RESONANCE CHARGE EXCHANGE OF DOUBLY CHARGED IONS IN SLOW COLLISIONS

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Submitted to JETP editor December 29, 1958

J. Exptl. Theoret. Phys. (U.S.S.R.) **37**, 95-97, (July, 1959)

The cross section for resonance charge exchange of doubly charged ions has been computed in the adiabatic approximation. A comparison is made between the experimental and theoretical charge exchange cross sections for doubly charged positive A, Kr, Xe, and Ne ions.

ONE-ELECTRON resonance charge exchange has been considered by many authors.[1-6] In the present paper we calculate the cross section for two-electron resonance charge exchange in the adiabatic approximation.

It has been shown earlier[7] that in the adiabatic approximation the cross section for charge exchange of an ion with an atom is

$$\sigma = \frac{1}{2}\pi R_0^2, \tag{1}$$

where R_0 is determined by the condition

$$\int_0^\infty \frac{E_a(R) - E_s(R)}{\hbar v}\,dx = k \approx \frac{1}{\pi}. \tag{2}$$

Here $x^2 = R^2 - R_0^2$; R is the distance between the nuclei in the ion and the atom; R_0 is the collision parameter; E_a is the energy of the electrons for the anti-symmetric wave function; E_s is the energy of the electrons for the symmetric wave function. Thus, the problem reduces to the calculation of the splitting of the electron levels as the nuclei approach each other.

We shall assume that for internuclear distances which are not too small it is possible to compute $E_a - E_s$ approximately, taking for He^{++}:

$$\psi_{s,a} \simeq [\varphi_A(r_1, r_2) \pm \varphi_B(s_1, s_2)]/\sqrt{2}, \tag{3}$$

as is done for the molecular hydrogen ion (the upper and lower signs refer respectively to ψ_s and ψ_a). Here φ_A and φ_B are the helium wave functions for electrons in the ground state when the electrons are attached to nucleus A or nucleus B; r is the distance of the electron from nucleus A, s is the distance from nucleus B. In this approximation the energy of the electrons is given by the expression

$$E_{s,a} = \frac{\int(\varphi_A \pm \varphi_B) H (\varphi_A \pm \varphi_B)\,d\tau_1\,d\tau_2}{\int(\varphi_A \pm \varphi_B)^2\,d\tau_1\,d\tau_2}$$

$$= E - \frac{4e^2\left[\int r_1^{-1}\varphi_B^2\,d\tau_1\,d\tau_2 \pm \int r_1^{-1}\varphi_A\varphi_B\,d\tau_1\,d\tau_2\right]}{1 \pm \int \varphi_A\varphi_B\,d\tau_1\,d\tau_2} \tag{4}$$

For large internuclear distances $\int r_1^{-1}\varphi_B^2 d\tau_1 d\tau_2 \sim 1/R$ and the remaining integrals are exponentially small. Hence,

$$E_a - E_s \approx \frac{8e^2}{R}\left(R\int\frac{\varphi_A\varphi_B}{r_1}\,d\tau_1\,d\tau_2 - \int\varphi_A\varphi_B\,d\tau_1\,d\tau_2\right). \tag{5}$$

The function φ is taken as the simple helium function

$$C\exp[-\alpha(r_1 + r_2)], \qquad \alpha = a_0^{-1}\sqrt{(E_1 + E_2)/2E_0},$$

where $E_1 + E_2$ is the total energy of the electrons in the atom, E_0 is the energy of the electron in the hydrogen atom and a_0 is the Bohr radius. The value of α for the helium atom is $1.71\,a_0^{-1}$, which corresponds to the minimum energy for the chosen wave function and also corresponds to the asymptotic region for a wave function having the mean binding energy [large r (or s)].

The analysis given here applies for relative velocities which satisfy the inequality $v \ll (\alpha e^2/\hbar)\,a_0$.

The results of the calculations are shown in Fig. 1; along the abscissa is plotted the relative velocity of the nuclei and along the ordinate axis is plotted $\alpha^2\sigma$, where σ is the cross section for two-electron charge exchange. On this same curve are plotted the measured experimental cross sections for two-electron charge exchange in the noble gases A, Ne, Kr, Xe.[8,9] Since one-electron charge exchange can occur in two-electron charge exchange

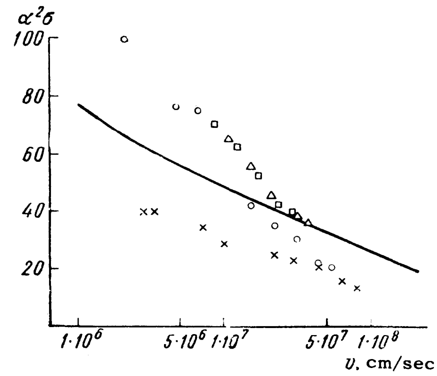

FIG. 1. ×) Ne; ○) A; △) Kr; □) Xe.

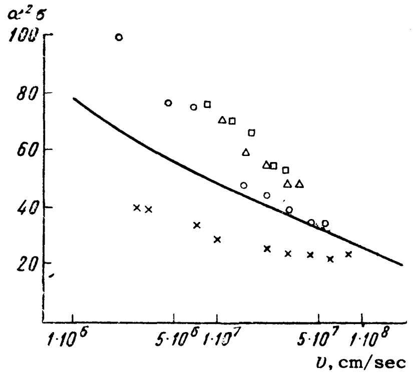

FIG. 2. ×) Ne; ○) A; △) Kr; □) Xe.

and in elastic scattering, and since this factor has not been taken into account in computing the cross section, the theoretical curve really corresponds to $\sigma_{20} + \frac{1}{2}\sigma_{21}$, where σ_{20} is the cross section for two-electron charge exchange and σ_{21} the cross section for one-electron charge exchange. A comparison of the experimental curves with the theory for this case is given in Fig. 2.

The theory given by Gurnee and Magee[9] for resonance charge exchange is similar to the present one but is less "rigorous." They make comparisons with some very old experimental results.[10,11] These authors assume $\psi = c \exp\{-\alpha(r_1 + r_2)\}/r^n$ and obtain $\alpha_{Ne} = 1.4$, $n = 1$; $\alpha_A = 1.3$, $n = 3$. As a result the cross sections obtained by Gurnee and Magee for Ne and A are larger than ours by approximately a factor of 2. The present results show better agreement with experiment.

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Translated by H. Lashinsky
14