat{\mathbf{k}}_{12}\sim 1/R_1)$$

and the measure of the set of directions where the eikonal asymptotic solutions (14) are invalid obviously approaches zero in the limit $R_1\to\infty$. In this sense the eikonal asymptotic solutions (14) are valid in almost all directions of the configuration space Ω_{23} (with the exception of a set of measure zero). For applications it is important to construct the general analytic expressions which have the correct asymptotic behavior in almost all directions of configuration space, with the possible exception of separate special directions where, even though its asymptotic behavior is not entirely correct, the approximate wave function has no unphysical singularities. In this case it can be expected that in specific calculations such an approximate wave function will give a smaller error in the final results.

Formally replacing the eikonal distorting factors in the eikonal asymptotic formulas (14) and (15) by the corresponding quantum-mechanical factors $F_{e0(1)}(v_{ij},\xi_{ij}(\mathbf{R}_1))\to\mathbf{F}_{q0(1)}(\nu_{ij},\xi_{ij}(\mathbf{R}))$ gives the following generalization:

$$\Psi_i^-=\psi^-_{\mathbf{k}_i(\mathbf{R}_1)}(\mathbf{r}_{23})\exp(i\mathbf{K}_1\mathbf{R}_1)F_{qi}(\nu_{12},\xi_{12}(\mathbf{R}_1))\times F_{q0}(\nu_{13},\xi_{13}(\mathbf{R}_1)), \qquad (18)$$

where

$$\mathbf{k}_i(\mathbf{R}_1)=\mathbf{k}_{23}+im_{23}\nabla_{\mathbf{R}_1}\ln F_{qi}(\nu_{12},\xi_{12}(\mathbf{R}_1))-i(1-m_{23})\nabla_{\mathbf{R}_1}\ln F_{q0}(\nu_{13},\xi_{13}(\mathbf{R}_1))\quad(i=0,1). \qquad (19)$$

We note in the limit $R_1\to\infty$ that away from the singular directions the generalized formulas (18) and (19) pass into the corresponding eikonal expressions (14) and (15). In the singular directions, however, the "local" momenta (19) are singular, since the distorting factors $F_{qi}(\nu,\xi)$ diverge logarithmically as $\xi\to 0$. Nor does the generalization of Refs. 22 and 23 that suggests the following general expression for the "local" momenta in Eq. (18):

$$\mathbf{k}_0(\mathbf{R}_1)=\mathbf{k}_1(\mathbf{R}_1)=\mathbf{k}_{23}+im_{23}\nabla_{\mathbf{R}_1}\ln F_q(\nu_{12},\xi_{12}(\mathbf{R}_1))-i(1-m_{23})\nabla_{\mathbf{R}_1}\ln F_q(\nu_{13},\xi_{13}(\mathbf{R}_1)), \qquad (20)$$

give the desired result, since even though the momentum is finite in the singular directions, the wave functions (18) with the general "local" momentum (20) have the wrong asymptotic behavior in the limit $R_1\to\infty$ away from the singular directions.

The reason why unphysical divergences appear when the eikonal distorting factors are formally replaced in Eq. (19) by the quantum-mechanical factors is that the "amplitude" distortions arising in the continuum states as a result of the Coulomb interaction of the particle pairs (1,2) and (1,3) is included in the definition of the generalized "local" momentum. To determine the correct quantum-mechanical generalization of the "local" momenta, we employ the relation between quantum and classical mechanics. Let

$$\psi_{\mathbf{k}}^{-}(\mathbf{r})=\exp(i\mathbf{kr})F_q(\nu,\xi)=a(\mathbf{r})\exp(iS(\mathbf{r}))$$

be the Coulomb wave describing the scattering of any particle pair (1,2) or (1,3) (to simplify the equations we do not indicate the suffices j and k characterizing the particle pair). Here we explicitly separated the amplitude $a(\mathbf{r})$ and phase $S(\mathbf{r})$ of the distorted wave. If the term $(-\Delta a/2ma)$, which is a second-order infinitesimal in the limit $r\rightarrow\infty$, is neglected in the Schrödinger equation (11) for the particle pair, then we obtain for the phase $S(\mathbf{r})$ the equation

$$\frac{(\nabla S)^2}{2m}+V(\mathbf{r})=\frac{k^2}{2m}, \tag{21}$$

which has the form of the classical Hamilton–Jacobi equation for the abbreviated action $S(\mathbf{r})$ of the particle, and the amplitude $a(\mathbf{r})$ satisfies the continuity equation

$$\mathrm{div}\left(a^2\frac{\nabla S}{m}\right)=0. \tag{22}$$

It follows from Eq. (21) that the "local" momentum of the particle $\mathbf{k}(\mathbf{r})\equiv\nabla S(\mathbf{r})$ is of a quasiclassical nature and is related to the phase of the wave function by the gradient operator. The continuity equation (22) shows that the probability density $a^2(\mathbf{r})$ of finding a particle at any point "moves" according to the laws of classical mechanics with the classical velocity $\mathbf{v}(\mathbf{r})=\nabla S(\mathbf{r})/m$ at each point.

Therefore if the distorting factors $F_{qi}(\nu_{jk},\xi_{jk}(\mathbf{R}_1))$ for the particle pair (j,k) are written in the form

$$F_{qi}(\nu_{jk},\xi_{jk}(\mathbf{R}_1))=a_{qi}(\nu_{jk},\xi_{jk}(\mathbf{R}_1))\times\exp(i\Phi_{qi}(\nu_{jk},\xi_{jk}(\mathbf{R}_1)), \tag{23}$$

then Eq. 18, in which the three-particle generalized momenta $\mathbf{k}_i(\mathbf{R}_1)$ are defined as

$$\mathbf{k}_i(\mathbf{R}_1)=\mathbf{k}_{qi}(\mathbf{R}_1)\equiv\mathbf{k}_{23}-m_{23}\nabla_{\mathbf{R}_1}\Phi_{qi}(\nu_{12},\xi_{12}(\mathbf{R}_1))+(1-m_{23})\nabla_{\mathbf{R}_1}\Phi_{q0}(\nu_{13},\xi_{13}(\mathbf{R}_1)), \tag{24}$$

gives the correct generalization of the asymptotic eikonal formulas (14) and (15). With this generalization the "local" momenta (24) are finite in the singular directions and away from the singular directions the expressions (18) and (24) in the limit $R_1\rightarrow\infty$ pass into the corresponding eikonal representations (14) and (15). In addition, since in a singular direction $\mathbf{k}_{q0}(\mathbf{R}_1)=\mathbf{k}_{q1}(\mathbf{R}_1)$ the total asymptotic wave function $\Psi_{as}^{-}=\Psi_0^{-}+\Psi_1^{-}$ contains no singularities in the singular direction. The logarithmic singularities in the distorting factors $F_{q1}(\upsilon_{12},\xi_{12}(\mathbf{R}_1))$ in the limit $\hat{\mathbf{R}}_1\rightarrow\hat{\mathbf{k}}_{12}$ cancel in the sum

$$F_q(\nu_{12},\xi_{12}(\mathbf{R}_1))=F_{q0}(\nu_{12},\xi_{12}(\mathbf{R}_1))+F_{q1}(\nu_{12},\xi_{12}(\mathbf{R}_1)).$$

Equations (18) and (24) give the quantum-mechanical generalization of the corresponding eikonal expressions (14) and (15). However, the relative simplicity of the expressions characteristic of the eikonal approximation is now lost. For applications it may be important to obtain the corresponding semiclassical expressions that retain their relative simplicity and at the same time reproduce the important characteristic features of the quantum-mechanical description. To this end, we now solve the semiclassical equations (21) and (22).

We seek the solution of Eq. (21) in the following form:

$$S_c(\mathbf{r})=\mathbf{k}\cdot\mathbf{r}+\Phi_c(\nu,\xi), \tag{25}$$

where $\mathbf{k}\cdot\mathbf{r}$ is the plane-wave part of the phase, $\Phi_c(\nu,\xi)$ is the part of the phase that is due to the interaction of the particles, the suffix "c" in Eq. (25) indicates that the corresponding quantities are semiclassical, ν is the Coulomb interaction parameter, and $\xi=kr+\mathbf{k}\cdot\mathbf{r}$. Substituting the expression (25) into Eq. (21) gives the following equation for $d\Phi_c/d\xi$:

$$\left(\frac{d\Phi_c}{d\xi}\right)^2+\frac{d\Phi_c}{d\xi}+\frac{\nu}{\xi}=0. \tag{26}$$

Similarly we have for the amplitude $a_c(\nu,\xi)$ the equation

$$\frac{d}{d\xi}\ln a_c(\nu,\xi)=-\frac{d\Phi_c/d\xi+\xi d^2\Phi_c/d\xi^2}{\xi(1+2d\Phi_c/d\xi)}. \tag{27}$$

Neglecting the quadratic term in Eq. (26) gives an equation for the phase in the eikonal approximation. The quadratic equation (26) has two solutions:

$$\left(\frac{d\Phi_c}{d\xi}\right)_{0,1}=\frac{\pm\sqrt{1-4\nu/\xi}-1}{2}, \tag{28}$$

where the indices 0 and 1 on the left-hand side correspond to the + and − signs, respectively, on the right-hand side of Eq. (28). Integrating Eq. (28) gives

$$\Phi_{c0,1}(\nu,\xi)=\frac{\xi}{2}(\pm\sqrt{1-4\nu/\xi}-1)\pm\nu\ln\frac{\sqrt{1-4\nu/\xi}-1}{\sqrt{1-4\nu/\xi}+1}. \tag{29}$$

We now integrate Eq. (27), substituting Eq. (28). This gives the following expressions for the semiclassical amplitudes:

$$a_{c0}(\nu,\xi)=C_0(\nu)\sqrt{1+\frac{1-2\nu/\xi}{\sqrt{1-4\nu/\xi}}}, \tag{30}$$

$$a_{c1}(\nu,\xi)=C_1(\nu)\frac{1}{\xi\sqrt{1-4\nu/\xi+(1-2\nu/\xi)\sqrt{1-4\nu/\xi}}}, \tag{31}$$

where $C_{0,1}(\nu)$ are integration constants. The complete solution of the system (26) and (27) can be represented as a superposition of the semiclassical solutions $F_{ci}(\nu,\xi)=a_{ci}(\nu,\xi)\exp(i\Phi_{ci}(\upsilon,\xi))$(i=0,1):

$$F_c(\nu,\xi)=a_{c0}(\nu,\xi)\exp(i\Phi_{c0}(\nu,\xi))+a_{c1}(\nu,\xi)\exp(i\Phi_{c1}(\nu,\xi)). \tag{32}$$

Here the plane-wave part of the solution has been dropped. We note that in the limit $\xi\rightarrow 0$ the semiclassical phases in the expression (32) have a finite value $\Phi_{ci}(\nu,\xi=0)$ and the amplitudes have the power-law singularity $a_{ci}(\nu,\xi)\rightarrow\xi^{-1/4}$ characteristic of classical WKB solutions. It follows from Eqs. (30) and (31) that

$$a_0(\nu,\xi)|_{\xi\rightarrow\infty}=\sqrt{2}C_0(\nu),$$
$$a_1(\nu,\xi)|_{\xi\rightarrow\infty}=\frac{C_1(\nu)}{\sqrt{2}\xi}, \tag{33}$$

i.e. the semiclassical solution $F_{c0}(\nu,\xi)$ corresponds to the unscattered waves, and $F_{cl}(\nu,\xi)$ corresponds to the scattered waves. If the integration constants in Eqs. (30) and (31) are set equal to

$$C_0(\nu)=\frac{1}{\sqrt{2}}\exp(i\nu(1-\ln(-\nu))),$$
$$C_1(\nu)=\sqrt{2}\nu\frac{\Gamma(-i\nu)}{\Gamma(i\nu)}\exp(i\nu(-1+\ln(-\nu))), \tag{34}$$

then the semiclassical representation (32) passes in the limit $\xi\rightarrow\infty$ into the corresponding eikonal representation (5). A one-to-one correspondence is established between the eikonal semiclassical (WKB) and quantum-mechanical solutions: $F_{ei}(\nu,\xi)\leftrightarrow F_{ci}(\nu,\xi)\leftrightarrow F_{qi}(\nu,\xi)$, $i=0,1$. Using this result and Eqs. (24) and (28) we obtain the following explicit expressions for the semiclassical "local" momenta:

$$\mathbf{k}_{c0,1}(\mathbf{R}_1)=\mathbf{k}_{23}-m_{23}k_{12}(\hat{\mathbf{R}}_1-\hat{\mathbf{k}}_{12})(\pm\sqrt{1-4\nu_{12}/\xi_{12}(\mathbf{R}_1)}-1)/2+(1-m_{23})k_{13}(\hat{\mathbf{R}}_1+\hat{\mathbf{k}}_{13})\times(\sqrt{1-4\nu_{13}/\xi_{13}(\mathbf{R}_1)}-1)/2. \tag{35}$$

Away from the singular directions, when $4|\nu_{ij}|\ll\xi_{ij}(\mathbf{R}_1)$, the expressions (35) pass into the corresponding eikonal expressions (15) for the momenta. We shall now consider the behavior of the semiclassical momenta (35) near the singular direction $\hat{\mathbf{R}}\simeq\hat{\mathbf{k}}_{12}$, where $\xi_{12}(\mathbf{R}_1)\ll4|\nu_{12}|$. Let $\cos\theta=\hat{\mathbf{R}}_1\cdot\hat{\mathbf{k}}_{12}$ and $\hat{\mathbf{R}}_1=\cos\theta\hat{\mathbf{k}}_{12}+\sin\theta\mathbf{n}_\varphi$, where $\mathbf{n}_\varphi$ is a unit vector pointing in the direction of the azimuthal component of the vector $\hat{\mathbf{R}}_1$. Then for fixed R_1 and $\theta\rightarrow0$ we have

$$\nabla_{\mathbf{R}_1}\Phi_{c0,1}(\nu_{12},\xi_{12}(\mathbf{R}_1))\rightarrow\mp\mathbf{n}_\varphi\sqrt{-\frac{8Z_1Z_2m_{12}}{R_1}}, \tag{36}$$

i.e. the semiclassical momenta (35) are finite in the singular direction $\hat{\mathbf{R}}_1=\hat{\mathbf{k}}_{12}$. We note that the semiclassical approximation becomes invalid near the turning points, where the semiclassical momenta become complex. The quantum-mechanical description must be used near these points.

3. AUTOIONIZATION AMPLITUDE

We now consider the resonance ionization of an atom $A(i)$ in a collision with an incident particle P^{Z_1} with charge Z_1, proceeding with the formation of an intermediate autoionization state α of the atom $A^{**}(\alpha)$

$$P^{Z_1}+A(i)\rightarrow P^{Z_1}+A^{**}(\alpha)\rightarrow P^{Z_1}+e^-+A^+(f), \tag{37}$$

as a result of the decay of which three charged particles form in the final state: 1) a scattered particle (ion) P^{Z_1}, 2) an autoionization electron e^-, and 3) a residual target ion $A^+(f)$.

Using the expressions (8), (18), and (24) for the wave function of the final state, the amplitude of the resonance process (37) can be represented as follows in the diagonalization approximation:[19]

$$A_{fi}=A_0+A_1, \tag{38}$$

$$A_j=-iA_{\alpha i}\int_0^\infty dt\, A_{f\alpha}(\mathbf{k}_j(\mathbf{R}_1))\times\exp\left(iE_et-i\int_0^t d\tau\, E_{c\alpha}(\tau)\right)F^*_{qj}(\nu_{12},\xi_{12}(\mathbf{R}_1))\times F^*_{q0}(\nu_{13},\xi_{13}(\mathbf{R}_1))\quad(j=0,1). \tag{39}$$

Here $A_{\alpha i}$ is the excitation amplitude of the autoionization state at the time $t=0$;

$$A_{f\alpha}(\mathbf{k})=\langle\hat{A}[\psi^-_{\mathbf{k}}\varphi_f]|\hat{V}_{ee}|\Phi_\alpha\rangle \tag{40}$$

is the amplitude for the autoionization state Φ_α to decay into the final state $\hat{A}[\psi^-_{\mathbf{k}}\varphi_f]$, as a result of which an electron with momentum $\mathbf{k}$ is in the continuum and the residual target ion is in the state φ_f; $\hat{A}$ is the (anti)symmetrization operator with respect to the electron coordinates; $\hat{V}_{ee}$ is the interelectron interaction operator; E_e is the energy of the autoionization electron, $E_{e\alpha}(t)=E_\alpha(t)-(i/2)\Gamma_\alpha(t)$ is the time-dependent complex energy of the α-th autoionization state (quasistationary electronic term); and, $E_\alpha(t)$ and $\Gamma_\alpha(t)$ are the real energy and the total width of the autoionization resonance, taking into account the PCI in the intermediate state. The coordinates $\mathbf{R}_1$ in Eqs. (39) and (40) are related to the time t of the motion of the scattered electron by $\mathbf{R}_1=\mathbf{v}t$, where $\mathbf{v}$ is the velocity of the ion.

The distorting factors $F_{qi}(\nu_{jk},\xi_{jk}(\mathbf{R}_1))$ in Eq. (39) account for the PCI of the particle pairs (1,2) and (1,3) in the final state. The interaction of the particle pair (2,3) is taken into account in the decay amplitude (40) and is ordinarily not included in the PCI, which takes into account the effect of the scattered ion. In the general case, however, when the effect of the scattered ion on the motion of the particle pair (2,3), the autoionization electron, and the residual target ion is taken into account, the "local" momenta $\mathbf{k}_i(\mathbf{R}_1)$ of the autoionization electron are different from the asymptotic value $\mathbf{k}_e=\mathbf{v}_e$, and the effects due to the interaction of the particle pair (2,3) cannot be isolated in a separate decay matrix element that does not depend on the characteristics of the scattered ion. The autoionization decay probability determined by the matrix element (40) depends on the time and position of the scattering ion: at a fixed time t the autoionization electron undergoes a transition from a bound to a continuum state with momentum $\mathbf{k}_1(t)$ or $\mathbf{k}_0(t)$, depending on whether or not it is rescattered by the receding ion.

Using the representation (23) for the distorting factors, we find that the integrands in Eq. (39) are proportional to the phase factor $\exp(iS_j(t))$ $(j=0,1)$, where

$$S_j(t)=E_e t-\int_0^t d\tau\, E_{c\alpha}(\tau)-\Phi_{qj}(\nu_{12},\xi_{12}(\mathbf{v}t))$$
$$-\Phi_{q0}(\nu_{13},\xi_{13}(\mathbf{v}t)). \quad (41)$$

The points t_c where the phase is stationary, $\dot{S}_j(t_c)=0$, determine the region making the main contribution to the time integral, i.e. the time interval when the transition probabilities are maximum. The stationary-phase condition can be expressed as

$$E_{fj}(t_c)=E_{c\alpha}(t_c) \quad (j=0,1), \quad (42)$$

where

$$E_{fj}(t)=E_e-\dot{\Phi}_{qj}(\nu_{12},\xi_{12}(\mathbf{v}t))-\dot{\Phi}_{q0}(\nu_{13},\xi_{13}(\mathbf{v}t))$$

is the time-dependent energy of the autoionization electron in the final state, i.e. transitions occur at the moment the electronic terms in the intermediate (resonance) and final states cross. The transition points are displaced from the real axis into the complex plane, since the intermediate state is quasistationary.

If the effect of the PCI in the intermediate state is neglected, then the energy of the resonance state does not depend on the time and is an atomic parameter, defined for an isolated atom to be $E_{c\alpha}=E_\alpha-(i/2)\Gamma_\alpha$. The effects due to the influence of the PCI in the intermediate state were studied in Refs. 19, 29, and 30. In addition, if the PCI in the final state of the particle pair (1,3) is described in the eikonal approximation and the pair (1,2) is described in the semiclassical approximation, then the expression (2) simplifies to

$$\pm\sqrt{1-4\nu_{12}z_c}=1+2\beta+2\nu_{13}z_c, \quad (43)$$

where

$$z_c=\frac{1}{a_{12}\tau_c}, \quad \beta=\frac{\varepsilon+i}{a_{12}}, \quad a_{12}=\frac{2}{\Gamma_\alpha}vv_e'(1-\hat{\mathbf{v}}\hat{\mathbf{v}}_e'),$$

$$\varepsilon=\frac{2(E_e-E_\alpha)}{\Gamma_\alpha}, \quad \tau_c=\frac{\Gamma_\alpha}{2}t_c.$$

The + or − signs in Eq. (43) correspond to the indices $j=0$ or 1 in Eq. (42). The complex root in Eq. (43) is determined so that $\sqrt{z^2}=z$. Solving Eq. (43) for z_c we obtain two roots:

$$(z_c)_{0,1}=-\frac{\beta}{\nu_{13}}-\frac{\nu}{\nu_{13}^2}h_{0,1}(\beta), \quad (44)$$

where

$$\nu=\nu_{12}+\nu_{13}, \quad h_0(\beta)=\frac{1}{2}\left(1-\sqrt{1+\frac{4\nu_{12}\nu_{13}}{\nu^2}\beta}\right),$$

$$h_1(\beta)=1-h_0(\beta).$$

In the kinematic region, where the interaction of the particle pair (1,2) is weak, the parameter $|\beta|\ll 1$ and Eq. (44) simplifies to

$$E_e-E_\alpha+\frac{i}{2}\Gamma_\alpha+V_f(t_{c0})=o(|\beta|) \quad \text{for } t_{c0}, \quad (45)$$

$$\left(E_e-E_\alpha+\frac{i}{2}\Gamma_\alpha\right)\left(1-\frac{v}{v_e'-v}\right)+\Delta E_{sc}\left(1-\frac{v}{v_e'}\right)$$
$$+V_{13}(t_{c1})=o(|\beta|) \quad \text{for } t_{c1}, \quad (46)$$

where

$$V_f(t)=V_{13}(t)+V_{12}(t)=\frac{Z_1}{vt}-\frac{Z_1}{v_e't},$$

$$\Delta E_{sc}=vv_e'-\mathbf{v}\mathbf{v}_e'=E_{\text{prior}}-E_{\text{post}},$$

$$E_{\text{prior}}=(\mathbf{v}+v_e'\hat{\mathbf{v}})^2/2, \quad E_{\text{post}}=E_e=v_e^2/2.$$

Here $V_f(t)$ is the potential energy of the three-particle PCI of the receding particles; E_{before} and E_{after} are the asymptotic kinetic energies of the autoionization electron in the laboratory coordinate system before and after the electron is elastically rescattered by the angle $\theta_e(\cos\theta_e=\hat{\mathbf{v}}_e\cdot\hat{\mathbf{v}})$ by the receding ion. It follows from Eq. (45) that if the imaginary part of the resonance energy is neglected, then $t_{c0}\simeq\nu/(E_\alpha-E_e)$, i.e. the semiclassical correspondence between the most likely moment of the transition of an autoionization electron into the continuous spectrum and its energy can be established: Away from the center of the resonance line, in the far wings, we enter the region of the spectrum that is formed as a result of the decay of the autoionization state at short times. The equation (45) also makes it possible to explain qualitatively the asymmetry that is observed in the resonance line when the PCI is taken into account: depending on the sign of the three-particle Coulomb interaction parameter ν, a "tail" appears in the profile of the resonance to the right or left of the center of the resonance line. For example, for $\nu>0$ and $E_e<E_\alpha$ (the classically allowed energy range) the point of stationary phase $t_{c0}>0$ falls within the region of integration $(0,\infty)$, while for $E_e>E_\alpha$ (the classically forbidden energy range) $t_{c0}\notin(0,\infty)$ and electron transitions into the continuous spectrum are suppressed on the right-hand wing of the resonance line.

At the transition points determined from Eq. (43) the "local" momenta (35) are complex:

$$\mathbf{k}_{0,1}(\beta)=v_e(\hat{\mathbf{v}}_e+h_{0,1}(\beta)(\mathbf{n}-\hat{\mathbf{v}}_e)), \quad (47)$$

where $\mathbf{n}=(v_e'\hat{\mathbf{v}}+v\hat{\mathbf{v}}_e')(|\mathbf{n}|=1)$. We note that the momenta (47) do not depend on the magnitude and sign of the charge Z_1. The scalar moduli of the vectors equal

$$|\mathbf{k}_0(\beta)|=|\mathbf{k}_1(\beta)|=k(\varepsilon)$$
$$\equiv v_e\sqrt{1+\frac{\Gamma_\alpha(\varepsilon+i)}{vv_e}\varphi(\theta_e,\theta_e')}, \quad (48)$$

where

$$\varphi(\theta_e,\theta_e')=\frac{\cos(\theta_e'-\theta_e)}{\sin(\theta_e'-\theta_e)-\sin\theta_e}\,\frac{\sin(\theta_e'-\theta_e)}{1-\cos\theta_e'},$$

$$\cos\theta_e=\hat{\mathbf{v}}_e\hat{\mathbf{v}}, \quad \cos\theta_e'=\hat{\mathbf{v}}_e'\hat{\mathbf{v}},$$

and the direction cosines of the vectors are

$$\cos\,\theta_{0,1}=\frac{\mathbf{k}_{0,1}(\beta)\cdot\hat{\mathbf{v}}}{k(\varepsilon)}$$
$$=\frac{v_e}{k(\varepsilon)}\left(\cos\,\theta_e+h_{0,1}(\beta)\,\frac{v-v_e'}{v_e}\,(\cos\,\theta_e'-1)\right). \qquad (49)$$

For the long-lived autoionization states Γ_α is a small parameter; for example, the width of the lowest $(2s^2)^1S$ resonance of the helium atom $\Gamma_\alpha=5.07\cdot 10^{-3}$. Since the angular function $\varphi(\theta_e,\theta_e')$ has no singularities, to terms $\sim\Gamma_\alpha$ we can set $k(\varepsilon)=v_e$. Then $k(\varepsilon)$ can differ substantially from v_e only in the remote wings of the resonance, where $|\varepsilon|\sim 1/\Gamma_\alpha\gg 1$. Away from the singular direction $\hat{\mathbf{v}}_e'=\hat{\mathbf{v}}$, the parameter $|\beta|\ll 1$, and in the zeroth approximation we can set $h_0(\beta)=h_0(0)=0$, $h_1(\beta)=h_1(0)=1$ in Eq. (47), i.e. the "local" momenta are $\mathbf{k}_0(0)=\mathbf{v}_e$ and $\mathbf{k}_1(0)=v_e\mathbf{n}$, respectively.

We now use the peaking approximation to extract from the integrand in Eq. (39) the matrix element determining the decay amplitude at the points t_{c0} and t_{c1}, respectively, for $j=0$ and 1. In this approximation we obtain

$$A_j=-iA_{\alpha i}A_{f\alpha}(\mathbf{k}_j(\beta))\,\frac{2}{\Gamma_\alpha}\,I_j(\varepsilon)\quad (j=0,1), \qquad (50)$$

where the integrals

$$I_j(\varepsilon)=\int_0^\infty d\tau\,\exp[(i\varepsilon-1)\tau]\tau^{i\nu_{13}}F_{qj}^*(\nu_{12},a_{12}\tau)$$

can be calculated analytically:[31]

$$I_0(\varepsilon)=\frac{\exp(\pi\nu_{12}/2)}{(1-i\varepsilon)^{1+i\nu_{13}}}\,\frac{\Gamma^2(1+i\nu_{13})}{\Gamma(1+i\nu_{13}-i\nu_{12})}\,{}_2F_1\left(-i\nu_{12},1+i\nu_{13},1+i\nu_{13}-i\nu_{12},\frac{1-i(a_{12}+\varepsilon)}{1-i\varepsilon}\right), \qquad (51)$$

$$I_1(\varepsilon)=i\nu_{12}\exp(2i\delta_c(\nu_{12}))\times\frac{\exp(\pi\nu_{12}/2)}{(1-i(a_{12}+\varepsilon))^{1+i\nu_{13}}}\,\frac{\Gamma^2(1+i\nu_{13})}{\Gamma(2+i\nu_{13}+i\nu_{12})}\,{}_2F_1\times\left(1+i\nu_{12},1+i\nu_{13},2+i\nu_{12}+i\nu_{13},\frac{1-i\varepsilon}{1-i(a_{12}+\varepsilon)}\right), \qquad (52)$$

where $\delta_c(\nu_{12})=\arg\Gamma(1+i\nu_{12})$ and ${}_2F_1(a,b,c,z)$ is the hypergeometric function.

We note that the interaction of the particle pairs (1,2) and (1,3) in the final state is described in Eq. (50) in the quantum-mechanical and eikonal approximations, respectively. The semiclassical WKB approximation is used to describe the interaction of the particle pair (1,2) in determining the "local" momenta $\mathbf{k}_j(\beta)$ and the transition points t_{cj}. The terms I_0 and I_1 describe, respectively, the contribution of the waves which are and are not rescattered by the receding ion to the total resonance-ionization amplitude. The contribution of the waves which are not rescattered dominates for $a_{12}\gg 1$:

$$I_0\rightarrow I_0^{eik}=\frac{\Gamma(1+i\nu)}{(1-i\varepsilon)^{1+i\nu}}\exp(i\nu_{12}\ln a_{12}),\quad I_1=O\left(\frac{1}{a_{12}}\right), \qquad (53)$$

where I_0^{eik} is the corresponding expression for the amplitude in the eikonal approximation.[14,15] The contributions I_0 and I_1 are comparable in the kinematic region where $a_{12}\sim 1$. As $a_{12}\rightarrow 0$, the quantities I_0 and I_1 diverge logarithmically, but in the sum I_0+I_1 these divergences ($I_{\rm sing}\sim\ln a_{12}$) cancel and I_0+I_1 remains finite for $\alpha_{12}=0$.

Separating out the angular dependence, we represent the decay amplitude of the autoionization state in the form

$$A_{f\alpha}(\mathbf{k})=\tilde{A}_{f\alpha}(k)Y_{LM}(\hat{\mathbf{k}}), \qquad (54)$$

where L and M are, respectively, the total orbital angular momentum and the magnetic quantum number of the autoionization state. The width of the resonance is determined by the expression $\Gamma_\alpha=2\pi v_e|\hat{A}_{f\alpha}(v_e)|^2$, where v_e is the velocity of the autoionization electron at the resonance point ($v_e=\sqrt{2E_\alpha}$). It follows from Eq. (54) that for small ejection angles the state with $M=0$ makes the main contribution to the transition amplitude. Therefore, neglecting the contribution of the states with $M\neq 0$ and using the expression (54), we shall write the relative intensity of the autoionization electrons for an isolated resonance in the form

$$I(E_e,\theta_e)=(2L+1)\,\frac{2}{\pi\Gamma_\alpha}\,K_\alpha(\varepsilon)|P_L(\cos\,\theta_0)I_0(\varepsilon)+P_L(\cos\,\theta_1)I_1(\varepsilon)|^2, \qquad (55)$$

where $K_\alpha=|\tilde{A}_{f\alpha}(k(\varepsilon))/\tilde{A}_{f\alpha}(v_e)|^2$ and $\cos\,\theta_{0,1}$ is determined by Eq. (49). In the general case the coefficient $K_\alpha(\varepsilon)\neq 1$ and the direction cosines $\cos\,\theta_{0,1}\neq\cos\,\theta_e$, and they take into account the effect of the scattered ion on the momentum of the autoionization electron at the moments of its transition into the continuous spectrum, which differ somewhat from one another depending on whether or not the electron is subsequently Coulomb-rescattered by the receding ion. Setting $K_\alpha(\varepsilon)=1$ and $P_L(\cos\,\theta_0)=P_L(\cos\,\theta_1)=P_L(\cos\,\theta_e)$, in Eq. (55) the expression (55) can be transformed into the corresponding expressions obtained previously in Refs. 9–13. In contrast to the corresponding representations in Refs. 9–13, however, the separation (55) makes it possible to investigate in detail the relative contribution of the waves that are and are not rescattered to the electronic intensity as well as the possible interference between them.

4. DISCUSSION OF THE COMPUTATIONAL RESULTS

To demonstrate the effects of rescattering of the autoionization electrons by the scattered particle, we calculated for small ejection angles θ_e the electron energy spectra near the $(2s^2)^1S$ resonance of the helium atom, excited in a collision with ions with velocity v less than the velocity v_e of the autoionization electrons. For the long-lived isotropic S resonance we must set $L=0$, $K_\alpha(\varepsilon)=1$, and $P_0(\cos\,\theta_0)=P_0(\cos\,\theta_1)=1$ in Eq. (55). The results of the present calculations according to Eq. (55) for 10-keV ${}^3He^+$ ions with the effective charges $Z_1=Z_{\rm eff}=1$ and 2 and ejection angle $\theta_e=5°$ are presented in Fig. 1. To compare with

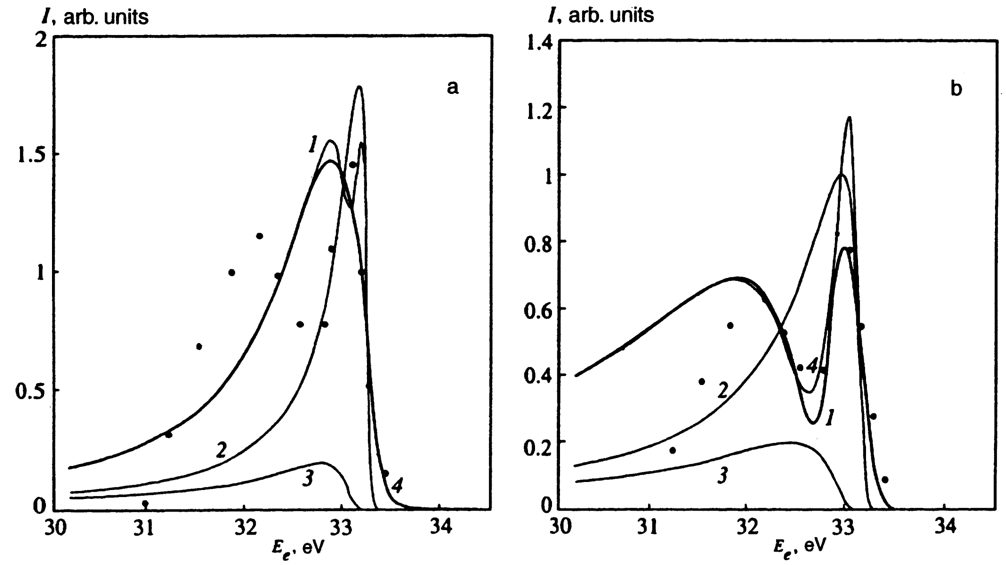


FIG. 1. Energy dependence of the relative intensity $I(E_e)$ of electrons ejected at angle $\theta_e=5°$ during the decay of the autoionization $(2s^2)^1S$ state excited in a helium atom in a collision with 10-keV $^3He^+$ ions. The results of the present calculations with effective $^3He^+$ ion charges $Z_{eff}=1$ (a) and $Z_{eff}=2$ (b) are shown: Curve *1*—complete calculation with Eq. (55); curves *2* and *3*—separate contribution of waves that are and are not rescattered, respectively; curve 4 was obtained by convolving the theoretical profile (curve *1*) and a Gaussian energy-resolution function with FWHM=0.3 eV. The experimental points were taken from Ref. 17.

the experimental data of Ref. 17, the result of convolving the theoretical profile of the resonance with the spectrometric Gaussian energy-resolution function with FWHM=0.3 eV is also presented in Fig. 1. The relevant experimental data from Ref. 17 were normalized so that the maximum intensities of the experimental and theoretical resonance profile would be the same.

The line obviously has a pronounced asymmetry—the "Coulomb tail" in the electron energy distribution is observed to the left of the maximum of the resonance. The contribution of the rescattered waves leads to the appearance of an additional "rescattering" peak in the left-hand wing of the resonance. In addition, interference between the waves that are and are not rescattered plays a large role in the formation of the "rescattering" peak in the complete calculations. A minimum appears in the contour of the line as a result of destructive interference of the waves. If the interference of the waves is neglected, then the rescattered waves contribute only some additional increase in the intensity of the electrons in the left-hand wing of the resonance.

The calculations showed that the form of the resonance depends strongly on the magnitude of the effective charge in whose field the electrons are rescattered. For example, for an asymptotic charge of the $^3He^+$ ion $Z_{eff}=1$ (or for protons with the same velocity) the relative intensity of the waves that are not rescattered is high and the interference of the waves that are and are not rescattered is weak—the additional peak does not appear in the (convolved) resonance profile. As the effective charge increases to $Z_{eff}=2$ (the nuclear charge of the $^3He^+$ ion), the maximum intensity of the waves that are not rescattered decreases and the interference structure in the profile of the resonance is pronounced. Hence it follows that the interference structure observed in Ref. 17 in the low-energy wing of the resonance results from the incomplete screening of the nuclear charge of the $^3He^+$ ion by a bound electron in the process of rescattering of the autoionization electrons in the field of the $^3He^+$ ion. As an experimental check of the dependence obtained in the present calculations of the line shape on the magnitude of the charge of the scattered particle, a comparative analysis could be made of the experimental spectra of the autoionization electrons produced under identical (just as in the experiment of Ref. 17) kinematic conditions in a collision of helium atoms with protons and $^3He^+$ nuclei.

As the ejection angle increases, the electrons rescattered by the receding ion lose more energy in the process and the "rescattering" peak shifts toward lower energies. The intensity of the peak decreases according to Eq. (53) as $\sim 1/a_{12}^2=(\Gamma_\alpha/2\Delta E_{sc})^2$, and the line shape is determined by the contribution of waves that are not rescattered. Conversely, as the ejection angle decreases, the "rescattering" peak shifts in the direction of higher energies and the intensity of the peak increases. As the ejection angle decreases from 5 to 0°, the positions of the maxima in the intensity distributions of the waves that are and are not rescattered converge toward one another. In this case the interference of the waves is constructive, the line shape does not change, and as a result the overall intensity of the resonance increases on account of the trapping of electrons in the continuum of the receding $^3He^+$ ion. For lack of space, we do not present the corresponding plots, which reflect the dynamics of the change in the shape and intensity of the resonance line as a function of the ejection angle. We merely note that the results obtained agree qualitatively with the relative experimental data of Ref. 17. However, the present interpretation of the appearance of the "rescattering" peak at 5° is different from the corresponding "interference of Coulomb paths" mechanism proposed in Ref. 17 and confirms the conclusions drawn in Ref. 10.

Interference plays an important but not always decisive role in the formation of the "rescattering" peak in the electron spectra. A kinematic situation in which the intensity of the waves that are not rescattered is low near the "rescattering" peak is possible. The computational results for 50 keV protons and ejection angle $\theta_e=2°$ are presented in Fig. 2. For comparison, the computational results for the resonance profile in the semiclassical eikonal approximation are also

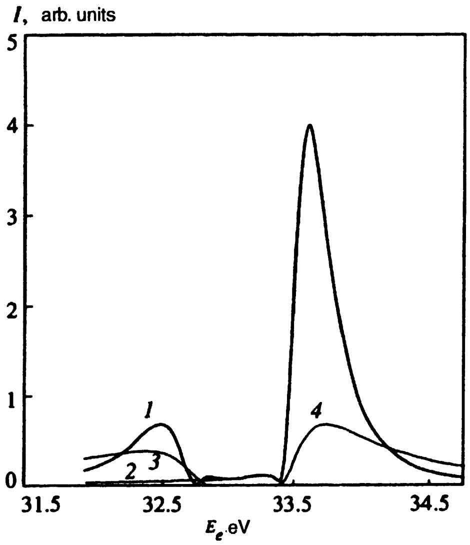


FIG. 2. Energy spectrum of autoionization electrons ejected at angle $\theta_e = 2°$ accompanying the decay of an autoionization $(2s^2)^1S$ state excited in a helium atom in a collision with 50-keV protons. The curves *1–3* are the same as in Fig. 1a, b. The curve *4* was calculated in the semiclassical eikonal approximation.[14,15]

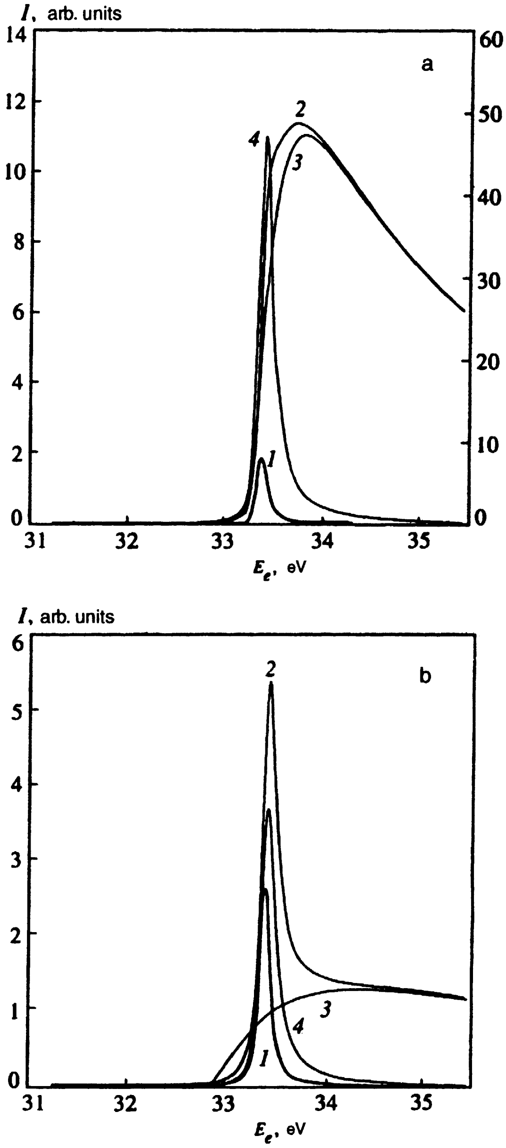


FIG. 3. Spectra of autoionization electrons ejected at angles $\theta_e = 5$ (a) and 10° (b) in a decay of the autoionization $(2s^2)^1$ state excited in a helium atom in a collision with 10-keV antiprotons. The curves *1–4* are the same as in Fig. 2. The ordinate for the curves *2* and *3* in a) is plotted on the right-hand side of the figure.

presented in the figure.[14,15] It is obvious that as the collision energy increases, the character of the asymmetry of the resonance, determined by the sign of the three-particle Coulomb interaction parameter ν, changes: the waves that are not rescattered form the "Coulomb tail" in the right-hand wing of the resonance. The intensity of the waves that have not been rescattered is lower in the left-hand wing of the resonance than the intensity of the waves that have been rescattered. In this situation the "rescattering" peak is formed in the complete calculations mainly on account of the contribution of the rescattered waves. Interference does not change the picture qualitatively; it merely changes somewhat the intensity and shape of the "rescattering" peak and leads to small oscillations of the line contour in the region where the waves that have and have not been rescattered have the same intensity.

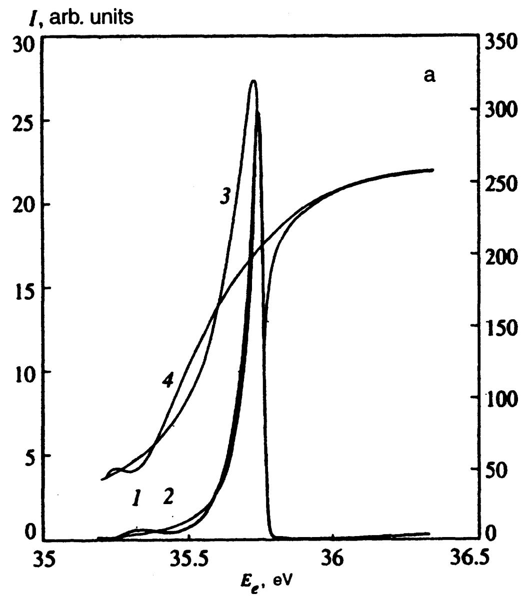
It is of great interest to investigate the relative contribution of the waves that have and have not been rescattered as a function of the sign of the charge of the incident particle. The results of analogous calculations of the shape of the $(2s^2)^1S$ resonance in the case of a collision with 10-keV antiprotons and ejection angles $\theta_e = 5$ and 10° are displayed in Fig. 3. It is obvious that for antiprotons no additional structure arises in the profile of the resonance. The surprising result of the calculations for antiprotons is the unexpectedly high intensity of the waves that have and have not been rescattered (curves *2* and *3*) as compared with the corresponding intensities obtained for protons. As a result of destructive interference of the waves, the total electronic intensity (curve 1) $|I_0(\varepsilon)+I_1(\varepsilon)|^2 \ll |I_0(\varepsilon)|^2$, $|I_1(\varepsilon)|^2$. As the ejection angle increases, the intensity of the rescattered (not rescattered) waves drops rapidly (by an order of magnitude; see Fig. 3), but these sharp changes have virtually no effect in the complete calculations.

We note that the effects of electron rescattering by an antiproton can be manifested for nonisotropic resonances. For $\delta_{0,1}(\varepsilon) = |I_0(\varepsilon)+I_1(\varepsilon)|^2/|I_{0,1}(\varepsilon)|^2$ the total intensity of the electrons is determined by the expression

$$I(E_e,\theta_e) = (2L+1)\,\frac{2}{\pi\Gamma_\alpha}\,|P_L(\cos\theta_1) - P_L(\cos\theta_0)|^2 |I_1(\varepsilon)|^2, \tag{56}$$

where, for example, for a P resonance

$$|P_1(\cos\theta_1) - P_1(\cos\theta_0)|^2 = |\cos\theta_1 - \cos\theta_0|^2 = \left|\left(1 - \frac{\Gamma_\alpha(\varepsilon+i)}{2(v-v_e')^2}\,\frac{1}{1-\cos\theta_e'}\right) \Big/ \left(1 + \frac{\Gamma_\alpha(\varepsilon+i)}{v v_e}\,\varphi(\theta_e,\theta_e')\right)\right| \left(\frac{v-v_e'}{v_e}\right)^2 (\cos\theta_e' - 1)^2. \tag{57}$$



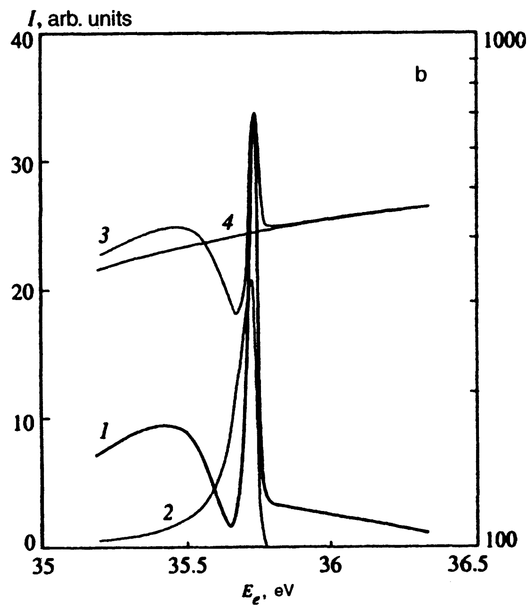


FIG. 4. Profiles of the autoionization $(2s2p)^1P$ resonance excited in a helium atom in a collision with 30 keV (a) and 40 keV (b) antiprotons for ejection angles $\theta_e=5$ and 8°, respectively. Curve *1*—complete calculation with Eq. (55); curve 2—calculation with Eq. (55), where $\cos\theta_{0,1}\equiv\cos\theta_c$; curves *3* and *4* (the ordinate is plotted on the right-hand side of the figure) represent the separate contribution of waves that are and are not rescattered, respectively.

We note that if Γ_α is a small parameter, then the angular functions $P_L(\cos\theta_{0,1}(\varepsilon,\theta_e))$ in Eq. (55) with $\theta_e'\ll 1$ differ from $P_L(\cos\theta_e)$ by a small amount. In addition, as follows from Eq. (57) $|\cos\theta_1-\cos\theta_0|\sim\sqrt{1-\cos\theta_e'}\simeq\theta_e'/\sqrt{2}$ for $\theta_e'\ll 1$, i.e. the total intensity of the electrons (55) is finite at $\theta_e'=0°$.

The results of model calculations of the profile of a nonisotropic $(2s2p)^1P$ resonance of a helium atom excited in a collision with antiprotons with energy $E_p=30$ and 40 keV and ejection angles $\theta_e=5°$ are presented in Fig. 4. One can see that a qualitatively new effect is obtained when the effect of the antiproton on the motion of an autoionization electron at the moment it makes a transition to the continuous spectrum is taken into account: an additional structure appears in the left-hand wing of the resonance (curve *1*); this structure does not occur in the calculations performed in the approximations of Refs. 9–13, i.e. neglecting this effect (curve 2). In addition, as the collision energy increases, this effect becomes more pronounced as the electron–antiproton interaction in the final state increases: it is essentially unobservable at $E_p=10$ keV and it is quite weak at $E_p=30$ keV, whereas at $E_p=40$ keV it is quite pronounced. This energy dependence of the effect is explained by the increase in the intensity of waves that are and are not rescattered with increasing collision energy: at $E_p=30$ keV $\delta_{0,1}(\varepsilon)\sim 5\cdot 10^{-2}$, whereas at $E_p=40$ keV $\delta_{1,0}(\varepsilon)\sim 5\cdot 10^{-2}$. Since $|\cos\theta_1-\cos\theta_0|\rightarrow 0$ as $\theta_e'\rightarrow 0$, the effect vanishes as the ejection angle decreases, and by virtue of the relation (53) it also vanishes as the ejection angle increases.

The qualitatively different sign–charge dependence obtained in the calculations for the ratio between the total electronic intensity $|I_0+I_1|^2$ and the separate contribution $|I_{(0)1}|^2$ of the waves that have (have not) been rescattered to the intensity at small ejection angles has a simple physical explanation—electrons are focused in an attractive field and defocused in a repulsive field, i.e. close electron trajectories in the field of a negatively (positively) charged particle will diverge (converge), and as a result small variations in the initial conditions as an electron moves along its trajectory will increase (decrease). As a result, a small difference in the direction of motion of the electrons at the moment the autoionization state decays ($\cos\theta_0\simeq\cos\theta_1$ for $\theta_e'\ll 1$) will have a stronger effect on the final results of electron scattering in a repulsive field than in an attractive field. The computational results completely confirm this conclusion.

The structure observed in the low-energy wing of the nonisotropic resonance for negatively charged particles is a substantially three-particle interference effect caused by the influence of the long-range Coulomb field of the scattered particle on the relative motion of the autoionization electron and the residual ion, which are weakly separated at the moment the electron makes a transition to the continuous spectrum. This qualitative three-particle Coulomb effect should be observable experimentally, being strongest for small (but not zero) ejection angles and low velocities of the scattered particle (e^-, p^-), close to the velocity of the ejected electrons. The structure observed in Ref. 20 for the more complicated atomic system $e_{sc}^- - e_{ej}^- - e_{\rm Aug}^- - {\rm Ar}^{2+}$ in the low-energy wing $L_3-M_{2,3}^2(^1D_2)$ of the Auger resonance of an argon atom can serve as an indirect experimental confirmation of the existence of this effect. This structure may be due to the interference of waves corresponding to Auger electrons, $e_{\rm Aug}^-$, that are and are not rescattered by the initially ejected electron, e_{ej}^-. Since, however, the wave interference is a subtle effect that can only be interpreted when the amplitudes and phases of the interfering waves are determined accurately, it will be possible to draw final conclusions about the origin of the structure observed in Ref. 20 only after a separate careful investigation of the shape of the Auger line, including a theoretical analysis of the effect of the PCI of all four charged particles, as well as the effects arising from the possible interference of the resonance with the background formed by direct transitions.

5. CONCLUSIONS

The wave function constructed in the present work for the three asymptotically-free charged particles possesses the correct asymptotic behavior in the region of configuration space where two particles are located close to one another and a third particle is located far away from the pair, and it can be used to describe bound–free transitions. The wave function determined by Eqs. (8), (18), and (24) is one of the main results of this work.

Taking into account the effect of the long-range Coulomb field of the third particle on the motion of the weakly separated particle pair in the wave function (8), (18), and (24) leads to a modification of the two-particle relative momentum—the momentum becomes a three-particle momentum, which depends on the position and the kinematic and dynamic characteristics of the motion of the third particle. In contrast to the results of Refs. 22 and 23, the modification of the momentum is different for the waves that are rescattered $\mathbf{k}_1(\mathbf{R}_1)$ and waves that are not rescattered $\mathbf{k}_0(\mathbf{R}_1)$; this is important in order to obtain the correct asymptotic behavior of the wave function. The field-modified momenta $\mathbf{k}_0(\mathbf{R}_1)$ and $\mathbf{k}_1(\mathbf{R}_1)$ exhibit different asymptotic behavior in the limit $R_1 \to \infty$.

As an application, the nonradiative decay of an atomic autoionization resonance in the field of the scattered charged particle was studied. The amplitude obtained for the process (37) by the stationary-phase method was used to analyze the effect of the three-particle PCI on the shape of the resonance line. The main result here—Eq. (55)—makes it possible to investigate in detail the relative contribution of the waves that are and are not rescattered to the electronic intensity as well as the possible interference between them. The three-particle effects associated the effect of the scattered charged particle on the momentum of the autoionization electron at the moment it makes a transition to the continuum are contained in the coefficient $K_\alpha(\varepsilon)$, which takes into account the change in the modulus of the momentum, and in the angular functions $P_L(\cos\theta_{0,1})$, which take into account the variations in the direction of motion of the autoionization electron under the action of the field of the scattered particle. For long-lived autoionization states the corrections introduced by the field of the scattered charged particle are small and, as a rule, can be neglected. For short-lived autoionization states, however, these corrections can be large, since in this case there is not enough time for the scattered particle to move far away from the atom at the moment the electron is ejected.

The quantitative investigation of the effects of the three-particle PCI in the spectra of the autoionization $(2s^2)^1S$ and $(2s2p)^1P$ resonances excited in the helium atom in collisions with 10–50 keV protons, $^3He^+$ ions, and antiprotons with small ejection angles established the following:

1. The structure observed in Ref. 17 in the low-energy wing of the $(2s^2)^1S$ resonance with 10 keV $^3He^+$ ions and ejection angle $\theta_e = 5°$ is associated with the rescattering of some of the autoionization electrons by the scattered $^3He^+$ ion. In addition, the interference of waves that are and are not scattered by the ion, and the incomplete screening of the nuclear charge of the ion by the bound electron play an important role in the formation of the "rescattering" peak.

2. A kinematic situation in which the intensity of the waves that have not been rescattered is low near the "rescattering" peak and the peak can be observed in its "pure form" is possible.

3. A new sign–charge interference effect was detected—additional structure can also appear in the left-hand wing of the resonance for negatively charged particles when the effect of the scattered particle on the motion of the autoionization electron at the moment it makes a transition to the continuous spectrum is taken into account.

The possibility of small variations in the direction of motion at the moment of ejection is associated with the topologically different character of the trajectories of an electron in an attractive field (electrons are focused) and a repulsive field (electrons are defocused). Using the optical–mechanical analogy, the positively charged scattered particles can be represented as a unique converging lens and the negatively charged particles can be represented as a diverging lens. The diverging lens plays the role of an instrument that makes it possible to resolve very fine details of the dynamics of the PCI at the moment of ejection of an electron. In this connection it is of great interest to study further the three-particle effects in the PCI in processes in which negatively charged particles participate: both light particles—$(e^-, 2e^-)$ processes and heavy particles—(p^-, p^-e^-) processes. The three-particle effects should be especially pronounced in the direct processes, where the electron ejection process is instantaneous

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