Charge-exchange collisions of multiply charged ions with atoms

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The problem of electron transfer between neutral atoms and multiply charged ions is considered at low and medium energies. It is assumed that a large number of final states are available for the electron transition so that the electron-capture process is treated as a tunnel effect caused by the strong attractive Coulomb field of the multicharged ion. The electron transition probability is obtained in a closed form using the modified-comparison-equation method to solve the Schrödinger equation. An approximately linear dependence of the one-electron transfer cross section on the charge of multicharged ions is found. Cross-section calculations of a number of charge-exchange reactions are performed.

I. INTRODUCTION

The charge-exchange processes between multiply charged ions and neutral species have recently received appreciable attention in connection with the contamination problems in tokamak-type thermonuclear plasmas,[1] possibility of creation of short-wavelength lasers,[2] and multicharged heavy-ion source development.[3] The most prominent feature of the charge-exchange process

$$A + B^{Z_2^+} \rightarrow A^+ + B^{(Z_2-1)+} \tag{1}$$

is that the electron transition preferentially takes place into highly excited Rydberg states of the ion $B^{(Z_2-1)+}$(resonance or quasiresonance condition). This leads to the creation of inverse population with a resulting radiation in the vacuum-ultraviolet (vuv) and x-ray region. In tokamak plasmas, where small admixtures of impurity multicharged ions are present, this radiation carries away a considerable fraction of the energy accumulated in the system.

Despite the recognized importance of the charge-exchange collisions between multiply charged ions and neutral species in the research fields mentioned above, little information on their cross sections and collision dynamics is available at present. This holds particularly for the region of relative impact velocities below the characteristic velocity of the bound electron. The experimental difficulties of working in this energy region and the progress made so far in this field of research have recently been reviewed by Panov.[4]

The theoretical studies of low- and medium-energy charge-exchange processes involving multiply charged ions are faced with the complexity of a multiple curve-crossing problem. Due to the small energy spacing of highly excited Rydberg states of the product ion $B^{(Z_2-1)+}$ ($\Delta\epsilon \sim Z_2^2/n^3$), which in reaction (1) are dominantly populated, the multistate collision problem involves significant interferences of different exit reaction channels. In a close-coupling treatment of the problem by Presnyakov and Ulantsev[5] these interference effects were neglected. Olson and Salop[6-8] have recently studied a large class of charge-exchange reactions between multicharged ions and neutral species applying the Landau-Zener theory (Refs. 6 and 7) and the absorbing-sphere model (Ref. 8). The absorbing-sphere model assumes a large number of the closely spaced curve crossings, so that one can define (although somewhat arbitrarily) a critical internuclear distance R_c inside of which the reaction probability equals one.

Chibisov[9] has recently treated the problem of interaction of the initial atomic state with the multiplicity of highly excited ionic states in a manner analogous to the methods of Radtsig and Smirnov[10] for treating ion-ion recombination reactions. Since the density of states of $B^{(Z_2-1)+}$ ions in which electron transition takes place is high enough, one can consider this part of the ionic energy spectrum as being almost continuous. Then, the electron transfer process can be considered as tunneling of the electron from the atomic potential well, into the quasicontinuous energy spectrum of the multicharged ion.

In the work of Chibisov[9] the Coulomb field of the multicharged ion was considered as homogeneous and constant in the whole region of the atom. In the present paper we adopt the tunneling mechanism of the electron transfer process. However, our treatment takes into account the inhomogeneous character of the ionic Coulomb field and therefore allows us to obtain the electron transition probability in a much broader region of variation of characteristic parameters of the problem (the binding energy of the atomic electron and the ionic charge).

The plan of the article is as follows. Section II deals with the determination of the quasistationary energy spectrum of a hydrogenlike atomic system in the field of multicharged ions. The imaginary part of the complex energy of these quasistationary

states determines the electron transition probability per unit time. In Sec. III the obtained result on the electron transfer probability is generalized to arbitrary atoms. In Sec. IV the calculation of the cross sections of a number of charge-exchange reactions and comparison of the obtained results with the experimental data (where available) as well as the previous theoretical calculations are given. Finally, in Sec. V some concluding remarks are presented.

Atomic units are used in this work unless otherwise indicated.

II. QUASISTATIONARY SPECTRUM OF A HYDROGENLIKE ATOM IN PRESENCE OF A MULTICHARGED ION

Within the model for the electron transfer process in atom–multicharged-ion adiabatic collisions adopted in the present paper, the perturbed atomic states are unstable against electron emission into the region of quasicontinuous ionic energy spectrum. Since the imaginary part of the energy of quasistationary state determines the electron transition probability, our electron transfer problem in the adiabatic energy region is essentially reduced to determination of the quasistationary energy spectrum of the atom in presence of a multicharged ion. In this section we shall solve this problem for the case of a hydrogenlike atom.

A. Separation of variables in the Schrödinger equation

Let us consider the motion of an electron in the field of two Coulomb charges Z_1 and Z_2

$$H\psi = E\psi, \quad H = -\tfrac{1}{2}\nabla^2 - Z_1/r_1 - Z_2/r_2, \tag{2}$$

with r_1 and r_2 being the electron distances from the charges Z_1 and Z_2, respectively. At large internuclear distances R a narrow cylindrical region around the internuclear axis gives the main contribution to the electron transition probability. We shall therefore solve Eq. (2) in this region and in the vicinity of Coulomb center Z_1. In these two regions the variables in Eq. (2) can be separated in parabolic coordinates.

Let us place the coordinate origin at the charge Z_1 (the nucleus of hydrogenlike atom), orient the z axis along the direction of the internuclear axis, place the Coulomb charge Z_2 at $z=-R$, and drop the index 1 in r_1. We shall first consider the region $r \ll R$, where the last term in the Hamiltonian H becomes

$$\frac{Z_2}{r_2} \equiv \frac{Z_2}{[x^2+y^2+(z+R)^2]^{1/2}} = \frac{Z_2}{R} - \frac{Z_2}{R^2}z + O\left(Z_2\left(\frac{r}{R}\right)^3\right). \tag{3}$$

The Schrödinger equation (2) in this region becomes

$$(\tfrac{1}{2}\nabla^2 + \tilde{E} + Z_1/r - \tilde{F}z)\psi = 0, \tag{4}$$

where

$$\tilde{E} = E + Z_2/R, \quad \tilde{F} = Z_2/R^2. \tag{5}$$

Hence, in the $r \ll R$ region our problem is reduced to the Stark-effect problem of a hydrogenlike system in an external homogeneous constant electric field $\tilde{F}$. Introducing parabolic coordinates

$$\xi = r+z, \quad \eta = r-z, \quad \theta = \arctan(y/x), \quad 0 \le \xi < \infty, \quad 0 \le \eta < \infty, \quad 0 \le \theta < 2\pi, \tag{6}$$

and representing the wave function ψ in the form

$$\psi = X(\xi)Y(\eta)/(2\pi\xi\eta)^{1/2}\exp(\pm im\theta), \tag{7}$$

the variables in Eq. (4) are separated and for $X(\xi)$ and $Y(\eta)$ one obtains the well-known equations

$$X''(\xi) + [\tfrac{1}{2}\tilde{E} + \beta_1/\xi + (1-m^2)/4\xi^2 - \tfrac{1}{4}\tilde{F}\xi]X(\xi) = 0, \tag{8a}$$

$$Y''(\eta) + [\tfrac{1}{2}\tilde{E} + \beta_2/\eta + (1-m^2)/4\eta^2 + \tfrac{1}{4}\tilde{F}\eta]Y(\eta) = 0. \tag{8b}$$

In Eqs. (7) and (8) m is the modulus of the magnetic quantum number, and the separation constants β_1 and β_2 are related to each other by

$$\beta_1 + \beta_2 = Z_1. \tag{9}$$

If, for the moment, we neglect the possibility of electron tunneling and impose the following boundary conditions

$$X(0) = 0, \quad X(\xi) \underset{\xi\to\infty}{\to} 0, \tag{10a}$$

$$Y(0) = 0, \quad Y(\eta) \underset{\eta\to\infty}{\to} 0, \tag{10b}$$

then Eqs. (8a)–(10a) and Eqs. (8b)–(10b) define two boundary-value problems. Considering β_1 and β_2 as "eigenvalues" of these problems and $\tilde{F}$ as a small parameter, one obtains the expansions[11]

$$\beta_1 = k(-2\tilde{E})^{1/2} + [\tilde{F}/(-2\tilde{E})][\tfrac{3}{2}k^2 + \tfrac{1}{2}\tau] + O(\tilde{F}^2), \tag{11a}$$

$$\beta_2 = \mathcal{K}(-2\tilde{E})^{1/2} - [\tilde{F}/(-2\tilde{E})][\tfrac{3}{2}\mathcal{K}^2 + \tfrac{1}{2}\tau] + O(\tilde{F}^2), \tag{11b}$$

where

$$k = n_1 + \tfrac{1}{2}(m+1), \; n_1 = 0,1,2,\ldots, \quad \mathcal{K} \equiv \mathcal{K}_0 = n_2 + \tfrac{1}{2}(m+1), \; n_2 = 0,1,2,\ldots, \quad \tau \equiv \tfrac{1}{4}(1-m^2) \tag{12}$$

and n_1, n_2 are the parabolic quantum numbers. The substitution of Eqs. (11a) and (11b) into Eq. (9) gives an equation for $\tilde{E}$. Solving this equation by iteration, and keeping in mind relations (5), we obtain

$$E \equiv E_r = E_0 + \Delta E, \tag{13}$$

$$E_0 = -Z_1^2/2n^2, \tag{13a}$$

$$\Delta E = -Z_2/R + \tfrac{3}{2}(Z_2 n\Delta/Z_1 R^2) + O(Z_2/R^3), \tag{13b}$$

where $n = n_1 + n_2 + m + 1$ is the principal quantum number and $\Delta = n_1 - n_2$. The expansions (11) and (13) are valid under the condition $R \gg n^2(2Z_2/Z_1^3)^{1/2}$. The term ΔE in (13) represents the energy-level shift due to the presence of the multiply charged ion Z_2.

B. Determination of the quasistationary energy spectrum: The electron transition probability

In treating Eq. (2) in the region far from the Coulomb charge Z_1 we should correctly describe the electron motion in the part of this region which gives dominant contribution to the electron tunneling effect. This is certainly a cylindrical region around the internuclear axis. In parabolic coordinates it is defined by $\xi \ll \eta < 2R$ and $(\xi\eta)^{1/2} \ll R$ and the last term in the Hamiltonian (2) takes the form

$$\frac{Z_2}{r_2} \equiv \frac{Z_2}{\{\xi\eta + [\frac{1}{2}(\xi - \eta) + R]^2\}^{1/2}} \simeq \frac{2Z_2}{2R - \eta}. \tag{14}$$

It is convenient to transform the potential (14) into the form

$$2Z_2/(2R - \eta) = Z_2/R + Z_2\eta/(2R - \eta)R. \tag{14a}$$

Then, from Eqs. (2) and (7), we obtain

$$X''(\xi) + [\tfrac{1}{2}\tilde{E} + \beta_1/\xi + (1 - m^2)/4\xi^2]X(\xi) = 0, \tag{15a}$$

$$Y''(\eta) + \left(\frac{\tilde{E}}{2} + \frac{\beta_2}{\eta} + \frac{Z_2\eta}{2R(2R - \eta)} + \frac{1 - m^2}{4\eta^2}\right) Y(\eta) = 0. \tag{15b}$$

The same notation for $\beta_1, \beta_2, X(\xi)$, and $Y(\eta)$ is used as before, since for $\xi \to 0$ Eq. (8a) goes over into Eq. (15a) and for $R \to \infty$ (or $\eta \ll 2R$) Eq. (15b) goes over into Eq. (8b). The relation (9) between β_1 and β_2 is still valid. The motion in "ξ direction" is finite in the classical sense whereas in "η direction" the electron experiences tunneling. Thus, we can retain the expansion (11a) for β_1 as before. However, in order to obtain β_2 Eq. (15b) has to be solved under the boundary conditions

$$Y(0) = 0, \quad Y(\eta) \underset{\eta > \eta_1}{\to} \text{(outgoing wave)}, \tag{16}$$

where η_1 is the turning point of Eq. (15b), nearest to the Coulomb center Z_2. The second boundary condition of conditions (16) describes the possibility of electron tunneling into the quasicontinuous part of the multicharged-ion energy spectrum.

Equations (15b) and (16) define a boundary-value problem with complex "eigenvalues" β_2. This problem can be solved by use of the modified comparison-equation method.[12,13] The details of calculations are given in the Appendix. The expression for β_2 is again given by an expansion in the form of (11b) but with a complex value of $\mathcal{K}$ (see the Appendix),

$$\mathcal{K} = \mathcal{K}_0 - i\delta, \tag{17}$$

$$\mathcal{K}_0 = n_2 + \tfrac{1}{2}(1 + m), \quad n_2 = 0, 1, 2, \ldots, \tag{17a}$$

$$\delta = \frac{(4b)^{2\mathcal{K}_0}}{2n_2!(n_2 + m)!} \exp[-bf(\alpha) - 4\mathcal{K}_0 g(\alpha)] \times [1 + O(1/b)], \tag{17b}$$

where

$$b = (-2\tilde{E})^{3/2}R^2/Z_2, \quad \alpha = (-\tilde{E})R/Z_2,$$

$$f(\alpha) = \frac{1 - \ln(\sqrt{1+\alpha} + \sqrt{\alpha})/\sqrt{\alpha(1+\alpha)}}{\alpha}, \tag{18a}$$

$$g(\alpha) = \alpha \ln(\sqrt{1+\alpha} + \sqrt{\alpha})/\sqrt{\alpha(1+\alpha)}, \tag{18b}$$

and n_2 is the second parabolic quantum number. The relations (17) and (11b) give an expansion for the complex eigenvalues β_2. Using this expansion and the expression (11a) for β_1 in Eq. (9) one obtains an equation for determination of the energy of the quasistationary electronic states. Solving it by iteration, one finds

$$E = E_r - \tfrac{1}{2} i\Gamma_{n_1 n_2 m}(R), \tag{19}$$

where E_r is given by the expression (13) and

$$\Gamma_{n_1 n_2 m}(R) = \frac{Z_1^2}{n^3 n_2!(n_2 + m)!}\left(\frac{4Z_1^3R^2}{Z_2 n^3}\right)^{2n_2 + 1 + m} \times \exp\left[-\left(\frac{Z_1^3R^2}{Z_2 n^3} - \frac{9}{2}\Delta\right) f(\alpha) - 2(2n_2 + 1 + m)g(\alpha)\right][1 + O(Z_2/R^2)]. \tag{20}$$

This expression for the energy width of the quasistationary electronic state is asymtotically exact, i.e., it is valid under the condition $R \gg n^2(2Z_2/Z_1^3)^{1/2}$. Two limiting cases can be obtained from the expression (20) for $\Gamma_{n_1 n_2 m}(R)$. For $\alpha \gg 1$, i.e., $R \gg 2n^2Z_2/Z_1^2$, we obtain

$$\Gamma_{n_1 n_2 m}(R) = \frac{Z_1^2(Z_1/nZ_2)^{2Z_2 n/Z_1}}{n^3 n_2!(n_2 + m)!} \times (2Z_1R/n)^{2n_2 + 1 + m + 2Z_2 n/Z_1} \times \exp(-2Z_1R/n)[1 + O(1/R)]. \tag{21}$$

For $\alpha \ll 1$, i.e., $R \ll 2n^2Z_2/Z_1^2$, expression (20) becomes

$$\Gamma_{n_1 n_2 m}(R) = \frac{Z_1^2}{n^3 n_2!(n_2 + m)!}\left(\frac{4Z_1^3R^2}{Z_2 n^3}\right)^{2n_2 + 1 + m} \times \exp\left(-\frac{2}{3}\frac{Z_1^3R^2}{Z_2 n^3} + 3\Delta\right)[1 + O(Z_2/R^2)]. \tag{22}$$

Expression (22) for Γ corresponds to the width of a hydrogenlike atomic energy level which is due to the influence of an external homogeneous electric field $\vec{F} = Z_2/R^2$.

The energy-level broadening $\Gamma_{n_1 n_2 m}(R)$ describes the decay of quasistationary states when the multiply charged ion is placed at a distance R from the hydrogenlike system. According to our model $\Gamma_{n_2 n_2 m}(R)$ gives the electron-capture probability per unit time.

III. ANGULAR MOMENTUM REPRESENTATION OF THE ELECTRON TRANSITION PROBABILITY AND ITS GENERALIZATION TO ARBITRARY ATOMIC STATES

In order to obtain the value of the electron transition probability $\Gamma_{n_1 n_2 m}(R) \equiv \Gamma(n_1, n_2, m)$ in the ordinary angular momentum representation (n, l, m), one has to sum the expression (20) over the possible values of parabolic quantum numbers n_1 and n_2. Accordingly, we have

$$\Gamma(n,l,m) = \sum_{n_1+n_2=n-1-m} |\langle l | n_1 n_2 \rangle|^2 \Gamma(n_1, n_2, m), \tag{23}$$

where $\langle l | n_1 n_2 \rangle$ are the coefficients which connect the angular momentum and the Stark eigenstates. These coupling coefficients are simply related to the Clebsch-Gordan coefficients.[14] The procedure of summation in (23) is explained elsewhere.[15] Here we give only the result,

$$\Gamma(n,l,m) = \frac{Z_1^2}{n^3 m!} \frac{(2l+1)(l+m)!}{(n+l)!(n-l-1)!(l-m)} \left(\frac{4Z_1^3 R^2}{Z_2 n^3}\right)^{2n-1-m} \times \exp\left\{-\left[\frac{Z_1^3 R^2}{Z_2 n^3} + \frac{9}{2}(n-1-m)\right] f(\alpha) - 2(2n-1-m) g(\alpha)\right\} [1 + O(Z_2 R^{-2})]. \tag{24}$$

It is evident from this expression that the axially symmetric states ($m = 0$) give the main contribution to the electron transition probability.

The expression (24) for $\Gamma(n, l, m)$ can be generalized for the case of an arbitrary neutral atom A in the field of a multicharged ion Z_2. Describing the active valence electron by its binding energy $-\frac{1}{2}\gamma^2$, angular momentum l, and projection m on the internuclear axis, we put $Z_1 = 1, n = \gamma^{-1}$ in Eq. (24). The term $\frac{9}{2}(n-1-m)$ in the exponent should be dropped in the case of an arbitrary atom, since this term originates from the linear Stark effect. In such a way, the expression for the electron transition probability in the case of an arbitrary atom is obtained in the form

$$\Gamma(\gamma, l, m) = A_{\text{Coul}}^2 (2\gamma)^{-2/\gamma} \frac{(2l+1)(l+m)!}{m!(l-m)!} \left(\frac{4\gamma^3 R^2}{Z_2}\right)^{2/\gamma-1-m} \times \exp\left[-\frac{\gamma^3 R^2}{Z_2} f(\alpha) - 2\left(\frac{2}{\gamma} - 1 - m\right) g(\alpha)\right] \times [1 + O(Z_2/R^2)], \tag{25}$$

where $\alpha = \gamma^2 R/(2Z_2)$ and

$$A_{\text{Coul}} = \gamma(2\gamma)^{1/\gamma} [\Gamma(1/\gamma + l + 1)\Gamma(1/\gamma - l)]^{-1/2}. \tag{26}$$

The expression (25) for $\Gamma(\gamma, l, m)$ is valid under the condition of $\gamma^2 R \gg (2Z_2)^{1/2}$. The constant A_{Coul} represents the Coulomb normalization constant in the asymptotic expression of the atomic electron radial wave function. For the ground and low-lying excited atomic states it is more correct to use the Hartree-Fock value A_{HF} of this constant, which can be obtained by a procedure described elsewhere.[16]

In the limiting case $\alpha \ll 1$, $\Gamma(\gamma, l, m)$ becomes (we drop the index of the constant A)

$$\Gamma(\gamma, l, m) = A^2 \gamma (2\gamma)^{-2/\gamma} \frac{(2l+1)(l+m)!}{m!(l-m)!} \times \left(\frac{4\gamma^3 R^2}{Z_2}\right)^{2/\gamma-1-m} \exp\left(-\frac{2}{3}\frac{\gamma^3 R^2}{Z_2}\right). \tag{27}$$

In fact, this limiting case has been considered in the work of Chibisov.[9] The condition $\alpha \ll 1$ is satisfied only for large Z_2 and/or small γ. In most of the charge-exchange reactions of multicharged ions on ground-state atoms the critical reaction radius R_0 is such that parameter α is of the order of magnitude of one. Thus, expressions (25) and (27) give considerably different values for Γ and consequently, different reaction cross section, $\sigma \simeq \pi R_0^2$.

IV. CROSS-SECTION CALCULATIONS

The cross section for the electron capture in atom–multicharged-ion collisions within the adiabatic approximation is given by[10]

$$\sigma = 2\pi \int_0^\infty \rho\, d\rho \left[1 - \exp\left(-\int_{-\infty}^{+\infty} \Gamma(R(t))\, dt\right)\right], \tag{28}$$

where $R(t)$ is the classical trajectory of the rela-

tive nuclear motion and ρ is the impact parameter. Assuming a straight-line trajectory for $R = R(t)$ and using the fact that the function $\chi(\rho)$

$$\int_{-\infty}^{+\infty} \Gamma\, dt = 2\int_{\rho}^{\infty} \frac{\Gamma(R) R\, dR}{v[R^2 - \rho^2]^{1/2}} \equiv \chi(\rho), \tag{29}$$

(v being the relative velocity) is a strongly varying function of ρ, the integration over ρ in Eq. (28) can be carried out to get[10]

$$\sigma = \pi\rho_0^2, \tag{30}$$

where the critical impact parameter ρ_0 is determined from the equation

$$\chi(\rho_0) = e^{-C} = 0.56, \tag{31}$$

$C = 0.577\ldots$ being Euler's constant. In order to make the dependence of the cross section on the characteristic parameters of the problem more explicit, let us estimate the integral $\chi(\rho_0)$ and introduce a new variable

$$x_0 = \gamma^3\rho_0^2/Z_2.$$

For the cross section we obtain

$$\sigma = (\pi Z_2/\gamma^3)x_0, \tag{32}$$

where x_0 is determined by the equation

$$x_0^{2/\gamma-1-m} e^{-x_0 f(\alpha_0)} = \frac{v}{B}\, e^{\varphi(\alpha_0)-C} \left(\frac{f(\alpha_0)}{\pi}\, \frac{\gamma^3}{Z_2}\right)^{1/2}, \tag{33}$$

and

$$B = A^2\gamma(2\gamma)^{-2/\gamma}\, 2^{2(2/\gamma-1-m)}\, \frac{(2l+1)(l+m)!}{m!\,(l-m)!},$$

$$\varphi(\alpha_0) = 2(2/\gamma - 1 - m)g(\alpha_0),$$

$$\alpha_0 = \tfrac{1}{2}(\gamma x_0/Z_2)^{1/2}.$$

As seen from Eq. (33), the quantity $x_0 = x_0(\gamma, Z_2, v)$ is a slowly varying (logarithmic) function of Z_2 and v. This implies a slow variation of the cross section with the change of relative velocity and an approximate linear dependence on Z_2 in the high Z_2 region. The slow energy dependence of σ seems to be confirmed by the experiments.[18] A linear Z_2 dependence of σ has also been obtained in the absorbing-sphere model.[8] However, the close-coupling treatment of Presnyakov and Ulantsev[5] predicts a Z_2^2 dependence of the cross section. This question will be discussed later, in Sec. IV C. Here, we note that in the low-Z_2 region ($\alpha_0 \gtrsim 1$) our model does not allow us to obtain any simple Z_2-scaling rule for the cross section, although the calculations (see, e.g., Figs. 1, 2, 4, 5) suggest that the approximate linear Z_2 dependence of σ is preserved down to $Z_2 = 4$–5.

The adiabatic approximation applied in our treatment will be valid if the collision time $\tau_c \sim \rho_0/v \sim (1/v)(Z_2 x_0 \gamma^{-3})^{1/2}$ is much longer than the characteristic atomic time $\tau_a \sim \gamma^{-2}$, which gives

$$v \ll (\gamma Z_2 x_0)^{1/2}. \tag{34}$$

Since Z_2 is assumed to be large and $\gamma \sim 1, x_0 \sim 10$, for ground-state atoms, condition (34) allows one to consider the collisions with relative energies up to several KeV 's as adiabatic.

In the rest of this section we give the results of the cross-section calculations for a number of charge-exchange reactions. We have used the approximation (30) and (31) for the cross section (28). It has been found that for hydrogen targets this approximation is correct within the second decimal of the cross-section value computed directly from the expression (28). The accuracy of the approximations (32) and (33) is almost the same.

A. Atomic-hydrogen reactions

The charge-exchange reactions of atomic hydrogen or deuterium with multiply charged ions are of fundamental importance for controlled-thermonuclear-fusion research. In this respect the Z_2 dependence of the cross section is of particular significance. We have performed cross-section calculations for electron transfer from the ground hydrogen atom state ($\gamma = 1, A = 2$) to multiply charged ions with Z_2 ranging from $Z_2 = 4$ to $Z_2 = 40$.

Figure 1 gives the result of our cross-section calculations for $v = 7 \times 10^7$ cm/sec (the full line). The dashed curve on the same figure represents the calculations of Olsen and Salop[8] within the absorbing-sphere model. Both theoretical models predict large charge-exchange cross sections. The linear Z_2 dependence of the cross section, predic-

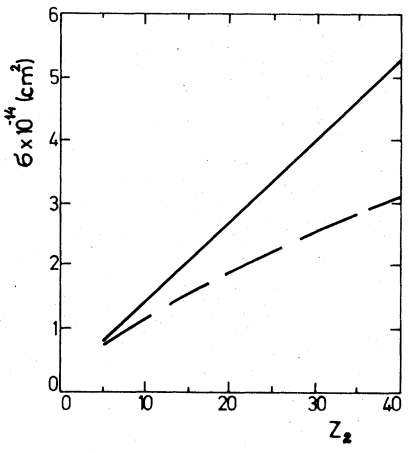

FIG. 1. Z_2 dependence of the cross section for $H(1s) + B^{Z_2+} \rightarrow H^+ + B^{(Z_2-1)+}$ reaction at $v = 7 \times 10^7$ cm/sec. The full line: present calculations; the dashed line: calculations of Olson and Salop (Ref. 8).

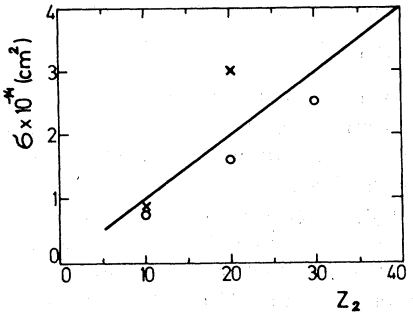

FIG. 2. Charge-exchange cross section for $H+B^{Z_2+}$ collision at $v=3\times10^8$ cm/sec. The full line: present calculations; the crosses and open circles are calculated cross-section values taken from Refs. 5 and 9, respectively.

ted by Eqs. (31) and (32), is already observed in the region of low-Z_2 values. The absorbing-sphere model predicts linear dependence of the cross section that starts from considerably higher Z_2 values ($Z_2 \sim 20$). Figure 2 gives a comparison of the results obtained by use of the present model for $v = 3\times10^8$ cm/sec (the full line) with the cross-section values for $Z_2=10$ and $Z_2=20$ calculated by Presnyakov and Ulantsev[5] (the crosses). The open circles on Fig. 2 represent the cross-section values calculated by Chibisov[9] for $Z_2=10$, 20, and 30.

The velocity dependence of the charge-exchange cross section is shown in Fig. 3 ($Z_2=10$, 20, and 30). As predicted by Eqs. (31) and (32) this dependence is fairly weak (logarithmic). In the interval from 1×10^7 to 1×10^8 cm/sec (two decades in the energy scale), the cross-section value decreases for about 30% only.

TABLE I. Parameters γ and A of the asymptotic wave function for ground-state alkali and rare-gas atoms.

Atom	γ	A	Atom	γ	A
Li	0.63	0.765	He	1.345	2.25
Na	0.626	0.751	Ne	1.26	1.50
K	0.567	0.533	Ar	1.075	2.07
Rb	0.556	0.491	Kr	1.015	2.12
Cs	0.536	0.416	Xe	0.945	2.15

B. Alkali-atom–multicharged-ion reactions

Another important class of charge-exchange reactions of multicharged ions is the one in which the neutral particle is a ground-state alkali atom. We have calculated the cross sections of this class of reactions for $v=5\times10^7$ cm/sec and for Z_2 ranging from $Z_2=5$ to $Z_2=40$. The parameters A and γ of the ground-state alkali-atom electron wave function are given in Table I.[16] The cross sections are shown in Fig. 4. The cross-section values for these reactions are about one order of magnitude larger than the electron transfer cross-section values for atomic hydrogen. This is the consequence of a great increase of the cross section with decreasing γ. For the same reason, the reaction with a Cs target has the largest cross section.

C. Rare-gas-atom–multicharged-ion reactions

We have performed cross-section calculations for rare-gas-atom–multicharged-ion electron transfer reactions since experimental data are available for them.[3,17] However, the experiments are done with Z_2 ranging from $Z_2=4$ to $Z_2=8$ only. The parameters A and γ for the ground-state rare-gas-atom wave functions are given in Table I.[18]

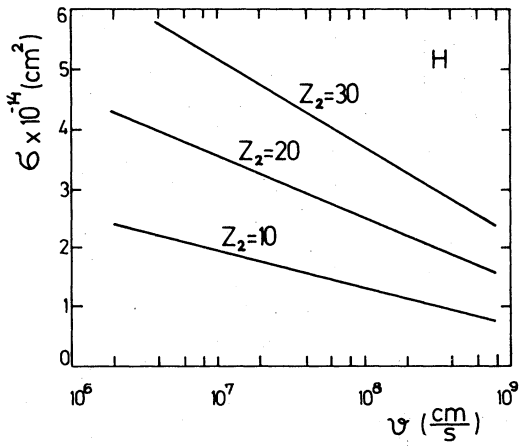

FIG. 3. Velocity dependence of the charge-exchange cross section in $H+B^{Z_2+}$ collisions.

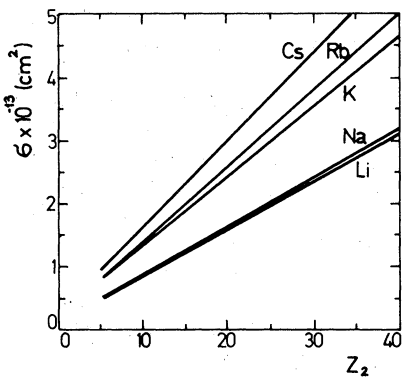

FIG. 4. Z_2 dependence of the charge-exchange cross section in alkali-atom–B^{Z_2+} collisions at $v=5\times10^7$ cm/sec.

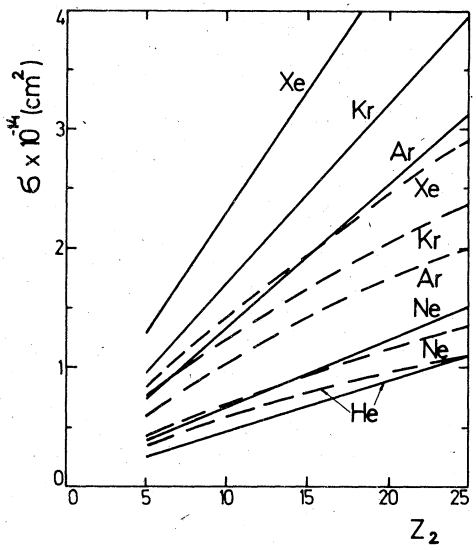

FIG. 5. Charge-exchange cross sections for rare-gas-B^{Z_2+} collisions at $v = 5.4\times10^7$ cm/sec. The full lines: present calculations; the dashed lines: calculations of Olson and Salop (Ref. 8).

Figure 5 shows the results of our Z_2-dependence cross-section calculations for the relative collision velocity $v = 5.4 \times 10^7$ cm/sec (the full lines). On the same figure the calculations of Olsen and Salop[8] are also presented (the dashed curves). Except for He and Ne atoms, our model gives higher cross-section values than the absorbing-sphere model.

The most characteristic feature of our electron tunneling model for the charge exchange of a multi-charged ion is the independence of the transition probability (and, consequently, the reaction cross section) on the final state of the captured electron. The experimental data of Klinger *et al.*[17] allow us to check this property of the model. Figure 6 gives a comparison of the theoretical calculations and experimental data ($E = 30$ keV) for the reactions

$$\mathrm{Ar} + \mathrm{B}^{Z_2+} \rightarrow \mathrm{Ar}^+ + \mathrm{B}^{(Z_2-1)+},$$

where B = Ar, Kr, Xe, and $Z_2 = 2-8$. The full line represents the result of our calculations using Eqs. (31) and (32), whereas the dashed curve indicates the calculations of Presnyakov and Shevel'ko[19] performed by using the theory given in Ref. 5. The figure suggests that for $Z_2 \geq 4$ the experimental cross-section data are fairly independent on the ionic species that supports the transition mechanism adopted in our model. On the other hand, the comparison of the theoretical curves with the trend of experimental data suggests that a linear Z_2 dependence is more likely than a quadratic one.

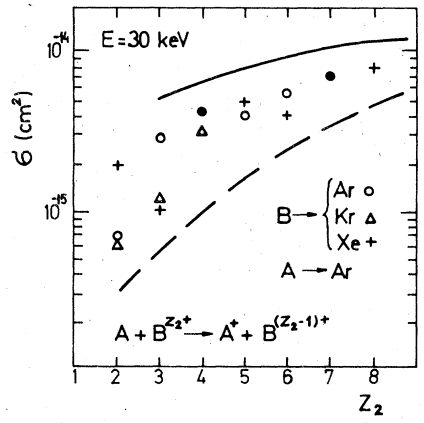

FIG. 6. Z_2 dependence of the cross section for $Ar + B^{Z_2+} \rightarrow Ar^+ + B^{(Z_2-1)+}$ reaction. The full curve: present calculations; the dashed curve: calculations of Presnyakov and Shevel'ko (Ref. 19); the experimental points are taken from Ref. 3.

V. CONCLUDING REMARKS

The theoretical method developed in this paper for calculating the charge-exchange cross section of multiply charged ions on neutral atoms is based on the assumption that the electron transition takes place in the ionic energy spectrum where the density of states is sufficiently high. Generally, this assumption is justified for multicharged ions with high values of the ionic charge ($Z_2 \gtrsim 10$). For lower values of Z_2, where this condition is not fully satisfied, our treatment overestimates the value of the transition probability. This explains why our curve in Fig. 6 is for approximately a factor of 1.5 higher than the experimental data. Another feature of the electron transfer process, included in our treatment, is its resonant character. This implies that no electron-loss process which involves energy transfer is included in the determination of the transition probability. However, Chibisov has shown[9] that the direct ionization and electron capture via target-excitation processes have negligible cross sections in the adiabatic region under consideration.

There is another ionization channel which is associated with the quasiresonant electron transfer. Namely, after the electron-capture process (which takes place at internuclear distances of the order of tens of atomic units) the ionization of the excited ion $B^{(Z_2-1)+}$ by the impact of the ion A^+ can occur. The one-electron transfer cross section calculated by use of the theory of the present paper should be reduced by the value of the above ionization cross section. However, this reduction is neglig-

ibly small because the ionization cross section is of the order of 10^{-16} cm^2 at $v \sim 1$ a.u.[9]

The treatment developed in the present article (for charge-exchange collisions of multicharged ions on neutral atoms) can be readily extended to the diatomic molecular target case. In this case the transition probability Γ contains the Frank-Condon factor for vibrational transition in the system of molecule-molecular ion (as a multiplicative factor) and the constant A in the asymptotic electron wave function becomes dependent on the angle between the molecular axis and the vector $\vec{R}$ that joins the center of mass of the molecule with the multicharged ion. Then, the cross-section calculations can be performed using a procedure outlined in Ref. 20.

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APPENDIX

Using the scale transformation

$$\eta = [(-2\tilde{E})R^2/Z_2]y,$$

the boundary-value problem [(15b) and (16)] is reduced to

$$\frac{d^2Y}{dy^2} + \left[-\frac{b^2}{4}\left(1 - \frac{y}{1-\alpha y}\right) + \frac{b\lambda}{y} + \frac{\tau}{y^2}\right] Y(y) = 0, \tag{A1}$$

$$Y(0) = 0, \; Y(y) \underset{y > y_1}{\rightarrow} \text{outgoing wave}, \tag{A2}$$

where

$$b = (-2\tilde{E})^{3/2}R^2/Z_2, \quad \lambda = \beta_2(-2\tilde{E})^{-1/2}, \quad \alpha = (-\tilde{E})R/Z_2, \tag{A3}$$

and y_1 is the turning point of Eq. (A1) corresponding to η_1 from Eq. (15b). In Eq. (A1), b is considered as a large parameter, α is treated as an independent parameter, and λ is the spectral parameter of the problem.

For the values of parameter b satisfying the condition $b \gg 4\lambda$, Eq. (A1) in the region of our interest $0 \leq y < 1/\alpha$ $(0 \leq \eta < 2R)$ has a pole at $y = 0$ and near it a turning point $y_0 \simeq 4\lambda/b$. Apart from this, Eq. (A1) has a distant turning point $y_1 \simeq (1+\alpha)^{-1}$ whose proximity to the pole $y = 1/\alpha$ (the Coulomb center Z_2) depends on the value of the parameter α. For the present, we assume that $\alpha = O(1)$.

In the region $y \in [O, y_1 - \epsilon_1]$, $\epsilon_1 > 0$, we can take the Whittaker equation as the etalon (or comparison) equation for Eq. (A1). Then, the regular solution, $Y_0(y)$, of Eq. (A1) in this region can be represented in the form[12,13]

$$Y_0(y) = [u'(y)]^{-1/2}\mathfrak{M}_{\mathcal{K}, m/2}[bu(y)]. \tag{A4}$$

Substituting this into Eq. (A1) we obtain the nonlinear equation for the function $u(y)$,

$$\frac{u'^2}{4} - \frac{p^2(y)}{4} + \frac{1}{b}\left(\frac{\lambda}{y} - \frac{\mathcal{K}u'^2}{u}\right) + \frac{\tau}{b^2}\left(\frac{u'}{u^2} - \frac{1}{y^2}\right) - \frac{1}{2b^2}\left[\frac{u'''}{u'} - \frac{3}{2}\left(\frac{u''}{u'}\right)^2\right] = 0, \tag{A5}$$

where

$$p(y) = [1 - y/(1-\alpha y)]^{1/2}.$$

Now we assume that $u(y, b)$ and $\lambda(b)$ can be expanded in asymptotic series in inverse powers of b, i.e.,

$$u(y, b) = \sum_{j=0}^{\infty} u_j(y) b^{-j}, \quad \lambda(b) = \sum_{j=0}^{\infty} \lambda_j b^{-j}. \tag{A6}$$

The condition that Eq. (A5) should be satisfied for any power of b gives an infinite system of recurrence first-order differential equations for $u_j(y)$. The coefficients λ_j are determined from the condition that $u_j(y)$ are regular at $y = 0$. Solving the mentioned system of equations for u_j, we obtain

$$\lambda = \mathcal{K} - (1/b)(\tfrac{3}{2}\mathcal{K}^2 + \tfrac{1}{2}\tau) + O(1/b^2), \tag{A7a}$$

$$u(y) = \int_0^y p(y)\,dy + \frac{2\mathcal{K}}{b}\int_0^{\infty}\left[\frac{p(y)}{\int_0^y p(y)\,dy} - \frac{1}{yp(y)}\right]dy + O(1/b^2) \tag{A7b}$$

We note here that, having in mind Eq. (A3), the expression (11b) for β_2 can be directly reproduced from the expansion (A7a).

In the region of the variable y which includes the turning point y_1 (i.e. $y \in [\epsilon_2, 1/\alpha - \epsilon_3]$, $\epsilon_2 > 0, \epsilon_3 > 0$), the Airy equation can be taken as comparison to Eq. (A1). The solution $Y_1(y)$ in this region can be represented as

$$Y_1(y) = \text{const} \times [v']^{-1/2}[\mathrm{Ai}(b^{2/3}v) - i\mathrm{Bi}(b^{2/3}v)], \quad \text{(A8)}$$

and, using the same method as before, we obtain for $v(y)$

$$v(y) = \left(\frac{3}{2}\int_{y_1}^{y} \frac{p(y)}{2}\,dy\right)^{2/3} - \frac{1}{b}\left(\frac{2}{3}\right)^{1/2}\left(\int_{y_1}^{y} \frac{p(y)}{2}\,dy\right)^{-1/3} \times \int_{y_1}^{y} \frac{\mathcal{K}}{yp(y)}\,dy + O(1/b^2). \quad \text{(A9)}$$

The linear combination of the Airy functions in Eq. (A8) is chosen so as to satisfy the second of the boundary conditions (A2).

In the region $y \in [\epsilon_2, y_1 - \epsilon_1]$ both $Y_0(y)$ and $Y_1(y)$ are valid and should be smoothly linked in this region. Using the asymptotic expressions for the Whittaker and the Airy functions, the matching condition $Y_0 Y_1' - Y_0' Y_1 = 0$ gives the following "dispersion relation" for determination of the parameter $\mathcal{K}$:

$$\frac{\cos\pi(\mathcal{K} - \frac{1}{2}m)}{\pi} = \frac{i}{\Gamma[\mathcal{K} + \frac{1}{2}(1+m)]\Gamma[\mathcal{K} + \frac{1}{2}(1-m)]}\left(\frac{4\mathcal{K}}{e^2}\right)^{2\mathcal{K}} \times \exp\left[-b\int_{y_0}^{y_1} p(y)\,dy + 2\mathcal{K}\int_{y_0}^{y_1} \frac{dy}{yp(y)} + i\pi\left(\mathcal{K} - \frac{1+m}{2}\right)\right]\left[1 + O\left(\frac{1}{b}\right)\right] \quad \text{(A10)}$$

where the relation $\Gamma(\frac{1}{2}+x)\Gamma(\frac{1}{2}-x) = \pi/\cos\pi x$ is used. Carrying out the integrations in Eq. (A10) and then solving this equation by iteration, we obtain Eqs. (17) and (18).

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