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Influence of the Coulomb interaction in the final state on the cross section of single-electron capture by fast ions

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ABSTRACT

It is shown that the Coulomb interaction of ions in the final state must be taken into account in the estimation of the cross section of electron capture by fast ions. The cross section of electron capture decreases considerably, and the dependence of the cross section on the collision energy becomes close to the experimental one if the interaction of charged particles after collision is taken into account.

1. Introduction

To estimate the charge distribution and the energy loss of ions passing through the material, it is necessary to obtain information about the cross section of electron capture for the collision of two multielectron systems, namely, the projectile $X^{q+}(Z)$ with the ionic charge q, the nuclear charge Z, and the number of electrons $N_i = Z - q$ and the target atom $A(Z_t)$ with the nuclear charge Z_t,

$$X^{q+}(Z) + A(Z_t) \to X^{(q-1)+}(Z) + A^{+}(Z_t), \tag{1}$$

where the scattered ion $X^{(q-1)+}(Z)$ is in the ground state or in one of the excited states.

Theoretical methods for describing the cross section $\sigma_{q,q-1}$ of single-electron capture have been developed as long ago as the last century [1–3]. They include various versions of perturbation theory or the method of distorted waves for fast collisions and the method of strong channel coupling for slow collisions. Each method has its own restrictions on the collision velocity V, the projectile parameters q and Z, and certain states of the active electron in the target atom and scattered particle. The Oppenheimer–Brinkman–Kramers (OBK) approximation [4–6] is one of the simplest methods for describing the electron capture (1) by fast ions. In this approximation taking into account the shell structure of both the projectile and the target atom, the electron is captured only because of its interaction with the projectile, and the internuclear interaction potential and the change in the recession kinematics in the final state because of the Coulomb interaction for $q \neq 1$ are not taken into account. Difficulties emerged when the efforts were made to define this approximation more exactly. It turned out that, sometimes, the first Born approximation taking the internuclear interaction into account describes experimental data for fast collisions worse than the OBK approximation [7]. This is related to the fact that the contribution of the internuclear interaction potential to the amplitude of the electron capture process is nonzero only because the wave functions of the initial and final states (1) are not orthogonal. The internuclear interaction potential cannot be considered in the first order of perturbation theory without considering the amplitudes of higher orders [2]. The electron capture from the outer shell of the target atom because of the internuclear interaction can be regarded as a correction to the amplitude in the OBK approximation only in the range of intermediate collision energy [8]. In addition, it was impossible to take into account the effect of Coulomb interaction of charged particles in the final states on $\sigma_{q,q-1}$. Up to now, it was assumed [2,3] that this interaction only leads to the appearance of the phase factor in the amplitude and, consequently, does not change $\sigma_{q,q-1}$. Such an approximation is substantiated strictly only in the case of Rutherford scattering and is used successfully in the problem of atom ionization by fast ions; however, its applicability to the problems related to the electron capture (1) is not obvious. The specific character of the process of electron capture is that the electron is captured by the fast ion when it passes through the electron cloud of the target atom, i.e., in the case of small internuclear distances. This is the difference between process (1) and scattering by the Coulomb potential and atom ionization by fast ions, in the case of which large internuclear distances and small transferred momenta contribute mainly to the amplitude.

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The aim of this paper is to estimate the effect of Coulomb interaction in the final state on the cross section $\sigma_{q,q-1}$ for $q > 1$.

2. Theoretical model

We assume that the influence of interaction between charged particles in final state is more significant than the influence of interaction between ion and neutral particle (atom) in initial state. In the case of fast collisions, the amplitude for the process of single-electron capture can be represented in the form

$$T(\mathbf{Q}) = \left\langle \Psi_{nLS}(\mathbf{r}) \exp(i\mathbf{K}_f\mathbf{R}) F(\xi,\mathbf{R}) \right| - \frac{q}{r} \left| \psi_{\nu\lambda\mu}(Z_t,\mathbf{x}) \exp(i\mathbf{K}_i\mathbf{R}) \right\rangle,$$

$$F(\xi,\mathbf{R}) = \exp\left\{ i\xi \ln(VR + \mathbf{V}{\cdot}\mathbf{R}) \right\}, \quad \xi = (q-1)/V, \tag{2}$$

where $\mathbf{x}$ and $\mathbf{r}$ characterize the positions of the active electron with respect to the nuclei of the target atom and the projectile, respectively; $\mathbf{R} = \mathbf{r} - \mathbf{x}$ is the internuclear distance; $\mathbf{K}_i$ and $\mathbf{K}_f$ are the momenta of the projectile and the scattered particle, respectively; $\mathbf{V}$ is the velocity of the scattered ion; $\psi_{\nu\lambda\mu}(Z_t,\mathbf{x})$ is the wave function of the active electron in the target atom with the principal quantum number ν, the orbital momentum λ, and the projection μ of this momentum; $\Psi_{nLS}(\mathbf{r})$ is the wave function of the active electron in the state of the scattered particle characterized by the quantum numbers n, L, and S; $\mathbf{Q} = \mathbf{K}_i - \mathbf{K}_f$ is the transferred momentum. Amplitude (2) differs from the amplitude in the OBK approximation [4–6] by the factor $F(\xi,\mathbf{R})$, which for $q \neq 1$ takes the Coulomb interaction of ions in the final states (1) into account. When the parameter $\xi = (q-1)/V$ increases the number of oscillations $F(\xi,\mathbf{R})$ increases also and the interaction becomes stronger. Approximation (2) was called the Coulomb–Brinkman–Kramers (CBK) approximation [9] in the problem describing the cross section that is differential with respect to the scattering angle.

If the effect of the active electron on the interaction of heavy particles in the final state (1) is neglected, amplitude (2) can be represented in the form

$$\begin{aligned} T(\mathbf{Q}) = {} & -(4\pi)^2 q Y_{lm}(\mathbf{Q}/Q) Y^*_{\lambda\mu}(\mathbf{Q}/Q) i^{l-\lambda} \\ & \times \int dr\, r \varphi_{nl}(Z,r) j_l(Qr) \\ & \times \int dx\, x^2 \varphi_{\nu\lambda}(Z_t,x) j_\lambda(Qx) \Phi(\xi,r,x), \end{aligned} \tag{3}$$

$$\Phi(\xi,r,x) = \int d\Omega_r\, d\Omega_x\, F(\xi,\mathbf{R}), \tag{4}$$

where $\varphi_{\nu\lambda}(Z_t,x)$ is the radial part of the wave function of the active electron in the target atom, $\varphi_{nl}(Z,r)$ is the radial part of the wave function of the active electron in the state of scattered ion characterized by the quantum numbers n and l, $j_l(Qr)$ and $j_\lambda(Qx)$ are the spherical Bessel functions, $Y_{lm}(\mathbf{Q}/Q)$ are the spherical harmonics, and $d\Omega_r$ and $d\Omega_x$ are the solid angles characterizing the positions of the active electron with respect to the nuclei of the projectile and the target atom, respectively.

The cross section of electron capture is calculated by integrating amplitude (3) over $\mathbf{Q}$, then by summing over the final states of the scattered particle and by averaging over all initial states of the active electron of the target atom

$$\sigma_{q,q-1} = \sum_{\nu\lambda\mu} \sum_{nLMS} \frac{f_S}{(2\lambda+1)} \int_{Q_{\min}}^{\infty} \left| T(\mathbf{Q}) \right|^2 d\mathbf{Q} / \left(8\pi^2 V^2 \right), \tag{5}$$

where $Q_{\min}$ is determined according to the energy and momentum conservation laws. It should be noted that $Q_{\min} \sim V$ in case of fast collisions [1] and $\sigma_{q,q-1}$ is determined in the region of large scattering angles, where $Q > V$. According to the property of Fourier transform this region of Q corresponds to region of small R. The single-electron capture by fast ions is absent at large R and large impact parameter. It can be explained by the presence of two exponential factors $((\varphi_{\nu\lambda}(Z_t,x) \sim \exp(-Z_t,x/\nu)$ and $\varphi_{nl}(Z,r)) \sim \exp(-Zr/n))$ in amplitude (3). These features distinguish the process of single-electron capture from the process of ionization of atom by fast ions.

The coefficient f_S in (5) is the probability that the scattered particle is in the state with the quantum number S. If the outer electron shell of the projectile is filled ($N_i = 2, 4, 10, \ldots$), then the state of the scattered particle is characterized by $S = 1/2$ irrespective of the spin of the active electron; then $f_S = 1$. For the projectile with the unfilled outer electron shell ($N_i = 1, 3, 5, 6, \ldots$), the scattered particle can be in two spin states, depending on the spin projection of the active electron. In this case, $f_S = 0.5$ if the averaging over all initial states of the target atom are taken into account.

The submitted model and first-order Born approximation with Coulomb boundary conditions model [3,10] have some differences. The approximation [10] can be used for electron capture from the K-shell of target atoms into K-shell of projectile. The most calculations [10] were related for protons ($q = 1$). The submitted model takes into account the electron capture from all shells of target atom into any shell of projectile. This model neglects the interaction in the final state for neutral scattered particle $X^{(q-1)+}(Z)$ at $q = 1$ and the internuclear interaction potential.

3. Results of our calculations

To describe the wave functions of the excited states of the scattered particle with several electrons, we used the functions obtained by numerical solution of the Hartree–Fock equation [11], which were approximated with the combination of Slater orbitals for $n \leqslant 5$ and $l \leqslant 2$ [12].

The oscillated integral with the infinite upper limit (3) was calculated by taking the interaction in the final state into account. To do this, three versions of calculations were carried out: the analytical calculation with $\Phi(\xi,r,x) = 1$, the numerical calculation with $\Phi(\xi,r,x) = 1$, and the numerical calculation with $\Phi(\xi,r,x) \neq 1$. The first two versions were required to choose a grid with the variables r and x, which provided the desired accuracy of the numerical integration for a given Q. It is assumed that the function $\Phi(\xi,r,x) \neq 1$, which is smooth and independent of Q, does not change the convergence conditions for integral (3). Then the numerical calculation with $\Phi(\xi,r,x) \neq 1$ for the same grid makes it possible to take the interaction of charged particles in the final states into account.

The results of calculating $\sigma_{q,q-1}$ for the collision of O^{8+} ions with the Ar atom (Fig. 1) show that the interaction in the final state decreases $\sigma_{q,q-1}$ by an order of magnitude or more as compared with the results of calculations in the OBK approximation. The differences between the theoretical cross section in the OBK approximation and the experimental data were not related previously with the effect of Coulomb interaction in the final state. This factor was neglected in analogy with the processes of Rutherford scattering and single atom ionization by fast ions. Our calculations show that the effect of interaction in the final state on $\sigma_{q,q-1}$ is and can be sufficiently strong. The Coulomb interaction pushes the scattered ion from the interaction region, decreasing the time required for this interaction, and $\sigma_{q,q-1}$ decreases, because the range of small R contributes mainly to (3). In this case the deviation of closest point of approach of heavy particles can be comparable with the size of target atom because the straight-line trajectory approximation is inaccurate at large scattering angles. Decreasing the projectile charge q (Fig. 2) or increasing V (Figs. 1 and 2) also leads to a decrease in the difference between two versions of the

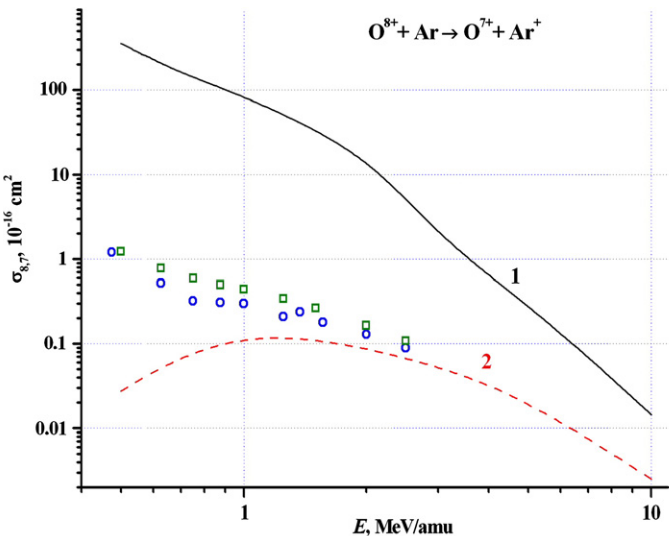

Fig. 1. Cross section σ_{87} of electron capture for the process of collisions of O^{8+} ions with Ar atoms. The calculated results: curve 1 corresponds to the OBK approximation and curve 2 corresponds to the approximation taking into account the Coulomb interaction of scattered ions. The experimental data are denoted by (○) [13] and (□) [14].

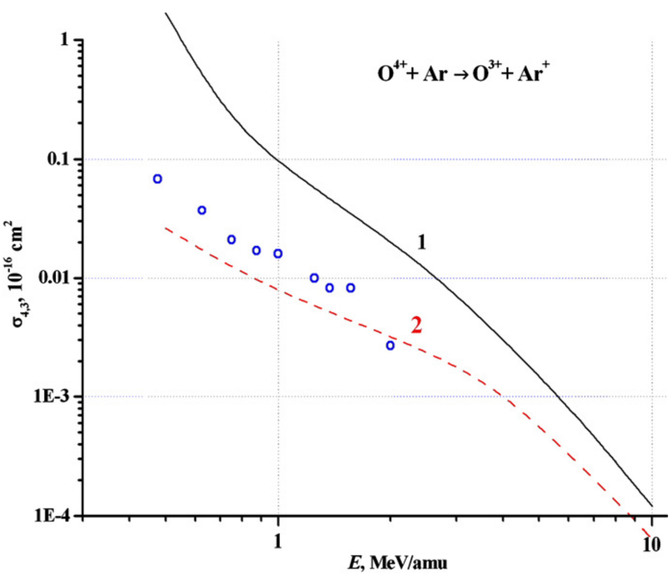

Fig. 2. Cross section σ_{43} of electron capture for the process of collisions of O^{4+} ions with Ar atoms. The same notation as in Fig. 1.

theory, and the results of calculations with the Coulomb interaction of particles in the final states taken into account and without considering it coincide as $\xi \to 0$.

The dependence on the energy of the cross section obtained in the OBK approximation and the experimental dependences are different (Figs. 1 and 2); i.e., their ratio depends on E. For the theoretical version taking the interaction in the final state into account, these dependences are close for fast collisions. This makes it possible to determine the difference between the theoretical cross section and the experimental one.

4. Conclusion

It was assumed previously that the Coulomb interaction of ions in the final state only leads to the appearance of the phase factor in the amplitude and does not affect the cross section of electron capture by fast ions. Our theoretical analysis and the calculated results show that the effect of interaction of ions in the final state on the cross section of electron capture exists and can lead to a considerable decrease in $\sigma_{q,q-1}$. In addition, the dependence of the theoretical cross section of single-electron capture on E taking the interaction in the final state for fast collisions into account is close to the experimental one, which makes it possible to analyze the relationship between the theoretical and experimental results.

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