Charge exchange and ionization in the collision of atoms and multiply charged ions

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In some physical applications it is important to know the charge-exchange and ionization cross sections of neutral atoms colliding with multiply charged ions ($Z_2 \gtrsim 10$) at velocities $v \sim v_0 = 2.18 \times 10^8$ cm/sec. This question has been the subject of a number of theoretical[1] and experimental[2] studies. Electron charge exchange is similar in many respect to the mesic-atom charge exchange analyzed by Gershteĭn.[3]

The processes of interest to us can be expressed in the form

$$A + B^{Z_2^+} \longrightarrow \begin{cases} A^+ + B^{(Z_2-1)+} & \text{(1a)} \\ A^+ + B^{Z_2^+} + e^- & \text{(1b)} \end{cases}.$$

In electron charge exchange, (1a) includes the interaction of one atomic state with a Coulomb condensation of excited states on the multiply charged ion B^{Z_2+}. The charge-exchange probability can therefore be calculated by using the model of Radtsig and Smirnov,[4] who treated the recombination of a negative ion with a positive one as the penetration of an electron from the negative ion through a barrier into the "continuous" spectrum of states on the positive ion. According to this model, the cross section of the charge exchange (1a) is equal to

$$\sigma_{ex} = 2\pi a_0^2 \int_0^\infty \rho\, d\rho \left[1 - \exp\left(-\int_{-\infty}^{+\infty} \Gamma(R(t))\, dt\right)\right], \tag{2}$$

where $\Gamma(R)$ is the probability per unit time of the electron penetration through the barrier at a given distance R between the atoms, and $a_0 = 0.53 \times 10^{-8}$ is the Bohr radius; the integration in (2) is with respect to time along the classical trajectory of nuclei with impact parameter ρ.

Formula (2) is valid in the adiabatic approximation: the characteristic frequency of the variation of the potential barrier with motion of the atoms (v/ρ) should be much less than the natural frequency of the electron. In our case ($\rho \sim \sqrt{Z_2}$) this means that $v \ll v_0\sqrt{Z_2}$, so that collisions with relatively large energies ($Z_2 \gg 1$) can be regarded as adiabatic.

At distances $\sqrt{Z_2} \ll J_A R \ll Z_2$ (J_A is the ionization potential of atom A) the barrier is formed by the self-field of the atom A and by the electric field $A_2 R^{-2}$ of the ion, which is almost homogeneous in the region of the atom. The decay frequency Γ of the atom in a homogeneous electric field was calculated earlier.[5] Using the result of [5] and calculating the cross section (2) by a method analogous to that of [4], we represent the charge-exchange cross section in the form

$$\sigma_{ex} = \frac{3\pi}{2} a_0^2 n_A^3 Z_2 f\left(n_A; \frac{v}{v_0 \sqrt{Z_2}}\right)$$
$$n_A \equiv (2J_A)^{-1/2}, \tag{3}$$

where the function f is given implicitly by the relation

$$f^{2n_A Z_1 - 1 - m} e^{-f} = \frac{1}{c}\left(\frac{v}{v_0 \sqrt{Z_2}}\right),$$

$$c = \frac{b^2 e^{0.577}}{6} \sqrt{\frac{\pi}{2}} (3n_A)^{2n_A Z_1 + 1/2} \frac{m!}{3^m} \frac{(2l+1)(l+m)!}{(l-m)!}, \tag{4}$$

where b is the amplitude of the asymptotic radial part of the atomic wave function [6]:

$$\psi_A \approx b r_A^{n_A Z_1 - 1} \exp(-r_A/n_A);$$

l and m are the angular momentum of the electron in the atom and its projection; Z_1 is the charge of the atomic core A ($Z_1 = 1$ for A of a neutral particle). For the hydrogen atom in the ground state we have $b = 2$.

The charge-exchange cross section of a definite atom ($n_A = \text{const}$) with ions of varying multiplicity Z_2 is determined by a single universal function $f(v/v_0\sqrt{Z_2})$. At velocities $v \sim v_0$ this function is determined, with an error $\lesssim 10\%$, by two approximations when solving the transcendental equation (4) by perturbation theory. We obtain for the cross section in this case

$$\sigma_{ex} = \frac{3\pi}{2} a_0^2 n_A^3 Z_2 \ln\left\{\frac{c\sqrt{Z_2}}{(v/v_0)}\left[\ln\frac{c\sqrt{Z_2}}{(v/v_0)}\right]^{2n_A Z_1 - 1}\right\}, \tag{5}$$

$$f = \ln\{\ldots\}. \tag{5a}$$

The main dependence of the charge-exchange cross section on the ion multiplicity Z_2 is linear.

Owing to the strong (exponential) dependence of the probability $\Gamma(R)$ of penetrating through the barrier, the charge exchange takes place mainly at a certain fixed distance R between the nuclei. The energy of the electron is then $-J_A - (Z/R)$ (the polarization displacement can be neglected). This allows us to determine the ion energy levels populated by charge exchange

$$E_{Z_2} = -\frac{Z_2^2}{2n_B^2};$$

$$n_B = n_A Z_2 \left[1 + 2n_A \sqrt{\frac{2Z_2}{3n_A^3 f(v/v_0\sqrt{Z_2})}}\right]^{-1/2}, \tag{6}$$

where f is determined by (4) or (5a). The error in the determination of n_B is of the order of ± 1.

For charge exchange of a hydrogen atom in the ground state with energy 50 keV ($v = 3\times10^8$ cm/sec), formulas (5) and (6) yield the following charge-exchange cross sections and the numbers of the most populated levels: $\sigma_{ex} = 7.5\cdot10^{-15}$ cm^2, $n_B = 6$ for $Z_2 = 10$; $\sigma_{ex} = 1.6\cdot10^{-14}$ cm^2, $n_B = 10$ for $Z = 20$; $\sigma_{ex} = 2.5\cdot10^{-14}$ cm^2, $n_B = 14$ for $Z_2 = 30$. The range of a hydrogen atom having this energy prior to charge exchange in a medium of ions with $Z_2 = 30$ and concentration 10^{11} cm^{-3} is ~ 4 m.

These figures are in good agreement with the numerical calculations of presnaykov and Ulantsev [1]: their charge-exchange cross sections for hydrogen at the same velocity are 8×10^{-14} cm^2 for $Z_2 = 10$ and 20, respectively.

The cross sections for the charge exchange for a neutral argon atom with argon ions Ar^{7+}, Ar^{6+}, Ar^{5+}, Ar^{4+} at an ion energy 50 keV ($v = 0.45\times10^8$ cm/sec) are, according to (5), respectively 5.5, 4.7, 3.8, and 3.0×10^{-15} cm^2 ($b = 2.7$ [6]). The corresponding experimental cross sections (which are constant in the energy range 10—100 keV) are 9.0, 6.5, 4.5, and 5×10^{-15} cm^2.

It must be noted that the cross sections reported in the experimental papers [2] pertain in fact to the neutralization of a multiply-charged ion by a many-electron atom without an analysis of the final charge state of the latter. It is clear, however, that the process

$$A + B^{Z_2+} \to A^{k+} + [B^{(Z_2-k)+}]^{**} \to A^{k+} + B^{(Z_2-p)+} + (k-p)e^-;$$

$$Z_2 \geq k \geq p \tag{7}$$

have just as large cross sections as in (5). For example, a decrease of the charge of the ion B^{Z_2+} by unity ($p = 1$) can result from charge exchange of two electrons from the atom A to excited levels of the ion (which are generally speaking different) with subsequent decay of the auto-ionization state of the ion $[B^{(Z_2-2)+}]^{**}$. The produced ion $B^{(Z_2-1)+}$ will then be in the electronic ground state. Several electrons leave the atom in succession. When the second ionization potential of the atom A is used, formula (5) yields for the cross section of the departure of the second electron a value only 1.5—2 times smaller than the cross section for the departure of the first electron. The measurements [2] reveal a similar (relatively weak) dependence of the charge-exchange cross section on the number of the departing electrons (so far, naturally, their number is $\ll Z_2$). The succeeding electrons populate excited states of the ion just as the first one, and this leads to formation of the auto-ionization complex $[B^{(Z_2-p)+}]^{**}$.

Thus, when a multiply charged ion collides with a many-electron atom, the sequence of events is much more complicated than in collisions with the single-electron hydrogen atom. The experimental [2] charge-exchange cross sections are equal to the sum of the cross sections of processes (1a) and (7).

We now discuss the ionization process (1b) for a single-electron atom, noting that for the true ionization it is necessary to impart to the electron an energy

$$\Delta E \geq J_A + (Z_2/R) \lessapprox J_A + \sqrt{Z_2}$$

(in atomic units). When an energy $\Delta E \sim J_A$ is acquired, an electron leaves the atom A, but it cannot go off to infinity from a multiply-charged ion located at a distance $R \leq J_A/Z_2$ from the atom. In the adiabatic approximation ($v \ll v_0\sqrt{Z_2}$)

the probability of transferring to the electron an energy ΔE is equal to

$$P(\rho) \sim Z_2^2 \exp(-|\Delta E| \rho/(v/v_0)).$$

We see therefore that the value of ρ_0 at which $P(\rho_0) = 1$ is

$$\rho_0 \approx (v/v_0)(\ln Z_2/\sqrt{Z_2}); \ (\sqrt{Z_2} >> J_A).$$

These distances are much smaller than those at which the charge exchange takes place: $\rho \sim \sqrt{Z_2}$. In one collision, therefore, the first to take place is charge exchange, followed by ionization of the excited ion $B^{(Z_2-1)+}$ by impact with the ion A^+. On the other hand, the cross sections with the ionization by single ions at velocities $v \sim v_0$ are of the order of $\sim 10^{-16}$ cm^2. The transfer of an energy $\sim J_A$ to the electron has a higher probability than ionization (but still much less than unity); this transfer leads to charge exchange into states $\sim J_A$ higher in energy than the states (6). An incorrect ionization cross section $\sigma_{\text{ion}} \sim Z_2^2$ was used in the calculations of [7].

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