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COUPLING OF THE DIRECT AND THE EXCHANGE SCATTERING IN SLOW ION-ATOM COLLISIONS

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Abstract: The effect of the direct interaction in a slow ion-atom collision on the exchange amplitude is considered. A modified formula is obtained for the $A^{2+}-A$ resonant charge exchange cross section and calculations are made for the case of A being an inert gas atom. The polarization (ion) capture radius and the elastic scattering cross section are estimated at thermal energies.

1. Introduction

In the theoretical treatment of the resonant rearrangement in heavy particle collisions it is usually assumed that impact parameters which give the main contribution to the reaction cross section are much larger than the effective potential range of the interacting particles. The relative nuclear coordinate R can be taken to have a linear time dependence. These assumptions are justified if the cross section of the exchange process (i. e. resonant charge exchange, resonant excitation transfer, spin exchange) is much larger than the elastic cross section. This is the case with single charged ion-parent gas atom collisions in the energy region $\gtrsim$ eV. However, in the scattering of multi-charged ions with atoms of their own gas, or with ions and excited atoms, the forces of the direct (potential) interaction are strong, and the elastic scattering amplitude has an appreciable value even at large impact parameters. The trajectories of heavy particles are not straight lines and in the exchange scattering calculations the ion-atom long-range potential interaction must be taken into account.

The effect of the elastic scattering on the single electron resonant capture has been analyzed by Bates and Boyd[1] and Smirnov[2]. The problem of elastic-inelastic scattering coupling has been treated by Demkov[3] in a general way. These authors, however, have made no estimates of the energy region in which the role of the direct scattering becomes dominant, nor of the elastic and exchange cross sections in this and higher energy regions. In the present paper we shall consider this problem for slow collisions of doubly charged ions with their parent atoms, where the coupling of the direct and the exchange amplitudes is expected to be great. The long-range potential interaction in the $A^{2+}-A$ system is strong, while the resonant charge exchange cross section is relatively small. For example, at the collision energy of 125 eV the charge-exchange cross section for the $He^{2+}-He$ reaction is about seven times smaller than for the $H^{+}-H$ reaction. It will be

shown that the elastic A^{2+} — A cross section is of the same order of magnitude as the exchange cross section in the thermal energy region.

In the next section the expression will be derived for the resonant two-electron capture cross section in A^{2+} — A collisions considered extensively in ref.[4] and[5]. In Section 3 this result will be modified on account of the polarization interaction between the A^{2+} ion and the A atom. The approximate expressions for elastic and charge exchange cross sections will be given in Section 4 considering the ion-atom collision as an orbiting collision. The modified charge exchange cross section calculations and some estimates of the elastic scattering cross section in the thermal region for the A — inert gas atom case will be given in the last section. Atomic units are used throughout the text.

2. *Effective cross section for resonant double charge exchange*

Let us consider the resonant charge exchange process in the collision of doubly charged ions with their parent gas atoms

$$A^{2+} + A \rightarrow A + A^{2+} \tag{1}$$

at low relative velocities. Due to the symmetry of the problem, the eigenfunctions of the Hamiltonian H of the system could be odd (ψ_u) and even (ψ_g) functions, depending on whether they change or do not change the sign under reflection of all electrons from the symmetry plane of the quasimolecule. As it is known, the corresponding energies E_u and E_g are degenerated at infinity. With decreasing internuclear separation, the interaction of these states eliminates the degeneracy and causes intense transitions of two electrons from the atom to the ion. These electron exchange effects begin to manifest themselves at large interatomic distances, where other energy levels of the quasimolecule are far enough from the u and g levels under consideration, and can be ignored in determining the probability of the reaction (1). Thus, the problem can be considered in the two-state approximation. From the molecular wave functions ψ_g and ψ_u, at $t \rightarrow \mp\infty$ two linear combinations can be constructed to describe the localized motion of two electrons in the atoms

$$\psi_{i,f} = \frac{1}{\sqrt{2}}(\psi_g \mp \psi_u). \tag{2}$$

In the adiabatic approximation, the energies E_g and E_u depend on the internuclear separation $R(t)$ as on a parameter. The solution of the Schrödinger equation $i\frac{\partial \Psi}{\partial t} = H\Psi$, which at $t \rightarrow -\infty$ describes the motion of the active electrons in the initial atom (i. e. $\Psi\ (t \rightarrow -\infty) = \psi_i$), at a finite time t has the form

$$\Psi = \frac{1}{\sqrt{2}}\left\{\psi_g\, e^{-i\int_{-\infty}^{t} E_g(t)\,dt} + \psi_u\, e^{-i\int_{-\infty}^{t} E_u(t)\,dt}\right\}. \tag{3}$$

At $t \to +\infty$ the total wave function (3) of the system has to be represented by a linear combination of the atomic wave functions ψ_t and ψ_f. Two-electron exchange amplitude is defined as

$$w = \left| \langle \psi_f | \Psi (t \to +\infty) \rangle \right|^2. \tag{4}$$

Using (2) and (3) and the orthogonality of the molecular wave functions as $R \to \infty$, we obtain from (4)

$$w = \sin^2 \zeta, \quad \zeta = \frac{1}{2} \int_{-\infty}^{+\infty} (E_u - E_g)\, \mathrm{d}t. \tag{5}$$

These adiabatic considerations show that resonant exchange reactions occur not because of any electronic transition between the g and u states, but because of their interference. Therefore, resonant exchange processes take place even at large interatomic separations and in this region they have large crosss sections compared to those of elastic and other inelastic processes. For this reason, the impact parameter method may be used in the derivation of the exchange cross section. Assuming a linear time dependence of the internuclear distance

$$\vec{R}(t) = \vec{v}\, t + \vec{\rho}, \quad (\vec{v}, \vec{\rho}) = 0, \tag{6}$$

where $\vec{v}$ is the relative velocity and $\vec{\rho}$ is the impact parameter, the integration of (5) over the impact parameters and the azimuthal angle gives for the charge exchange cross section

$$\sigma = 2\pi \int_0^\infty \sin^2 \zeta(\rho)\, \rho\, \mathrm{d}\rho, \tag{7}$$

$$\zeta(\rho) = \int_0^\infty \frac{\Delta(R)\, R \mathrm{d}R}{v\, [R^2 - \rho^2]^{1/2}}, \quad \Delta(R) = E_u(R) - E_g(R). \tag{8}$$

The knowledge of the energy separation $\Delta(R)$ of the symmetrical and antisymmetrical states at large R is of basic importance for the determination of the cross section. The perturbation methods can give this quantity within an exponential accuracy only. Since $\Delta(R)$ at large R is an exponentially small quantity, an exact asymptotic expression is needed for ΔR. For the two-electron exchange, as in the reaction (1), an exact asymptotic expression for $\Delta(R)$ is given by[4]

$$\Delta(R) = A\, R^{\varkappa}\, \mathrm{e}^{-\gamma R}, \tag{9}$$

where γ, $\varkappa$ and A are constants depending on the parameters of the two-electron atomic wave function. Although $\Delta(R)$ is small at large R, there exists an impact parameter region $(0, \rho_0)$ in which the integral $\zeta(\rho)$ has large values, so that the $\sin^2 \zeta$ function can be averaged, and the expression (7) gives

$$\sigma = \frac{1}{2} \pi \rho_0^2 + 2\pi \int_{\rho_0}^\infty \sin^2 \zeta\, \rho\, \mathrm{d}\rho. \tag{10}$$

The critical impact parameter ρ_0 should be chosen in such a manner that at $\rho > \rho_0$ the $\zeta(\rho)$ already enters its asymptotic region and the integral term in (10) can be neglected. This condition is fulfilled if ρ_0 is determined from the equation[5]

$$\int_{\rho_0}^{\infty} \frac{\Delta(R)\, R\,dR}{v\,[R^2 - \rho_0^2]^{1/2}} = \frac{e^{-C}}{2} = 0.28, \tag{11}$$

and then the charge exchange cross section is

$$\sigma_0 = \frac{1}{2}\pi\rho_0^2. \tag{12}$$

In (11) C is Euler's constant.

With the expression (9) for $\Delta(R)$, the integral in (11) at large ρ_0 can be expressed in terms of the zero-order McDonald function. Using its asymptotic behaviour one obtains the following transcendental equation for ρ_0

$$B\,\rho_0^{\varkappa+1/2}\,e^{-\gamma\rho_0} = 0.28\,v, \quad B = A\sqrt{\frac{\pi}{2\gamma}}. \tag{13}$$

For the determination of the parameters γ, $\varkappa$ and A, see ref.[4]

3. Modification of the exchange cross section for the direct ion-atom interaction

The formulas (12) and (13) of the preceding section for the double charge exchange cross section, are derived ignoring the strong polarization interaction in the $A^{2+}-A$ system. For this reason we shall modify these formulas and shall take into consideration the interparticle potential $U(R)$. Now the trajectories of heavy particles are not defined by (6) and, therefore, the interatomic distances giving the main contribution to the exchange cross section are determined not by (11) but by[6]

$$\int_{R_1}^{\infty} \frac{\Delta(R)\, R\,dR}{v\left[R^2 - \rho_0^2 - R^2\,\dfrac{U(R)}{E}\right]^{1/2}} = 0.28. \tag{14}$$

Here R_1 is the greatest pole of the integrand and E the kinetic energy of the relative motion. The integral in (14) rapidly converges in the neighbourhood of distant poles, such as R_1, and expanding the denominator in a power series we can calculate the asymptotic value of the integral, with $\Delta(R)$ from (9)

$$\frac{B}{v}\,\frac{R_1^{\varkappa+1/2}\,e^{-\gamma R_1}}{\left[\dfrac{\rho_0^2}{R_1^2} - \dfrac{R_1 U'(R_1)}{2E}\right]^{1/2}} = 0.28. \tag{15}$$

Comparing (13) and (15) we see that the case of $U(R) \neq 0$ can be reduced formally to the case of $U(R) = 0$ by the following correspondence: $R_1 \to \rho_0$ and

(16)

Further, using the definition of the turning point R_1

$$1 - \frac{\rho_0^2}{R_1^2} - \frac{U(R_1)}{E} = 0 \tag{17}$$

the expression for the resonant charge exchange cross section can be written in the form

$$\sigma_1 = \frac{1}{2}\pi\rho_0^2 (U \neq 0) = \frac{1}{2}\pi R_1^2 \left[1 - \frac{U(R_1)}{R}\right]. \tag{18}$$

At large interatomic distances the potential interaction in the $A^{2+} - A$ system is of the polarization type $U(R) = -\frac{2\alpha}{R^4}$ (α is the polarizability of the atom), so that the charge exchange cross section in $A^{2+} - A$ collisions is determined by the formulas

$$\sigma_1 = \frac{1}{2}\pi R_1^2 \left(1 + \frac{2\alpha}{E R_1^4}\right), \tag{19}$$

$$B R_1^{\varkappa + 1/2} e^{-\gamma R_1} = 0.28\, v \left(1 - \frac{2\alpha}{E R_1^4}\right)^{1/2}. \tag{20}$$

As may be seen from these expressions, the inclusion of the direct particle interaction into consideration makes the exchange cross section larger than that for the $U(R) = 0$ case, when the interparticle potential is attractive. If $U(R)$ is a repulsive potential, its effect is opposite. These direct scattering effects on the exchange cross section may be ignored if the collision energy is much greater than the potential energy in the region of interatomic separations giving the dominant contribution

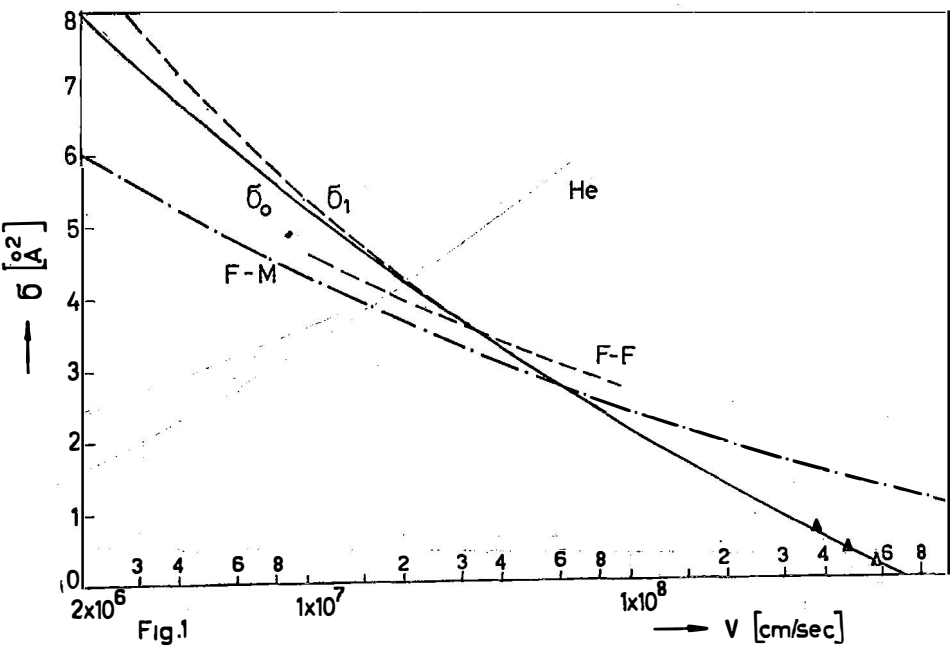

Fig.1

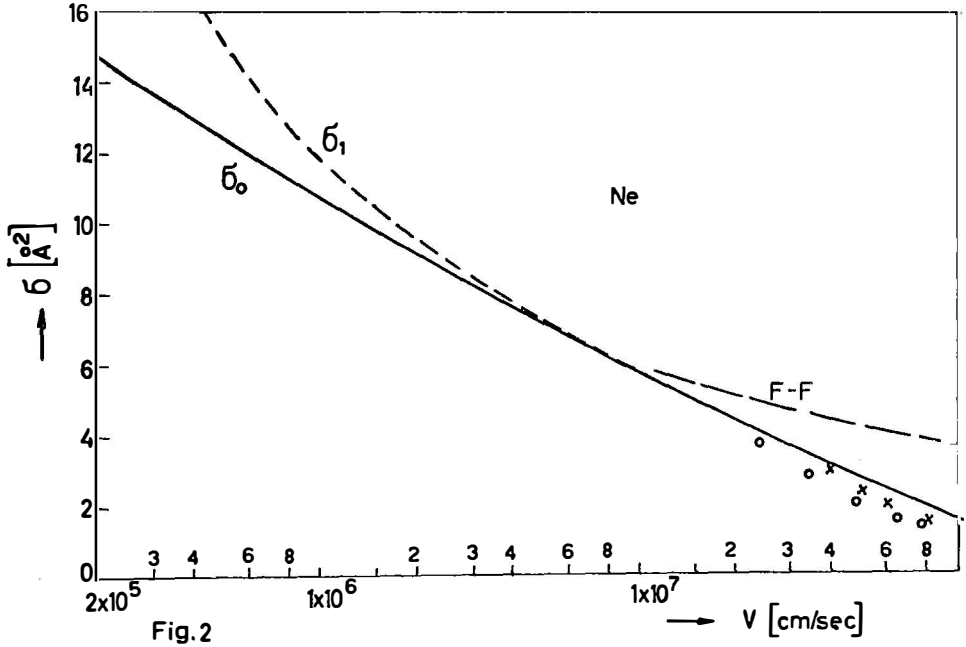
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Fig. 2

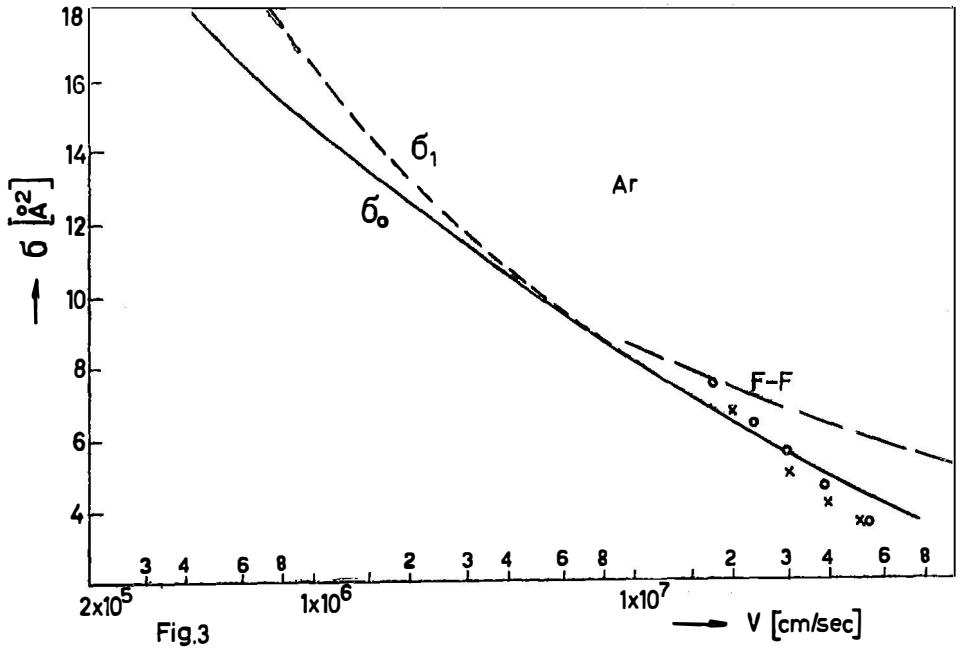
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Fig. 3

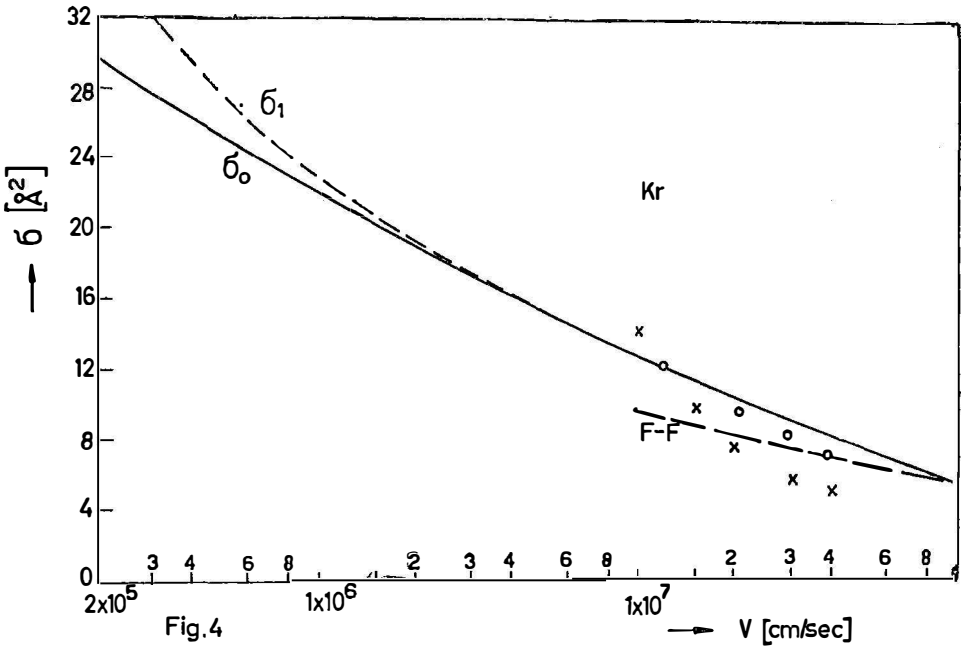

Fig. 4

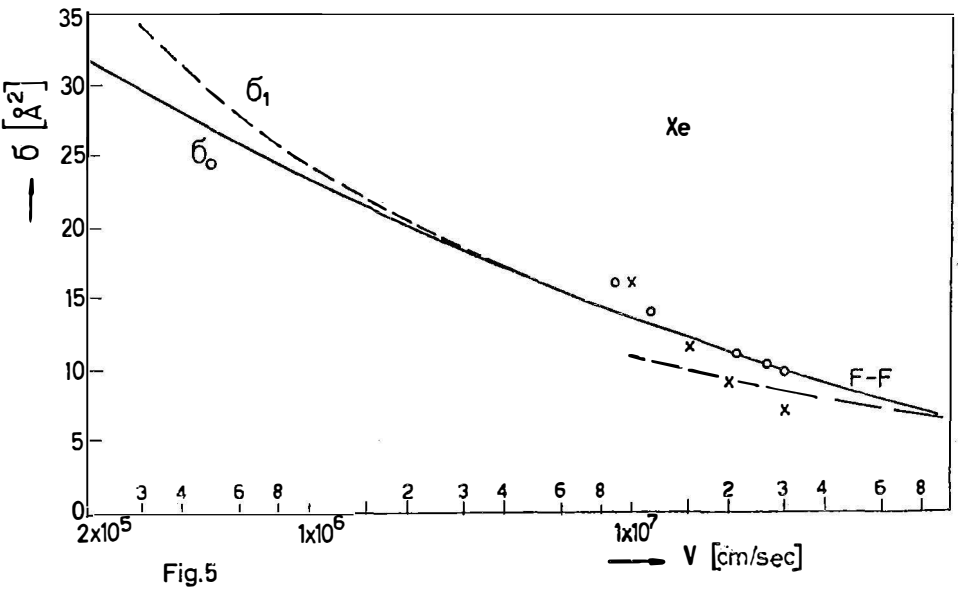

Fig. 5

Fig. 1–5. Resonant double charge exchange cross sections. Curves σ_1 and σ_0 represent our calculations of the cross section with and without taking into account the direct interparticle interaction. Curves F-F and F-M are variational results of refs. [10] and [11]. Symbols ▲, *o*, *x* represent the experimental data od refs. [7], [8] and [9] respectively.

to the cross section, $E \gg U(R_1)$. This condition can be rewritten in our case of $A^{2+} - A$ collisions as

$$v \gg v_c = \frac{2\pi}{\sigma}\sqrt{\frac{\alpha}{\mu}}, \tag{21}$$

where σ is the double charge exchange cross section and μ the reduced mass of the nuclei. If A is an inert gas atom v_c is about 10^{-3}, which corresponds to the thermal energy region.

4. *Polarization capture of the ion and elastic scattering cross section*

The strong attractive character of the potential interaction in the $A^{2+} - A$ system makes possible a capture of the ion by the atom in a slow collision during a finite time. After that the ion can leave the atom. Due to the long collision time of such an »orbiting« collision, the probabilities of the elastic and the exchange scattering are equal and amount to 1/2. In an interparticle attractive potential of the form $-\ a\ R^{-n}$ the orbiting collision occurs when the interatomic distance R becomes smaller than a value of $R_c = \left[\frac{a(n-2)}{2E}\right]^{1/n}$. In this case the capture cross section is given as

$$\sigma_c = \pi \left(\frac{n}{n-2}\right) \left[\frac{a(n-2)}{2E}\right]^{2/n}. \tag{22}$$

In the case of $A^{2+} - A$ slow collisions this cross section is $2\pi \left(\frac{2\alpha}{E}\right)^{1/2}$, so that for elastic and exchange processes at $R_1 < R_c$ we have

$$\sigma_{el} = \sigma_{ex} = \pi R_c^2, \quad R_c = \left(\frac{2\alpha}{E}\right)^{1/2} > R_1. \tag{23}$$

Hence, the formula (19) determines the double charge exchange cross section only in the region $R_1 > R_c$. At $R_1 = R_c$ the expressions (19) and (23) give the same cross section value; moreover, at this point their first derivatives in v are equal.

5. *Modified double charge exchange cross section calculations*

The critical velocity v_c defined by (21), at which $E = U(R_1)$, can be estimated in the case of A being an inert gas atom, by determining the double charge exchange cross section using an appropriate low energy extrapolation of the experimental data of[7-9]. The values obtained are given in Table 1. The critical velocities define the polarization ion capture radii R_c, see (23), which are also given in Table 1. The elastic scattering cross section σ_{el} calculated for the critical velocity is of the same order of magnitude as σ_0, and for Xe it is about twice σ_0. Thus, at $v \lesssim v_c$ the charge exchange cross section must be calculated using (19)-(20). The results of these calculations are represented in Figs. 1-5. The cross sections σ_0 in these figures are taken from ref.[4]. In the low velocity region the difference $\sigma_1 - \sigma_0$ be-

Table 1

Gas	$v_c\ 10^3$	R_c	$\sigma_{el}\ [\pi a_0^2]$	$\sigma_0\ [\pi a_0^2]$
He	3.860	5.9	11.6	10.2
Ne	1.370	7.7	18.9	14.6
Ar	1.300	9.5	30.2	20.4
Kr	0.627	12.6	51.0	34.6
Xe	0.453	14.2	64.6	38.2

comes appreciable. The experimental data in the figures are those of[7-9]. The curves F-F and F-M represent the theoretical calculations of Fetisov and Firsov[10] and Ferguson and Moiseiwitsch,[11] respectively. These authors determined the energy separation $\Delta(R)$ by the variational methods, which are not adequate for this purpose. Therefore, their results for σ_0 are fairly rough.

Thus, our σ_1 calculations confirm that in a multi-charged ion-atom collision, when the exchange cross-section is small, the effect of the direct interaction on the exchange amplitude is appreciable, especially at low energies.

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VEZA POTENCIJALNOG I IZMENSKOG RASPRŠENJA U SPORIM SUDARIMA IONA I ATOMA

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Sadržaj

Razmotren je uticaj direktne interakcije na amplitudu izmene u sporim sudarima iona i atoma. Za $A^{2+} - A$ rezonantnu izmenu naelektrisanja dobivena je modifikovana formula preseka uzimajući u obzir ovaj uticaj. Kada je A atom inertnog gasa, izvršena su izračunavanja preseka po ovoj formuli. Procenjene su vrednosti radiusa polarizacionog zahvata i elastični preseci pri ovim sudarima u termalnoj oblasti energija.