Effect of the target ion core on electron capture into the continuum of a fast neutral atom

Sh. D. Kunikeev and V. S. Senashenko

Scientific-Research Institute of Physics, Moscow State University
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We propose a unified mechanism of electron capture, induced by the field of the target ion core, into the continuum by a fast neutral atom. We show that in the process of scattering of two atoms virtual capture of an electron of the fast atom into a bound state of the ion core is possible. This reduces the screening of the nucleus of the atom and results in a Coulomb interaction potential between the free electron and atom: $V_s \sim Z_s(\mathbf{R}, E_s)/r_s$ with the effective charge Z_s, which is proportional to the probability of electron capture into a bound state of the ion core and depends on the internuclear separation $\mathbf{R}$ and the collision energy E_s (r_s is the distance between the free electron and the nucleus of the fast particle). We discuss the influence of the effective potential V_s on the intensity and shape of the peak in the energy spectra of electrons ejected at 0° as a function of the collision energy.

1. INTRODUCTION

Electron capture into low-lying states of the continuum in collisions of different ions with atoms has been investigated in detail, both experimentally[1–3] and theoretically.[4–6] It has been shown that as soon as the velocity of the ejected electron approaches in magnitude and direction the velocity of the scattered charged particle a sharp peak appears in the energy spectra of the electrons ejected at 0°. At the peak the velocity of the scattered particle is equal to the velocity of the ejected electron.[1,4] Different theoretical methods for describing the interaction of the electron with the scattered charged particle explain qualitatively the experimental data obtained.[4–6] When the interaction of the heavy charged particles in the final state is taken into consideration, the peak in the energy distribution of the electrons becomes significantly narrower.[7] The shape of this peak and the dependence of its position and width on the collision kinematics have been investigated in detail in experiments on ionization of inert-gas atoms by protons and multiply charged ions.[2,8]

Ionization collisions of neutral atoms have not been studied nearly as well. Recent experiments,[9–11] in which the ejected electron and the charged state of the scattered particle were recorded by the coincidence method, have shown that when positively charged atomic particles as well as neutral atomic particles are present in the final state for H–Ar, He–He, and He–Ar collisions at 75 keV, a peak is observed in the energy spectra of the electrons emitted in the forward direction. In addition, for neutral atoms the peak is even somewhat narrower than for positively charged scattered ions. At the same time, it has been observed in experiments with 0.15–2.5 MeV H^- and H^+ ion beams passing through thin carbon films that the peak in the spectra of electrons accompanying H atoms is strongly suppressed at zero ejection angle.[12]

Different theoretical models have been proposed in order to describe the observed phenomena. In Ref. 13 the peak observed for neutral atoms is associated with the presence of a low-lying virtual state in the ejected electron + scattered atom system in a long-lived excited state. In particular, it is proposed for the system *e*–He that the helium atom is in a metastable 2^1S state, for which the electron scattering length is quite long, which is a necessary condition for the appearance of a narrow peak in the electron energy distribution. In Ref. 14 the explanation of electron capture into the continuum of the neutral atom is based on the assumption that in a collision of atomic systems intermediate autodetached doubly and triply excited states of the negative ions He^{-**} and He^{-***} can form, and when these states decay electrons which are quite slow relative to the scattered neutral atom are ejected. In order to check these models it is necessary to perform additional investigations which would confirm the possibility of the formation of a significant number of metastable atoms in the beam or negative ions in intermediate resonance states.

In Ref. 15 an attempt was made to obtain, on the basis of the impulse approximation, a peak at small ejection angles for atoms in the ground state. It was shown that a wide peak forms for $\mathbf{v}_e = \mathbf{v}$, where $\mathbf{v}_e$ and $\mathbf{v}$ are, respectively, the velocity of the ejected electron and the velocity of the scatter particle. The appearance of this peak is explained by the presence of a long-range attractive polarization potential $V_{\rm pol} \sim \alpha/r_s^4$, where α is the dipole polarizability of the atom, between the free electron and the scattered atom. In Ref. 15, however, the fact that the scattering of the electron by the atom can depend strongly on the character of the dynamic screening of the nuclear charge of the fast particle,[16] which charge changes under the action of the ion core of the target atom, is neglected.

In the present paper we consider the effect of the target ion core on electron capture into the continuum of a fast neutral atom which modifies the effective interaction potential between the free electron and the scattered atom. It is shown that in the scattering process virtual capture of an electron from the fast atom into the bound state of the target ion core is possible and this decreases the screening effect of the electrons of the scattered particle and modifies the effective interaction potential between the free electron and the scattered atom, whose asymptotic form is $V_s \sim -Z_s(\mathbf{R})/r_s$, where $Z_s(\mathbf{R})$ is the effective charge of the fast particle and $\mathbf{R}$ is the separation between the nuclei.

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The influence of the effective potential V_s on the intensity and shape of the peak in the energy spectra of electrons ejected at 0° as a function of the collision energy is discussed. The atomic units $e = \hbar = m = 1$ are employed.

2. BASIC FORMULAS

Consider the collision of two neutral atoms:

$$A_s^0 + A_t^0 \to A_s^0 + A_t^+ + e, \tag{1}$$

as a result of which the target atom A_t^0 is ionized and three free particles are formed in the final state: the scattered atom A_s^0, the target ion core A_t^+, and an electron e ejected into a low-lying state of the continuum of A_s^0. In what follows, in constructing the wave function of the final state $\Psi_f^{(-)}$ we neglect the perturbation of the distribution of the electrons in bound states of A_s^0 and A_t^+ by the field of the free electron. In this approximation, we represent $\Psi_f^{(-)}$ as follows:

$$\Psi_f^{(-)}(\mathbf{R}, \mathbf{r}_i, \mathbf{r}) = \hat{A}[\chi_A^{(-)}(\mathbf{R}, \mathbf{r}_i)\chi_e^{(-)}(\mathbf{R}, \mathbf{r})], \tag{2}$$

where $\chi_A^{(-)}$ and $\chi_e^{(-)}$ are, respectively, the wave function of the subsystem $A_s^0 + A_t^+$ and the wave function of the free electron, $\mathbf{r}_i$ is the collection of coordinates of the electrons in a bound state, $\mathbf{r}$ are the coordinates of the free electron, and $\hat{A}$ is the antisymmetrization operator. We substitute the function (2) into Schrödinger's equation and integrate its right- and left-hand sides together with the functions $\chi_A^{(-)}$. Then, neglecting the nonlocal short-range exchange potential,[17] we obtain an equation for the wave function $\chi_e^{(-)}$:

$$[-iv\nabla_R - {}^1\!/_2\nabla_r^2 + V_e(\mathbf{R}, \mathbf{r})]\chi_e^{(-)}(\mathbf{R}, \mathbf{r}) = E\chi_e^{(-)}(\mathbf{R}, \mathbf{r}), \tag{3}$$

where $V_e(\mathbf{R},\mathbf{r})$ is the interaction potential between the free electron and the atom A_s^0 and the ion A_t^+, averaged over the states of the bound electrons for fixed values of $\mathbf{R}$ and $\mathbf{r}$:

$$V_e(\mathbf{R}, \mathbf{r}) = -\frac{Z_s}{r_s} - \frac{Z_t}{r_t} + \langle\chi_A^{(-)}(\mathbf{R}, \mathbf{r}_i)\sum_{i=1}^{Z_s+Z_t-1}\frac{1}{|\mathbf{r}-\mathbf{r}_i|}|\chi_A^{(-)}(\mathbf{R}, \mathbf{r}_i)\rangle / \langle\chi_A^{(-)}(\mathbf{R}, \mathbf{r}_i)|\chi_A^{(-)}(\mathbf{R}, \mathbf{r}_i)\rangle, \tag{4}$$

where $\mathbf{r}_s$ and $\mathbf{r}_t$ are the coordinates of the free electron relative to the nuclei of A_s^0 and A_t^+ with charges Z_s and Z_t, respectively, $\mathbf{r}$ are the coordinates of the free electron relative to the center of mass of the system $A_s^0 + A_t^+$; and, $E = k^2/2$ is the kinetic energy of the electron.

For $R \gg 1$ the wave function $\chi_A^{(-)}$ can be represented approximately in the form of the expansion[18]

$$\chi_A^{(-)} = \chi_f + \sum_\alpha \varphi_\alpha\psi_t\Lambda_\alpha^{(-)}(\mathbf{R}) + \sum_\beta \varphi_s\psi_\beta\Lambda_\beta^{(-)}(\mathbf{R}), \tag{5}$$

where

$$\Lambda_\gamma^{(-)}(\mathbf{R}) = 2\mu\int\frac{d\mathbf{K}}{(2\pi)^3}\frac{\exp(i\mathbf{K}\mathbf{R})T_{\gamma f}^{(-)}(\mathbf{K}, \mathbf{K}_f)}{K_\gamma^2 - K^2 - i0}, \quad \gamma = \alpha, \beta. \tag{6}$$

Here the indices α and β describe the channels for single-electron excitation of the atom $A_s^0(\alpha)$ and capture of one electron from the state f of the atom $A_s^0(f)$ into the bound state β of the target atom $A_t^0(\beta)$; φ_α, ψ_t, and φ_s, ψ_β are the wave functions of the bound states of $A_s^0(\alpha)$, A_t^+, and A_s^+, $A_t^0(\beta)$, respectively; χ_f is the asymptotic wave function of the system $A_s^0(f) + A_t^+$; $T_{\gamma f}^{(-)}$ is the transition amplitude from the state f into the state γ; $\mathbf{K}_\gamma$ and $\mathbf{K}_f$ are the relative momenta of the atoms in the channels γ and f; and, μ is the reduced mass of the heavy colliding particles. We note that in the expansion (5) the contribution of many-electron transitions, the excitation or ionization of the ion A_t^+ under the action of the atom A_s^0, as well as the small asymptotic terms describing the ionization of the atom A_s^0 and decreasing with distance as $|\mathbf{X}|^{-5/2}$, where $|\mathbf{X}| = (R^2 + r^2)^{1/2}$ (Ref. 18), is neglected.

If the expansion (5) is limited only to the asymptotic state χ_f, then after averaging in Eq. (4) we obtain the usual static interaction potential. The next terms in the expansion (5) describe the perturbation of the asymptotic state χ_f by the interaction of the atom A_s^0 with the ion A_t^+. For what follows, it is convenient to represent the integral (6) in cylindrical variables:

$$\Lambda_\gamma^{(-)}(\rho, t) = \frac{2\mu}{(2\pi)^3}\int d\mathbf{Q}_\perp \exp(i\mathbf{Q}_\perp\boldsymbol{\rho})I_\gamma^{(-)}(\mathbf{Q}_\perp, t), \tag{7}$$

where

$$I_\gamma^{(-)}(\mathbf{Q}_\perp, t) = \int_{-\infty}^{\infty} dK_\parallel \frac{\exp(iK_\parallel vt)T_{\gamma f}^{(-)}(K_\parallel, \mathbf{Q}_\perp, \mathbf{K}_f)}{P_\gamma^2 - K_\parallel^2 - i0},$$

$$\mathbf{R} = \boldsymbol{\rho} + vt\hat{\mathbf{K}}_f, \quad \mathbf{K} = K_\parallel\hat{\mathbf{K}}_f + \mathbf{Q}_\perp, \quad P_\gamma^2 = K_\gamma^2 - Q_\perp^2, \quad \hat{\mathbf{K}}_f = \mathbf{K}_f/K_f,$$

and $\mathbf{Q}_\perp$ is the transverse component of the transferred momentum. We note that the poles at $K_\parallel = \pm(P_\gamma - i0)$ make the main contribution to the integral $\Gamma_\gamma^{(-)}$. Its value is easily obtained by closing the integration contour and applying the residue theorem: for $t > 0$ the contour is closed in the upper half-plane and for $t < 0$ the contour is closed in the lower half-plane. In this case the integrals over the additional sections of the contour are higher order infinitesimals. Taking into consideration the fact that the amplitude $T_{\gamma f}^{(-)}$ decreases rapidly with increasing $Q_\perp$ and setting $P_\gamma = K_\gamma - Q_\perp^2/2K_\gamma$, we obtain

$$\Lambda_\gamma^{(-)}(\rho, t) = i\,\mathrm{sign}(t)\exp(-iK_\gamma v|t|)A_{\gamma f}^{(-)}(\rho, t), \tag{8}$$

where

$$A_{\gamma f}^{(-)}(\rho, t) = \frac{1}{2\pi v}\int_0^\infty Q_\perp dQ_\perp J_0(Q_\perp\rho)$$

$$\exp\left(i\frac{Q_\perp^2}{2\mu}|t|\right)T_{\gamma f}^{(-)}(-\mathrm{sign}(t)K_\gamma, Q_\perp, K_f).$$

Since $T_{\gamma f}^{(-)} \sim \mu^{-6} \ll 1$ for $t > 0$ (the backscattering case), we set $\Lambda_\gamma^{(-)}(\rho, t > 0) = 0$. If $t < 0$ and $1 \ll |t| \ll \mu$, then $\exp(iQ_\perp^2|t|/2\mu) \approx 1$ and $A_{\gamma f}^{(-)}(\rho, t) \approx A_{\gamma f}^{(-)}(\rho, -0)$ is the quasiclassical amplitude of the transition $f \to \gamma$. In the region $|t| \gg \mu$ the expression (8) describes a spherical wave.

We now examine in greater detail the effective potential $V_e(\mathbf{R},\mathbf{r})$. In averaging the expression (4) over the coordinates of the bound electrons, we take into account the fact that the wave functions φ_α and ψ_t describe states with Z_s and $Z_t - 1$ electrons bound relative to nuclei with Z_s and Z_t electrons, respectively, while the wave functions φ_s and ψ_β

describe states with $Z_s - 1$ and Z_t electrons bound relative to nuclei with charges Z_s and Z_t, respectively. Calculating the averages in the expression (4) with the wave function (5) and the transition amplitude (8) at distances greater than the dimensions of the region of localization of the atomic electrons, we obtain

$$V_e(\rho,t,\mathbf{r}) = -\frac{Z_s(\rho,t)}{r_s} - \frac{Z_t(\rho,t)}{r_t}, \tag{9}$$

where

$$Z_s(\rho,t)=\frac{P_{cap}(\rho,t)}{P_{cap}(\rho,t)+P_{exc}(\rho,t)+1}, \quad Z_t(\rho,t)=1-Z_s(\rho,t),$$

$$P_{exc}(\rho,t)=\sum_\alpha |A_{\alpha f}^{(-)}(\rho,t)|^2, \quad P_{cap}(\rho,t)=\sum_\beta |A_{\beta f}(\rho,t)|^2. \tag{10}$$

It is obvious from the formulas (9) and (10) that in the presence of interaction of A_s^0 and A_t^+ the electron charge density is redistributed, as a result of excitation and charge exchange at finite internuclear distances, between the atoms A_s^0 and A_t^+ in a manner such that the total effective charge of the system A_s^0 and A_t^+ remains unchanged, and for long times $|t| \ll \mu$ the charge $Z_s(\rho,t) \propto |t|^{-2}$ and the charge $Z_t(\rho,t) \to 1$. If $t<0$ and $|t| \ll \mu$, then $P_{exc}(\rho,t)$ and $P_{cap}(\rho,t)$ are virtually independent of t and determine, respectively, the probability of excitation and charge exchange in the interaction of A_s^0 and A_t^+. In the region $t>0$ the charge $Z_s(\rho,t) = 0$. Here the perturbation of the state of the atom $A_s^0(f)$ by the field of the free electron is neglected. This approximation is quite well-founded, since, as follows from Eq. (9), the polarization potential determining the magnitude of the perturbation, decreases asymptotically much more rapidly than does the potential $-Z_s(\rho,t)/r_s$.

We represent the approximate solution of Eq. (3) with the interaction potential (9) in a form analogous to the wave function of an electron in the field of two constant charges:[19]

$$\chi_e^{(-)} = \exp(i\mathbf{kr})\Phi_{\mathbf{k}_e}^{(-)}(\nu_t(\rho,t),\mathbf{r}_t)\Phi_{\mathbf{k}'_e}(\nu_s(\rho,t),\mathbf{r}_s), \tag{11}$$

where

$$\Phi_{\mathbf{k}}^{(-)}(\nu,\mathbf{r})=f_c^{(-)}(\nu)\,{}_1F_1(-i\nu,1,-ikr-i\mathbf{kr}),$$

$$f_c^{(-)}(\nu)=\exp\left(-\frac{\pi\nu}{2}\right)\Gamma(1-i\nu),$$

$$\nu_t(\rho,t)=-\frac{Z_t(\rho,t)}{k_e}, \quad V_s(\rho,t)=-\frac{Z_s(\rho,t)}{k_e'},$$

and $\exp(i\mathbf{kr})$ describes the motion of the electron relative to the center of mass of the system $A_s^0 + A_t^+$. The distorting factors $\Phi_{\mathbf{k}_e}^{(-)}$ and $\Phi_{\mathbf{k}'_e}^{(-)}$ take into account the perturbation of the plane-wave continuum as a result of the interaction of the electron with A_t^+ ion and the A_s^0 atom, where $\mathbf{k}_e$ and $\mathbf{k}'_e$ are the momenta of the electron relative to A_t^+ and A_s^0, respectively.

As follows from the formula (11), the effect of the field of the target ion core A_t^+ on the state of the electron in the continuum can be both direct and indirect. The indirect effect of the ion A_t^+ on the electron results from the perturbation of the atom A_s^0, due to which the electron density in the system $A_s^0 + A_t^+$ is redistributed and the screening of the nuclear charge of the atom A_s^0 is reduced. If the indirect effect of the charge of the ion A_t^+ on the electron is neglected, then in the formula (11) we must set $Z_s = 0$ and $Z_t = 1$. It should be noted that the approximation (11) is valid when the charges Z_s and Z_t vary slowly in time, i.e.,

$$\left|\frac{d}{dt}\ln Z_s(\rho,t)\right| \ll 1, \quad \left|\frac{d}{dt}\ln Z_t(\rho,t)\right| \ll 1.$$

The total ionization amplitude, obtained with the electron wave function (11), can be represented as a sum of two amplitudes, corresponding to the contributions of different sections of the trajectory with $t<0$ and $t>0$:

$$a_{fi}={}^1/_2[a_{fi}{}^B(Z_t(\rho),\rho)K_s(\rho)+a_{fi}{}^B(Z_t(\rho)=1,\rho)], \tag{12}$$

where

$$K_s(\rho)=f_c^{(-)*}\left(-\frac{Z_s(\rho)}{k'_e}\right)\left(1-\frac{k_{e\parallel}'}{Q_\parallel}\right)^{-iZ_s(\rho)/k'_e}.$$

Here a_{fi}^B is the Born amplitude of ionization and $Q_\parallel$ and $K_{e\parallel'}$ are the longitudinal components of the transferred momentum and the momentum of the electron relative to A_s^0. If the dependence of the charge Z_s on the impact parameter ρ is neglected in the transition from the region $t<0$ into the region $t>0$, i.e., $Z_s(\rho) \approx Z_s(0)$, and the change in the charge Z_t is also neglected, then the doubly differential ionization cross section describing the angular and energy distributions of the electrons ejected in collisions of neutral atoms is given by the expression

$$\frac{d^2\sigma}{dE_e\,d\Omega_e} = F_c\cdot\left(\frac{d^2\sigma}{dE_e\,d\Omega_e}\right)_B, \tag{13}$$

where $(d^2\sigma/dE_e d\Omega_e)_B$ is the ionization cross section in the Born approximation, and the factor $F_c = \frac{1}{4}|1 + K_s(0)|^2$ accounts for the increase in the ionization cross section as a result of the capture of an electron into the continuum of the neutral atom. The factor $F_c \to \pi Z_s(0)/2k'_e \to 0$ and $F_c \to 1$ for large values of k'_e.

3. DISCUSSION

The results of the calculations of the distribution of the effective charge Z_s as a function of the impact parameter ρ for different He^0–He^+ collision energies are presented in Fig. 1. To simplify the calculations, we included only two bound states in the expansion (5): the ground state of the

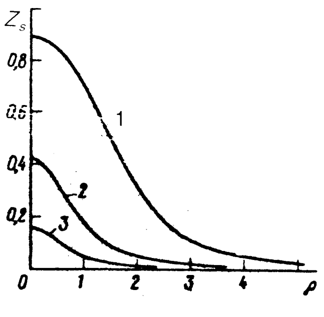

FIG. 1. Distribution of the effective charge Z_s as a function of the impact parameter ρ for different He^0–He^+ collision energies. The curves *1, 2,* and *3* correspond to collision energies of 100, 300, and 500 keV.

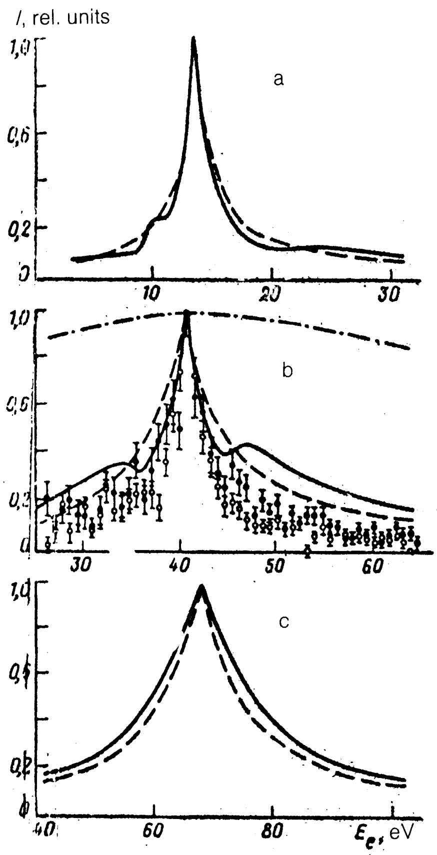

FIG. 2. Energy distributions of the intensity I of the spectra of forward-ejected electrons for different He^0–He^0 collision energies: 100 (a), 300 (b), and 500 keV (c). Present calculations: solid lines—theoretical intensities (13); dashed lines—the Coulomb normalization factor of the state of the continuum of an electron in the field of a charge $Z_s = 1$; dot-dashed line—the results of Ref. 15. The experimental data were taken from Ref. 9: ●—He^+–He; ○—He–He.

atom A_s^0 and the ground state of the atom A_t^0, neglecting the excitation of the atom A_s^0 and electron capture into excited states of the atom A_t^0. The capture amplitude was calculated in the approximation of intermediate states of the continuous spectrum.[20] The calculations show that the effective charge Z_s is concentrated near the internuclear axis, i.e., at $\rho = 0$, and as the impact parameter increases the effective charge monotonically decreases together with the probability of capture of an electron from the atom A_s^0 into a bound state of the atom A_t^0. The charge Z_s also decreases as the collision energy increases.

The results of calculations of the intensity of the spectra of forward-ejected electrons for different He^0–He^0 collision energies are presented in Fig. 2. In comparing with the experimental data of Ref. 9 (Fig. 2b), the theoretical intensities (13), minus the background formed by Born transitions, were averaged over the ejection angle with angular resolution $\Delta\theta_e = 3.5°$ (solid lines). One can see that the capture of an electron into the continuum of the neutral atom can lead to the formation of a sharp peak in the energy spectra of the forward-ejected electrons. For comparison, the dependence of the Coulomb normalization factor of the state of the continuum in the field of the charge $Z_s = 1$ (dashed lines) as well as the results of Ref. 15 (dot-dashed line) are shown in Fig. 2. One can see that the width Γ_0 of the peak in the case of collisions of neutral atoms can be both greater and less than the width Γ_+ of the peak in the case of collisions with a charged particle. For collision energies of 100, 300, and 500 keV we have $\Gamma_+/\Gamma_0 = 1.2$, 1.4, and 0.7, respectively. At 300 keV the experimental value is $\Gamma_+/\Gamma_0 = 1.6$. The calculations show that the narrowing of the peak in the electron energy spectrum is caused by the interference of ionization amplitudes on different sections of the trajectory of the fast particle.

The results of the present calculations are in good agreement with the experimental data in the central part of the peak, though in the wings appreciable differences are observed, probably due to the fact that the dependence of the charge Z_s on ρ was neglected. Obviously, as the effective charge decreases with increasing impact parameter, the intensity in the wings of the peak decreases. As the collision energy increases, the intensity of the peak and the magnitude of the interference oscillations of the contour decrease at the same time as the effective charge Z_s decreases. The small asymmetry, associated with the presence of the factor $(1 - k'_{e\|}/Q_\|)^{-iZ_s(0)/k'_e}$ in the expression for F_c, in the peak gradually decreases with increasing collision energy to the extent that the longitudinal transferred momentum $Q_\|$ increases.

4. CONCLUSIONS

In this paper we have thus proposed a mechanism, different from previously discussed mechanism,[13–15] for the formation of the peak observed in the energy distributions of electrons ejected in the forward direction in ionization collisions.[9–11] We have shown that the target ion core, whose presence results in distortion of the electron distribution in the fast particle in the final state and in a corresponding modification of the interaction potential between the free electron and the scattered atom, plays an important role in the electron capture into the continuum of the neutral atom. When the virtual capture of an electron of the scattered atom in the bound state of the ion core is taken into account, the screening of the nuclear charge of the atom is reduced and a Coulomb interaction potential, in which the nuclear charge is proportional to the probability of electron capture and depends on the internuclear distance, appears. The presence of such an interaction between the free electron and the scattered atom leads, in turn, to the formation of a narrow peak in the energy distributions of forward-ejected electrons; this agrees qualitatively with the experimental results.[9] In contrast to Ref. 13, the present study predicts that as the collision energy increases, the intensity of the peak will decrease and oscillations of the contour will appear in the wings at low collision energies.

The present model can be checked experimentally by investigating the dependence of the height of the peak on the collision energy. We also note that the experimental data of Ref. 9 reveal that the width of the observed peak depends on the structure of the target atom. The proposed model is consistent with these results, since the character of the interaction of the free electron and the scattered atom depends significantly on the target ion core, in particular, on the particular shell of the target atom from which the electron is ejected into the continuous spectrum. As far as the results of Ref. 12 are concerned, the observation of strong suppression of the peak is probably associated with the spatial delineation of the region of formation of convoy electrons in the solid and their subsequent transport and capture into the continuum of the fast atom at the exit from the target. Under these conditions the virtual capture of an electron from the fast atom into the bound state of an atom of the medium is unlikely.

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