CALCULATION OF THE CROSS SECTIONS FOR ELECTRON LOSS BY FAST IONS IN LIGHT MEDIA

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The effective cross sections for electron loss by fast ions in hydrogen and helium were calculated in the free-collision approximation. At low binding energies of the lost electron the screening of the Coulomb field of the nuclei of the medium governs the magnitude of the cross section. In such cases, at high velocities the free-collision approximation gives results identical with those obtained in the Born approximation.

1. INTRODUCTION

USE of the Born approximation for calculating the effective cross section for electron loss by fast ions in collisions with atoms of a medium requires relatively complicated and cumbersome calculations which have been carried out only for some of the simplest cases.[1-3] Therefore, the experimental data are usually analyzed by means of Bohr's formulas,[4] which were obtained in the free-collision approximation. In the latter approximation, which is valid at high energies when the ion velocity v is considerably greater than the orbital velocity of the lost electron, the cross section for electron loss is assumed to be equal to the effective cross section for scattering of a free electron of velocity v by an atom of the medium, accompanied by a change of the electron momentum by a quantity $q \geq \mu u$, where $u = (2I/\mu)^{1/2}$, I is the binding energy of the lost electron, and μ is the electron mass. (In a system of coordinates moving with the electron before the collision the electron obtains an energy $\Delta E \geq I$.)

In the free-collision approximation we neglect "resonance effects,"[4] i.e., cases of electron loss in long-range collisions with a small change in the momenta of the colliding particles ($q < \mu u$). The contribution of such collisions to the cross section of electron loss becomes negligible at high velocities because of the screening of the Coulomb field of the nuclei of the medium by the atomic electrons. The screening should also have a definite effect on the cross sections for free collisions. However, the formula obtained by Bohr for the cross section for electron loss in light media does not allow for this screening at all. Therefore, the cross sections calculated using this formula are in many cases greater than the experimental values. Because of this the process of electron loss in the free-collision approximation is considered here with an allowance for the screening. We obtain an expression for the electron-loss cross section in light media, which includes Bohr's formula as a special case.

2. CALCULATION AND RESULTS

In the Born approximation,[5,6] the differential cross section for electron scattering by hydrogen and helium atoms with a change of electron momentum from $\hbar k$ to $\hbar(k + dk)$ can be written as follows:

$$d\sigma = 8\pi (v_0/v)^2 \{Z^2 (1 - F)^2 + Z (1 - F^2)\} k^{-3} dk, \qquad (1)$$

where $F = [1 + (ka_0/2Z^*)^2]^{-2}$; $a_0 = \hbar^2/\mu e^2$ and $v_0 = e^2/\hbar$ are the atomic units of length and velocity; Z is the nuclear charge of an atom; and Z^* is the effective nuclear charge ($Z^* = 1$ for hydrogen and 1.69 for helium).

In calculating the cross sections for electron loss the first term of Eq. (1), proportional to Z^2 and representing elastic collisions of an electron and an atom, should be integrated between the limits $k_{min} = \mu u/\hbar$ and $k_{max} = 2\mu v/\hbar$. For the second term (representing inelastic collisions, i.e.,collisions of a free electron with the electrons of an atom in the medium) we have $k_{max} = \mu v/\hbar$, and the minimum value of the transferred momentum $\hbar k_{min}$ is equal to μu only in the case when $\mu u > q_{min}$, where q_{min} is the minimum value of the transferred momentum permitted by the laws of energy and momentum conservation. If μu

$< q_{min}$, then in place of k_{min} we should use the quantity $q_{min}/\hbar$.

If the internal energy of an atom increases by ΔE on collision with an electron, then $q_{min} = \mu v(1 - \sqrt{1 - 2\Delta E/\mu v^2})$. The minimum value of ΔE is of the same order of magnitude as I_c, which is the binding energy of the electron in the ground state of an atom, so that in our case $q_{min} \approx \mu v(1 - \sqrt{1 - 2I_c/\mu v^2})$. Since the replacement of the lower limit by $q_{min}/\hbar$ occurs at $2I_c/\mu v^2 \approx 1$, then, for the sake of simplicity, we may assume that $q_{min} \approx 2I_c/v$. Thus in integrating the inelastic part of the cross section the lower limit is $k_{min} = \mu u/\hbar$ for $v > 2I_c/\mu u$ and $k_{min} \approx 2I_c/\hbar v$ for $v < 2I_c/\mu u$.

After integrating we obtain the following expression for the electron-loss cross section:

$$\sigma = \pi a_0^2 (v_0/Z^*v)^2 \{Z^2 [G_e(u/2Z^*v_0) - G_e(v/Z^*v_0)] + Z [G_i(u/2Z^*\varepsilon v_0) - G_i(v/2Z^*v_0)]\}; \quad (2)$$

$$G_e(x) = (1 + x^2)^{-1} + (1 + x^2)^{-2} + \tfrac{1}{3}(1 + x^2)^{-3},$$

$$G_i(x) = 4\ln(1 + x^{-2}) + 6(1 + x^{-2})^{-1} + 2(1 + x^{-2})^{-2} + \tfrac{1}{3}(1 + x^{-2})^{-3},$$

where $\epsilon = 1$ for $vu > 2I_c/\mu$ and $\epsilon \approx \mu vu/2I_c$ for $vu < 2I_c/\mu$. For $u \gg 2Z^*v_0$ and $v \gg u$ the expression (2) simplifies:

$$\sigma = 4\pi a_0^2 Z^2 (v_0^2/vu)^2 [1 + Z^{-1} - (u/v)^2(\tfrac{1}{4} + Z^{-1})]. \quad (3)$$

If in the square brackets of Eq. (3) we leave only the first two terms, we obtain the cited Bohr's formula in which the screening of the nuclear Coulomb field of the atoms in the medium is not allowed for. Thus Bohr's formula is valid for $u > 2Z^*v_0$. For ions with $u = 2Z^*v_0$ at $v > 3u$ this formula gives cross sections which differ by not more than 20% from those calculated using Eq. (2).

In the case $u < 2Z^*v_0$ the cross sections of Eq. (2) can be approximated, with an error not exceeding 15%, by the following expressions: for $u = (0.4 - 2)Z^*v_0$

$$\sigma = 2\pi a_0^2 Z^2 \frac{v_0^3}{Z^*v^2 u}\left\{0.6 + \frac{1.7}{Z} - \frac{u}{v}\left(\frac{2Z^*v_0}{v}\right)\left(\frac{1}{4} + \frac{1}{Z}\right)\right\}, \quad (4)$$

and for $u < 0.4Z^*v_0$

$$\sigma = \pi a_0^2 Z^2 \left(\frac{v_0}{Z^*v}\right)^2 \left\{\frac{7}{3} - \frac{13}{3Z} + \frac{8}{Z}\ln\frac{2Z^*\varepsilon v_0}{u} - \left(\frac{2Z^*v_0}{v}\right)^2\left(\frac{1}{4} + \frac{1}{Z}\right)\right\}. \quad (5)$$

These formulas are valid for $v \geq 2Z^*v_0$. For $v = (0.4 - 2)Z^*v_0$ the quantity $(2Z^*v_0/v)(\frac{1}{4} + 1/Z)$ in the braces of Eqs. (4) and (5) should be replaced by $0.3 + 1.7Z^{-1}$.

From a comparison of Eq. (3) with Eqs. (4) and (5), as well as from Figs. 1 and 2, which show the electron-loss cross sections in atomic hydrogen and helium calculated using Bohr's formulas and Eq. (2), it is evident that in the case $u \lesssim Z^*v_0$ the screening of the nuclear Coulomb field of the atoms of the medium considerably reduces the magnitude of the cross section. Without an allowance for the screening, i.e., according to Eq. (3), the electron loss cross section rises without limit with decrease of the electron binding energy. The screening limits the magnitude of the cross section: according to Eq. (2) for each value of the velocity there is a limit to the value of the cross section. From Eq. (5), on the other hand, we see that for $u < 2I_c/\mu v$, when $\epsilon = \mu vu/2I_c$, the cross section is independent of u.

It is necessary to emphasize that the reduction in cross section due to screening occurs at any velocity which can be arbitrarily high. The screening does not affect the dependence of the cross sections on the velocity at sufficiently high values of v: according to Eq. (3), as well as Eqs. (2), (4) and (5), the cross section is proportional to v^{-2}.

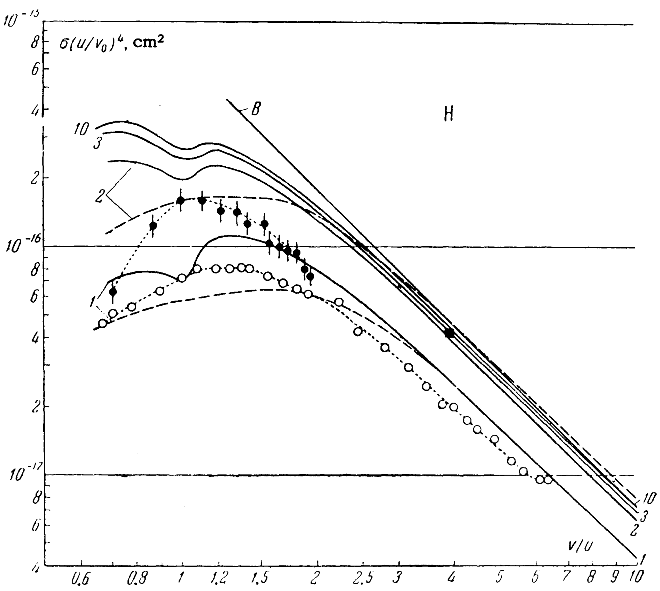

FIG. 1. Values of $\sigma(u/v_0)^4$ in hydrogen as a function of v/u for ions with u/v_0 = 1, 2, 3 and 10 (the values of u/v_0 are given near the curves). B denotes the values of $\sigma(u/v_0)^4$ according to Bohr's formula. The dashed curves represent the results obtained in the Born approximation for H atoms (u/v_0 = 1) and He^+ ions (u/v_0 = 2). The points are experimental results: ○ – for H taken from Allison's review[8]; ● and ■ – for He^+ taken from the work of Pivovar et al.[9] and Jacobsen[10] respectively.

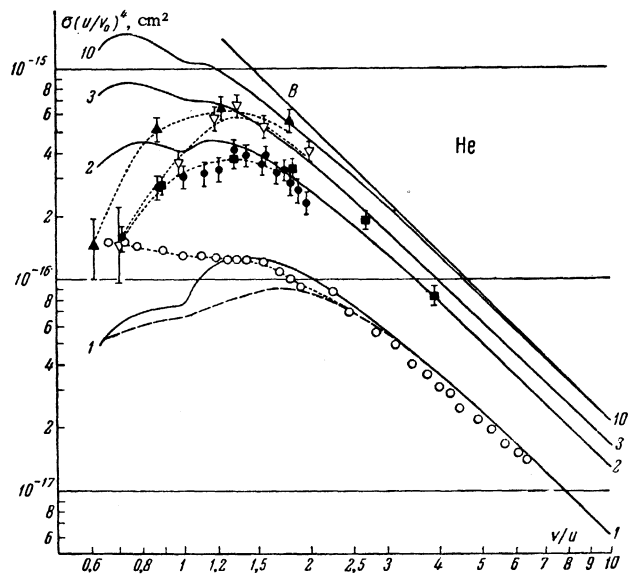

FIG. 2. Values of $\sigma(u/v_0)^4$ in helium. The values of u/v_0 are given near the curves. B represents Bohr's formula; the dashed curves give the Born approximation for H atoms. The points are experimental results: ○ – for H taken from Allison's review[8]; ● and ■ – for He^+ taken from[9] and[7] respectively; ▲ – for Li^{2+}, ▽ – for N^{4+} taken from[7].

From Eq. (5) it is also evident that the loss of weakly bound electrons occurs mainly as a result of their collision with the electrons of the medium.

3. DISCUSSION OF RESULTS

We shall compare the cross sections obtained with those calculated on the Born approximation.[1-3] The latter are given in Figs. 1 and 2.

As shown by Fig. 1 for He^+ ions in hydrogen, when $u/Z^*v_0 = 2$, for $v \geq 2u$ the free-collision approximation gives somewhat lower values of σ than does the Born approximation. This discrepancy is obviously due to the fact that in the free-collision approximation we neglect cases of electron loss in long-range collisions with small changes in the momenta of the colliding particles ($q < \mu u$). On reduction of u the role of these collisions decreases strongly due to screening. Therefore, even in the cases $u/Z^*v_0 = 1$ and 0.6 (hydrogen atoms in hydrogen and helium, Figs. 1 and 2), Eq. (2) gives for $v \geq 3u$ practically the same result as the Born approximation.

There is a considerable difference between the Born approximation and the free-collision approximation in the velocity region $v \approx u$. Because we neglect the motion of the lost electron relative to the nucleus of the ion, the threshold velocity below which the cross section is zero in the free-collision approximation is displaced from the region of very low velocities to the region $v \approx u$: for the elastic part of the cross section the threshold velocity becomes u/2 and for the inelastic part it becomes u or $(2I_c/\mu)^{1/2}$. According to Eq. (2), on increase of the velocity the cross section near the threshold rises very rapidly, and consequently two maxima appear on the $\sigma(v)$ curve and the value of the cross section in the range $v/u = 0.6 - 2$ is 1.5–2 times greater than the Born value. An allowance for the motion of the electrons in the ion smooths out the dependence of σ on v. As a result of this the curve $\sigma(v)$ for the Born approximation has only one broad maximum.

It is necessary to note that the calculations carried out in the Born approximation refer only to the loss of K-electrons, while in the derivation of Eq. (2) we made no assumptions about the initial state of the lost electrons. Therefore, the results of the present work are valid for any ion. The conclusion that, in the region of high velocities at given values of v and Z, the electron-loss cross section depends only on its binding energy, has been confirmed experimentally.[7]

To compare the calculated and experimental results, Figs. 1 and 2 show the experimental cross sections for electron loss in hydrogen and helium for H atoms and He^+ and Li^{2+} ions, each having one K-electron, and for N^{4+} ions having one electron in the L-shell ($u/v_0 = 2.68$). In the latter case the possibility of K-electron loss can be neglected, since the cross section for the loss of these electrons is 5–10 times smaller than the cross section for the loss of an L-electron.

In view of the special interest in the loss of a very weakly bound electron, both from the theoretical standpoint and in several applications, we give in Fig. 3 the theoretical and experimental cross sections for electron loss by negative hydrogen ions in hydrogen and helium (the ionization potential of H^- ions is 0.75 V, $u = 0.235v_0$). Since an H^- ion has two equivalent electrons, the cross section obtained from Eq. (2) was doubled.

As shown by Fig. 2, in helium at $v \gtrsim 2u$ the experimental results agree with the calculated ones within the experimental error. In hydrogen (Figs. 1 and 3) the theoretical cross sections at high velocities are as a rule somewhat larger than the experimental ones. Such a systematic discrepancy is, at least partly, due to the fact that the theoretical calculations were carried out for atomic hydrogen while the experimental results refer to the molecular gas.

For ions with $u < Z^*v_0$ at $v \approx u$ one cannot expect good results from the Born approximation or from the free-electron approximation. However, even in this range of velocities the experimental

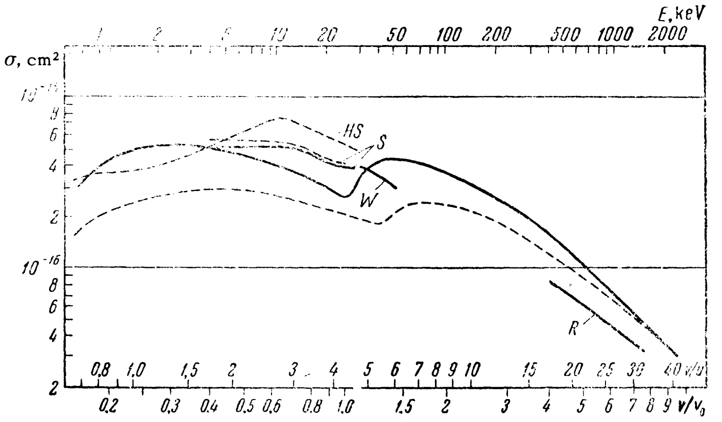

FIG. 3. Cross sections for electron loss by H^- ions in hydrogen (continuous curves) and in helium (dashed curves). The experimental curves are taken from Allison's review[8]: using the data of Steer (S), Rose (R), Hasted and Stedeford (HS), and, for $v = (1 - 1.5)v_0$, from Whittier[11] (W).

cross sections differ from the calculated ones by a factor not greater than 2.

In the case of negative hydrogen ions, for which the value of u is small, the theoretical cross sections approach the experimental ones at considerably higher values of v/u than for the other ions considered here. This is because, according to Eq. (2), there should be a second $\sigma(v)$ maximum due to the rapid rise of the contribution of inelastic collisions in the region $v \approx 6u$. In fact, as pointed out above, the contribution of inelastic collisions rises with increase of the velocity much more slowly and the second maximum is not obtained. In spite of this discrepancy the calculation allows us to understand the reason for the very weak variation of the cross section in a wide range of velocities in the case of ions with low ionization potential.

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