ELECTRON DETACHMENT FROM FAST NEGATIVE IONS IN INERT GASES

G. B. LOPANTSEVA and O. B. FIRSOV

Submitted to JETP editor October 14, 1965

J. Exptl. Theoret. Phys. (U.S.S.R.) 50, 975–978 (April, 1966)

We considered the detachment of electrons from weakly bound negative ions of the first group in the periodic table, interacting with inert gases. The perturbation theory and the Fermi potential are used in the calculations. The cross section for the detachment of an electron from a negative ion is found to be equal to the total cross section for the elastic scattering of slow free electrons by the corresponding inert gas atoms at electron velocities equal to the relative velocity of the colliding atomic systems.

THE cross section for the detachment of an electron from a negative hydrogen ion in helium was calculated by Sida[1] in the Born approximation. In the form used by Sida, the calculations can yield correct results only for collision velocities greater than $2e^2/\hbar$, which corresponds to hydrogen ion energies greater than 100 keV. In fact, the agreement between Sida's calculations and experimental results at low velocities, particularly the quantitative agreement, leaves much to be desired.

The perturbation theory is also used in the present paper. However, the theory is applied to an effective potential of the δ-function type, which corresponds to the interaction of an electron belonging to a negative ion with an inert-gas atom. This potential is selected to obtain the correct scattered S-wave (the Fermi potential) on applying the Born approximation to the problem of the scattering of a slow electron in a given inert gas. In fact, the dimensions of the region effectively occupied by the wave function of a weakly bound electron in a negative ion are much larger than the dimensions of a target atom. The region occupied by the atom can be eliminated from the problem by applying to its boundaries the conditions for a logarithmic derivative of a wave function. We can also introduce a potential of sufficiently small dimensions, to which the perturbation theory can be applied and which gives the same boundary conditions.

Naturally, such a calculation will be applicable, in contrast to Sida's calculations, to collision velocities such that the de Broglie wavelength of the electron is much larger than the dimensions of the inert-gas atom, $v \ll e^2/\hbar$, but at the same time the velocity of the ion should be considerably higher than the "velocity of an electron in the orbit of a negative ion," i.e., $\sqrt{2\epsilon/m}$, where ϵ is the energy binding an electron to a negative ion and m is the electron mass. In this case a calculation based on classical mechanics gives a cross section for the electron detachment equal to the cross section for the elastic scattering of an electron by an inert-gas atom. A similar result follows from the calculation given below.

Assuming the negative ion (H^-, Li^-, Na^-, K^-, Rb^-, Cs^-) to be fixed at the origin of coordinates, the position of the inert-gas atom can be given by the radius vector $\mathbf{R}$, which depends on time $\mathbf{R} = (\rho_0, vt)$, $v = |\dot{\mathbf{R}}|$, ρ_0 is the impact parameter.

The cross section for the detachment of an electron from a negative ion in the field of an inert-gas atom is given by the formula:[1)]

$$\sigma = \int_{\rho_0}^{\infty} 2\pi\,\rho_0 d\rho_0 \int_{\mathbf{k}} |W|^2 \frac{d\mathbf{k}}{(2\pi)^3}, \qquad (1)$$

where $d\mathbf{k} = k^2 \sin\theta dk d\theta d\varphi$, and $|W|^2$ is the probability of detachment. Allowing for the electron exchange in the negative ion, W is given by

$$W = L\int\int\int \Psi_f^*(\mathbf{r}_1, \mathbf{r}_2, t)[\delta(\mathbf{r}_1 - \mathbf{R}) + \delta(\mathbf{r}_2 - \mathbf{R})] \times \Psi_i(\mathbf{r}_1, \mathbf{r}_2, t)\, d\mathbf{r}_1\, d\mathbf{r}_2\, dt. \qquad (2)$$

Since the Ψ-function is symmetrical with respect to the electron coordinates $\mathbf{r}_1$, $\mathbf{r}_2$, we have

$$W = 2L\int\int \Psi_f^*(\mathbf{R}, \mathbf{r}_2, t)\Psi_i(\mathbf{R}, \mathbf{r}_2, t)\, d\mathbf{r}_2\, dt. \qquad (3)$$

The double integral with respect to $\mathbf{r}_2$ in Eq. (3) represents some function of $\mathbf{R}$ which, at large distances, degenerates into a product of the wave functions of a free electron and an electron bound to an atom of an alkali metal. The latter is given by

$$\varphi_i = \sqrt{\frac{\alpha}{2\pi}}\, \frac{e^{-\alpha R}}{R}\, e^{i\alpha^2 t/2}$$

1)We use the atomic system of units in which $e^2 = \hbar = m_e = 1$.

and satisfies the time-dependent Schrödinger equation

$$\left(-\frac{1}{2}\Delta - i\frac{\partial}{\partial t}\right)\varphi_i(\mathbf{R}, t) = 0.$$

Here, Δ is the Laplace operator in spherical coordinates, and $\alpha = \sqrt{2\epsilon}$, where ϵ is the energy binding an electron in a negative ion.

The wave function of a free electron will be represented in the form

$$\varphi_f = \left[e^{i\mathbf{kR}} - \frac{\sin kR}{kR} + e^{i\delta_0}\frac{\sin(kR+\delta_0)}{kR}\right]e^{-ik^2t/2}$$

$$= \left[e^{i\mathbf{kR}} + e^{i\delta_0}\sin\delta_0\frac{e^{ikR}}{kR}\right]e^{-ik^2t/2},$$

i.e., a plane wave "corrected" by introducing the right zero phase.

The δ-function in Eq. (2) behaves as the Fermi interaction potential, which describes the influence of a rapidly moving inert-gas atom on a bound electron. The coefficient L in Eq. (2) is a theoretical parameter which is found from the experimental data. It is equal to $2\pi l$, where l is the length characterizing the scattering of slow electrons by corresponding atoms of inert gases.

Since vt = z, the probability of electron detachment has the form

$$W = \frac{l\sqrt{2\pi\alpha}}{v}\int_{-\infty}^{\infty}\exp\left(-\alpha R + i\frac{k^2+\alpha^2}{2v}z\right)\frac{e^{i\mathbf{kR}}}{R}dz + \frac{l\sqrt{2\pi\alpha}}{v}$$

$$e^{-i\delta_0}\sin\delta_0\int_{-\infty}^{\infty}\exp\left(-ikR - \alpha R + i\frac{k^2+\alpha^2}{2v}z\right)\frac{dz}{kR^2}. \tag{3'}$$

However, to shorten the calculations it is convenient to use directly the square of the modulus of this expression:

$$|W|^2 = 2\pi\alpha l^2 v^{-2}[(C+A)^2 + B^2]. \tag{4}$$

Here, we have introduced the following notation:

$$A = a\sin\delta_0\cos\delta_0 - b\sin^2\delta_0,$$
$$B = b\sin\delta_0\cos\delta_0 + a\sin^2\delta_0,$$

$$C = \int_{-\infty}^{\infty}\exp\left(-\alpha R + i\frac{\alpha^2+k^2}{2v}z\right)\frac{e^{-i\mathbf{kR}}}{R}dz,$$

$$a = \int_{-\infty}^{\infty}\exp\left(-\alpha R + i\frac{\alpha^2+k^2}{2v}z\right)\frac{\cos kR}{kR^2}dz,$$

$$b = \int_{-\infty}^{\infty}\exp\left(-\alpha R + i\frac{\alpha^2+k^2}{2v}z\right)\frac{\sin kR}{kR^2}dz. \tag{5}$$

Using Eq. (5), the expression in the square brackets of Eq. (4) can be written thus:

$$(C+A)^2 + B^2 = (a^2+b^2)\sin^2\delta_0$$
$$+ 2Ca\sin\delta_0\cos\delta_0 - 2Cb\sin^2\delta_0.$$

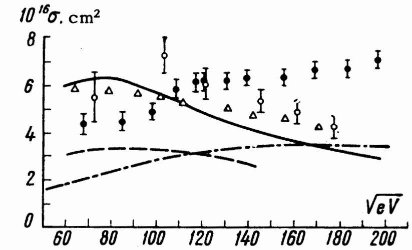

FIG. 1. Cross section for the detachment of an electron from H⁻ in He and Ne. Δ – experimental data from[3] for He target; ○, ● – experimental data from[2] for H⁻ in He and Ne, respectively; dashed curve is theoretical, taken from[1] for He target; the continuous and chain curves represent the results of the present investigation for H⁻ in He and Ne, respectively. The values of the scattering lengths l were taken from[4].

Since, C is an integral which includes a plane wave, having the following form when expanded in terms of Legendre's polynomials

$$e^{ikR\cos\theta} = {}'\sum_{j=0}^{\infty}(-i)^j(2j+1)$$

$$\times P_j(\cos\theta)\left(\frac{R}{k}\right)^j\left(\frac{1}{R}\frac{d}{dR}\right)^j\frac{\sin kR}{kR},$$

and a includes, under the integral sign, the factor (cos kR)/kR, in subsequent integration with respect to sin $\theta d\theta$, the product aC gives zero in those cases when $j \neq 0$, because of the completeness of the system of Legendre's polynomials. The term in the expansion with j = 0 yields an integral of type b:

$$2Ca\sin\delta_0\cos\delta_0 = 2ba\sin\delta_0\cos\delta_0.$$

Similar considerations show that

$$2Cb\sin^2\delta_0 = 2b^2\sin^2\delta_0,$$

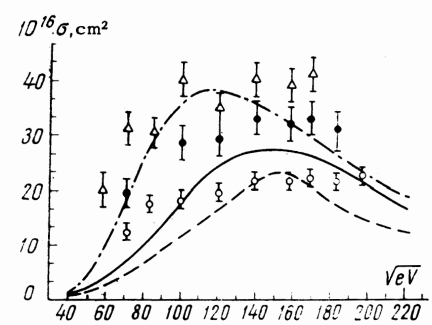

FIG. 2. Cross section for the detachment of an electron from H⁻ in Ar, Kr, Xe. ○, ●, Δ – experimental data from[2] for Ar, Kr, and Xe, respectively. The results of the present investigation for H⁻ in Ar, Kr, and Xe are represented by dashed, continuous, and chain curves, respectively. The values of the scattering lengths were taken from[5].

and finally

$$|W|^2 = 2\pi a l^2 v^{-2}\{C^2 + (a^2 - b^2)\sin^2\delta_0 + 2ab\sin\delta_0\cos\delta_0\}. \tag{6}$$

After further integration with respect to ρ_0 and k, the first term in Eq. (1) gives the contribution $4\pi l^2$ to the electron detachment cross section. Calculations show that the two other terms, responsible for the additional correction made to obtain the right S-wave phase, make a small contribution representing a fraction of one per cent of the first term.

The final result allows us to conclude that the cross section for the electron detachment from negative ions of the first group interacting with inert gases is equal to the cross section for the elastic scattering of slow electrons by these inert gases.

In particular, using fast K^-, Rb^-, and Cs^- ions, we can observe the Ramsauer effect in Ar, Kr, Xe, and other inert gases. For this purpose, we need ~120 keV Cs^- or ~36 keV K^- ions, on the assumption that this effect is observed for electrons when the electron energy is ~0.5 eV. The effect cannot be observed using H^-, Na^-, or Li^- ions, since the required ion energies are outside the range of applicability of the theory.

Figures 1 and 2 show the results of the present investigation and compare them with the published experimental data,[1-3] which are available—in the range of velocities of interest to us—only for hydrogen ions.

[1] D. W. Sida, Proc. Phys. Soc. (London) **A68**, 240 (1955).

[2] J. B. H. Stedeford, Proc. Roy. Soc. (London) **A227**, 466 (1955).

[3] P. M. Stier and G. F. Barnett, Phys. Rev. **103**, 869 (1956).

[4] C. Ramsauer and R. Kollath, Ann. Physik **12**, 529 (1932).

[5] H. S. W. Massey and E. H. S. Burhop, Electronic and Ionic Impact Phenomena, 1952 (Russ. Transl., IIL, 1958).

Translated by A. Tybulewicz
123