Double ionization of magnesium atoms by helium ions

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The cross-section for double ionization of magnesium atoms by helium atoms, $He^+ + Mg \to He^+ Mg^{++} + e$, is numerically calculated in the range of energies $10^5 < V < 10^8$ cm/sec within the framework of the impact-parameter method. For low relative motion speeds $V < 5 \times 10^6$ cm/sec, an analytic equation is obtained for the ionization cross-section, which is equal to the product of the capture cross section and reaction probability with zero impact parameter. Some conclusions are drawn regarding the double ionization cross section of other atoms by helium ions.

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1. The double ionization process for an atom colliding with a helium ion

$$He^+ + A \to He + A^{2+} + e \qquad (1)$$

is energetically possible if the ionization potential of helium is greater than the sum of the two ionization potentials of the atom A. This relation holds for many elements (Mg, Mn, Fe, ...), so that the process may play an important role in the formation of doubly charged ions in a discharge.[1] Reactions of the type (1) have undergone little experimental study. The double ionization cross section of magnesium has been previously[1] measured at thermal velocities. A number of studies[2] have dealt with the measurement of charge-exchange cross sections with excitation,

$$He^+ + A \to He + A^{*+}. \qquad (2)$$

The process (1) is a limiting case for the process (2). Theoretical calculations of actual reactions belonging to the type of (1) have not previously been carried out, and only general statements regarding the calculation of the autoionization width of this process are available.[3]

2. Ionization of an atom A in the process (1) is due to the transfer of an electron from A to the helium ion, so that the disintegration probability of the autoionization state formed as the helium ion approaches A falls rapidly with increasing interatomic distance. Consequently a calculation of a reaction of the type of (1) requires knowledge of the behavior of the terms and ionization rate within short interatomic distances. This constitutes a basic complication of the theory, so that separate calculations are necessary in each concrete case.

Let us consider double ionization of magnesium. The ionization potential of helium exceeds the sum of the two magnesium potentials by only $\Delta E = 0.072$ atomic units, while the polarizability of the magnesium atom[4] $\alpha_1 = 130$ (calculated using the Hartree–Fock method) is significantly greater than the polarizability of a helium atom[5] $\alpha_2 = 1.39$, so that the terms of the He^+–Mg system rapidly drops and intersects the term of the He–Mg^{++} system already at great distances. Thus the He^+–Mg state ceases to be an autoionization state and does not disintegrate at short distances. The distance of approach at which disintegration ceases is determined from the equation

$$\Delta E - \frac{\alpha_1}{2R_0^4} = -\frac{2\alpha_2}{R_0^4}, \qquad R_0 = 5.4 \text{ a.u.} \qquad (3)$$

The ionization rate of the autoionization state is given by the equation

$$\Gamma(R) = 2\pi |W_{if}|^2 = 2\pi |\langle \Psi_f | H_{el} - E(R) | \Psi_i \rangle|^2, \qquad (4)$$

where Ψ_i and Ψ_f are the wave functions of the initial and final states of the system, H_{el} is the electronic Hamiltonian, and $E(R)$ is the total electronic energy (an atomic system of units is used). An exact calculation of $\Gamma(R)$ requires knowledge of the two-electron wave functions in a field of two nuclei, so that $\Gamma(R)$ cannot be exactly calculated at the present time. The matrix element (4) is defined by the region near the helium nucleus, since the final state is the strongly-bound state of the helium atom, so that

$$\Gamma(R) = A(R) \exp(-2\gamma R). \qquad (5)$$

Here $\gamma = (2I)^{1/2}$ where I is the first ionization potential of the magnesium atom. If we do not take into account the narrow near-threshold region, which does not substantially contribute to the disintegration probability, we may assume that $A(R)$ is a slowly varying function in comparison with an exponential function. Further, $A(R)$ is assumed constant and its value is selected such that the calculated cross sections coincide with the experimental cross section[1] at thermal velocities $\sigma_{exp} = 1.6 \pm 0.5$ (10^{-15} cm^2).

3. The reaction cross section as a function of velocity is given by

$$\sigma(E) = \int_0 P(\rho, E) 2\pi \rho \, d\rho. \qquad (6)$$

Here $P(\rho, E)$ is the ionization probability as a function of the impact parameter[6]

$$P(\rho) = 1 - \exp\left[-2 \int_{\rho_1}^{\infty} \frac{\Gamma(r)\, dr}{V(1 + \alpha_1/\mu V^2 r^4 - \rho^2/r^2)^{1/2}}\right]. \qquad (7)$$

Here ρ_1 is the greater of the distance of shortest approach and the distance at which disintegration ceases, and V is the relative motion velocity. The ionization rate (5) rapidly decreases with distance, and disintegration ceases at a comparatively great distance, so that the probability of the reaction (1) is $P(\rho) \ll 1$ for all impact parameters, even for thermal velocities. One consequence of this result is that the capture cross section at thermal velocities is significantly greater (very nearly by a factor of 20) than the reaction cross section. Therefore, the exponential in Eq. (7) can be expanded,

$$P(\rho)=2A\int_{\rho_1}^{\infty}\frac{\exp(-2\gamma r)\,dr}{V(1+\alpha_1/\mu V^2r^4-\rho^2/r^2)^{1/2}}. \qquad (8)$$

Figure 1 shows results of a numerical calculation of the cross section as a function of velocity using Eqs. (6) and (8). The constant A turns out to equal 0.37. The cross section falls rapidly with increasing velocity.

4. For low energies $V \ll 5\times10^6$ cm/sec, when the capture radius[7] is given by

$$\rho_{\text{cap}}=(4\alpha_1/\mu V^2)^{1/4} \gg R_0 \sim 1/\gamma,$$

we can obtain an analytic expression for the dependence of reaction cross section on velocity. The distance of shortest approach on trajectories with impact parameters greater than ρ_{cap} exceeds $\rho_{\text{cap}}\sqrt{2}$, so that the contribution of these trajectories to the reaction cross section is negligible. On trajectories corresponding to capture, $\rho_1=R_0$ in Eq. (8), and the third term in the radicand is negligible in comparison with the second term. We thereby find that the reaction cross section at low velocities is equal to the capture cross section multiplied by the reaction probability at zero impact parameter,

$$\sigma\approx2\pi\left(\frac{\alpha_1}{\mu V^2}\right)^{1/2}P(0)=\frac{2\pi A}{\gamma V}R_0^2\exp(-2\gamma R_0). \qquad (9)$$

Figure 1 compares the numerical integration and Eq. (9).

The physical meaning of this result is that at low initial helium-ion energies, the energy of this ion is significantly greater than its initial energy as it moves in the polarization potential near the point at which the autoionization channel is closed, so that disintegration at impact parameters less than the capture radius is independent of the initial energy.

The distribution function of the released electrons can be obtained at low energies. As stated before, disintegration at low energies is independent of the impact parameter, so that the probability $f(E)$ that an electron with given energy is emitted is uniquely connected with the distance of approach. The electron-emission probability is proportional to $\Gamma(R)$ and is inversely proportional to the particle velocity, which is determined by the polarization potential, and is inversely proportional to the change of energy of the emitted electrons,

$$f(E)\sim\Gamma(R)\Big/\bar{U}^{1/2}(R)\frac{d}{dR}\Delta U(R). \qquad (10)$$

Here R is considered as a function of the energy with which the electron is emitted, and is defined by the equation $E=\Delta U(r)$. Figure 2 shows $f(E)$ calculated from Eq. (10) using Eqs. (3) and (5). It is seen that electrons in the range up to 0.06 atomic units are emitted for the most part. It would be of interest to obtain the experimental distribution function at low velocities.

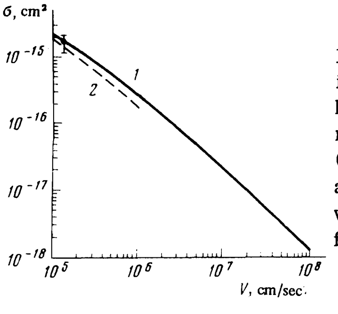

FIG. 1. Cross section double ionization of magnesium by a helium ion. Curve 1 was numerically calculated using Eqs. (6) and (8) while curve 2 was analytically calculated for low velocities using Eq. (9); ● from previous experiment.[1]

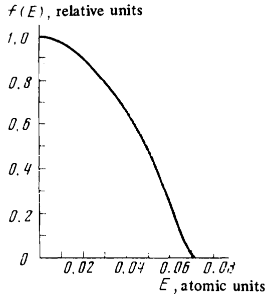

FIG. 2. Energy distribution function of ionized electrons at low velocities $V \ll 5\times10^6$ cm/sec.

5. In conclusion, we should note that the features of double-ionization of magnesium, associated with the fact that disintegration ceases at distances R between approximately 5 and 10 atomic units, are also characteristic for many other atoms (Ge, Mn, Fe, Si, ...) that can participate in the process (1). We can conclude that the cross section of the reaction (1) will fall rapidly as the sum of the two ionization potentials of the atom A approaches the ionization potential of helium, since the He$^+$–A state will rapidly become non-autoionized. This leads, for example, to the following relations for the cross sections of double ionization of different atoms by helium ions:

$$\sigma(\text{Mg})>\sigma(\text{Mn})>\sigma(\text{Ge})>\sigma(\text{Fe})>\sigma(\text{Si}).$$

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