

*CALCULATION OF THE EFFECTIVE CROSS SECTION FOR THE LOSS OF K ELECTRONS
BY FAST HYDROGEN-LIKE IONS DURING ENCOUNTERS WITH HYDROGEN AND
HELIUM ATOMS*

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Submitted to JETP editor December 28, 1964; resubmitted April 10, 1965

J. Exptl. Theoret. Phys. (U.S.S.R.) **49**, 500-514 (August, 1965)

The cross sections for loss of K electrons by fast hydrogen-like ions of any element, due to encounters with hydrogen or helium atoms, is calculated in the nonrelativistic Born approximation. Approximate expressions suitable for practical applications are obtained for the cross sections in limiting cases. For low-charge ions the Born approximation yields cross sections which are identical with those calculated in the free-collision approximation. The calculated cross sections can also be used to estimate the cross sections for electron loss from other shells.

1. INTRODUCTION

UNTIL recently the theoretical calculations of the cross section for the loss of an electron by a fast atomic particle colliding with the atoms of a medium, were made in a wide range of velocities only for three very simple cases: loss of an electron by a hydrogen atom colliding with hydrogen^[1] or helium^[2] atoms, and loss of an electron by a singly-charged helium ion colliding with hydrogen atoms^[3]. For particles with arbitrary atomic number Z , the only published calculations pertain to the cross sections for the knock-out of K and L electrons by protons and α particles^[4,5] for a relative colliding-particle velocity $V < Zv_0$ ($v_0 = e^2/\hbar = 2.19 \times 10^8$ cm/sec), and for the electron loss in collisions between ions with velocity $V > Zv_0$ and hydrogen and helium atoms, in the free-collision approximation^[6]. These calculations did not give a sufficiently complete and correct picture of the effect of variation of V and Z on the electron-loss cross sections. To calculate the general laws governing the variations of the cross sections, and to obtain handy approximate formulas for practical calculations, we determine in the present paper, in the nonrelativistic Born approximation, the cross sections for the loss of a K electron by a hydrogen-like ion of an arbitrary element colliding with atoms of hydrogen or helium.

According to the well known criteria^[7,8], the Born approximation is valid for the calculation of the cross sections of inelastic collisions between ions of charge Z and nuclei of charge $Z_S e$, if

$Z \lesssim Z_S$ and $\kappa_S < 1$, where $\kappa_S = 2Z_S v_0/V$, i.e., only for fast collisions ($V > Zv_0$). For ions with $Z \gg Z_S$, as shown by Henneberg^[4], the Born approximation can be used also for slow collisions ($V < Zv_0$). In this case the Born approximation is equivalent to the method of impact parameters with straight-line trajectories^[9]. According to Smirnov^[10], the curvature of the trajectories can be neglected when

$$V > Zv_0(ZZ_c\mu / M_0)^{1/4} \approx (0.2 - 0.4)Zv_0$$

(where $M_0 = MM_S / (M + M_S)$ is the reduced mass of the system and μ is the electron mass). The available experimental data on the ionization of the K-shells of medium and heavy atoms by protons^[11] show that the Born approximation is in satisfactory agreement with experiment up to

$$V \gtrsim (0.1 - 0.2)Zv_0.$$

The possibility of using the Born approximation to calculate the K-electron loss cross sections in collisions between ions and neutral atoms calls for further analysis. It will be shown later that the region of applicability of the Born approximation is in this case approximately the same as for the ionization of particles by collision with atomic nuclei.

2. GENERAL FORMULA FOR THE ELECTRON LOSS CROSS SECTIONS

Using the known general formula for the cross sections for elastic collisions in the Born approximation^[12] and applying them to electron-loss phe-

nomena, we obtain for the total cross section for the loss of an electron by an ion colliding with atoms of the medium the following expression:

$$\sigma = S_{n_s} \frac{M_0^2 V'}{4\pi\hbar^4 V} \iint |\langle mm_s | N | nn_s \rangle|^2 d\mathbf{K} d\Omega, \quad (1)$$

where V and V' are the velocities of the ion relative to the atom of the medium before and after collision; $\langle mm_s | N | nn_s \rangle$ is the matrix element of the transition of the ion and the atom of the medium from the initial states m and m_s to the final states n and n_s . The final states n of the ion, which enter in (1), belong to the continuous spectrum and can be characterized by the electron wave vector \mathbf{K} relative to the nucleus of the ion when the distance between them is large. For the atoms of the medium, the final state n_s can be arbitrary, and, in particular, it may coincide with the initial state. In this connection, we integrate in (1) over all values of \mathbf{K} which are allowed by the energy and momentum conservation laws, and some S_{n_s} over all possible final states n_s of the atom of the medium, including integration over the states of the continuous spectrum.

According to [12] we have

$$\langle mm_s | N | nn_s \rangle = \int \chi_m(\mathbf{r}) \chi_n^*(\mathbf{r}) \varphi_{m_s}(\mathbf{r}_s) \varphi_{n_s}^*(\mathbf{r}_s) U e^{i\mathbf{R}\mathbf{Q}} d\mathbf{R} d\mathbf{r} d\mathbf{r}_s, \quad (2)$$

where \mathbf{R} is the radius vector of the ion relative to the nucleus of the atom of the medium; \mathbf{r} is the radius vector of the removed electron, drawn from the nucleus of the ion; \mathbf{r} — the aggregate of the radius vectors \mathbf{r}_{sj} of the atomic electrons relative to the nucleus of the atom of the medium; $\chi_m(\mathbf{r})$ and $\chi_n(\mathbf{r})$ are the wave functions of the removed electron in the initial and final states, respectively; $\varphi_{m_s}(\mathbf{r}_s)$ and $\varphi_{n_s}(\mathbf{r}_s)$ are the electron wave functions of the atom of the medium in the initial and final state; $T = M(V' - V)/\hbar$ is the change in the wave vector of the ion as a result of the collision; U is the potential of the interaction of the ion with the atom of the medium. For a single-electron ion with a nuclear charge Ze , and for an atom of the medium with a nuclear charge $Z_s e$, we have

$$U = -e^2 \left[\frac{ZZ_s}{|\mathbf{R}|} - \sum_j \frac{Z}{|\mathbf{R} + \mathbf{r}_{sj}|} - \frac{Z_s}{|\mathbf{R} - \mathbf{r}|} + \sum_j \frac{1}{|\mathbf{R} + \mathbf{r}_{sj} - \mathbf{r}|} \right].$$

If $\varphi(\mathbf{r}_s)$ can be represented in the form of a

product of wave functions of the individual atomic electrons $\varphi(\mathbf{r}_{sj})$ then, taking into account the orthogonality of the wave functions, we obtain after integrating (2) with respect to \mathbf{R}

$$\begin{aligned} & \langle mm_s | N | nn_s \rangle \\ &= \frac{4\pi e^2}{Q^2} \left[-ZZ_s \delta_{mn} \delta_{m_s n_s} + Z \delta_{mn} \sum_j^{z_s} \varepsilon_{sj}(m_s n_s) \right. \\ & \left. + Z_s \delta_{m_s n_s} \varepsilon(mn) - \varepsilon(mn) \sum_j^{z_s} \varepsilon_{sj}(m_s n_s) \right]; \quad (3) \\ & \varepsilon(mn) = \int \chi_m(\mathbf{r}) \chi_n^*(\mathbf{r}) \exp(i\mathbf{Q}\mathbf{r}) d\mathbf{r}, \\ & \varepsilon(m_s n_s) = \int \varphi_{m_s}(\mathbf{r}_{sj}) \varphi_{n_s}^*(\mathbf{r}_{sj}) \exp(i\mathbf{Q}\mathbf{r}_{sj}) d\mathbf{r}_{sj}. \quad (3a) \end{aligned}$$

For the electron-loss process $m \neq n$, therefore the first two terms in (3), corresponding to the scattering of the ion by the atom of the medium without a change in the state of the ion, do not make any contribution to the electron-loss cross section.

Taking into account the relation between Q and the ion scattering angle θ in the c.m.s.

$$\hbar^2 Q^2 = M^2(V - V')^2 + 4M V V' \sin^2(\theta/2) \quad (4)$$

and combining terms corresponding to collisions which leave the atom of the medium in its initial state, we obtain for the total electron-loss cross section the following expression:

$$\begin{aligned} \sigma &= 8\pi Z_s^2 \left(\frac{v_0}{V}\right)^2 \int_{Q_{min}}^{Q_{max}} (1-F)^2 \frac{dQ}{Q^3} \int_{K_{min}}^{K_{max}} |\varepsilon(mn)|^2 d\mathbf{K} \\ &+ 8\pi \left(\frac{v_0}{V}\right)^2 S_{n_s}' \int_{Q_{min}}^{Q_{max}} \frac{dQ}{Q^3} \int_{K_{min}}^{K_{max}} |\varepsilon(mn)|^2 \sum_j^{z_s} |\varepsilon(m_s n_s)|^2 d\mathbf{K}; \\ & F = Z_s^{-1} \sum_j^{z_s} \varepsilon(m_s n_s). \quad (5) \end{aligned}$$

Here F is the atomic form factor. For hydrogen and helium atoms $F = [1 + (Qa_0/2Z_s^*)^2]^{-2}$, where $Z_s^* e$ is the effective charge of the nuclei (for hydrogen atoms $Z_s^* = 1$, for helium atoms $Z_s^* = 1.69$), $a_0 = \hbar^2/\mu e^2$ is the atomic unit of length.

The first term in formula (5), which we denote σ_{el} , is the electron-loss cross section for ion-atom collisions in which the medium remain in the initial state. These collisions correspond to elastic collisions between the electron in the ion and the atoms of the medium, and can be called pseudo-elastic. The second term in (5), henceforth denoted σ_{inel} , is the electron loss cross section in pseudo-inelastic collisions, i.e., in collisions which end in

excitation or ionization of the atoms of the medium (we leave out the value $n_s = m_s$ in the summation of S'_{n_s} over n_s).

Under the usually satisfied condition $V - V' \ll V$, we can replace $M^2(V - V')^2$ in (4) by $(\Delta E/V)^2$, where

$$\Delta E = \frac{1}{2}M(V^2 - V'^2) = I + \hbar^2 K^2 / 2\mu - \Delta E_{n_s},$$

I is the binding energy of the lost electron in the initial state. ΔE_{n_s} is the change in the energy of the atom of the medium as it goes over into the state n_s . In this approximation we obtain for the integration limits in (5)

$$Q_{min} = \Delta E / \hbar V, \quad Q_{max} = 2MV / \hbar.$$

We shall show that the cross section for the electron loss is practically independent of Q_{max} , and we can therefore assume that $Q_{max} = \infty$. The value of K_{min} for hydrogen-like ions is zero, and K_{max} is determined from the equation

$$QV\hbar = \Delta E = I + \hbar^2 K_{max}^2 / 2\mu + \Delta E_{n_s}.$$

3. LOSS OF K ELECTRON IN PSEUDOELASTIC COLLISIONS

The cross section for the loss of an electron in pseudoelastic collisions depends essentially on the quantity $|\epsilon(mn)|^2$. For the case when the K electron goes over into the continuous-spectrum state, this quantity was calculated by Bethe^[13] and by Massey and Mohr^[14] in connection with the solution of the problem of the ionization of a hydrogen-like ion by electrons or protons. As a result of these calculations, using exact nonrelativistic wave functions of an electron in the Coulomb field, we obtained after integrating over the angle variables Ω_k of the momentum space K :

$$\begin{aligned} \int_{\Omega_k} |\epsilon(mn)|^2 K^2 d\Omega_k dk &= \epsilon_{k,q}^2 dk \\ &= \frac{256q^2(q^2 + 1/3 + 1/3k^2)}{[(q^2 - k^2 + 1)^2 + 4k^2]^3 (1 - e^{-2\pi/\hbar})} \\ &\times \exp\left[-\frac{2}{k} \tan^{-1} \frac{2k}{q^2 - k^2 + 1}\right] k dk, \end{aligned} \quad (6)$$

where $q = Q\hbar/\mu y_e = Qa_0/Z$, $k = K\hbar/v_e = Ka_0/Z$, and $v_e = Zv_0$ is the average orbital velocity of the K electron.

After introducing the quantity $v = V/v_e = V/Zv_0$, we obtain for σ_{el} the expression

$$\sigma_{el} = 8\pi a_0^2 \left(\frac{Z_s}{Z^2 v}\right)^2 \int_{1/2v}^{\infty} (1-F)^2 \frac{dq^{(2qv-1)^{1/2}}}{q^3} \int_0^2 \epsilon_{k,q}^2 dk. \quad (7)$$

The cross sections σ_{el} were calculated by formula (7) with values $F = [1 + (Zq/2Z_s^*)^2]^{-2}$ and $\epsilon_{k,q}^2$ from (6), for the loss of a K electron by hydrogen-like ions of different elements colliding with hydrogen atoms or helium atoms, using the M-20 computer of the Moscow University (see the Appendix). The results of the calculations are shown in Figs. 1a and b. We see from the figures that the values of σ_{el} for the loss of an electron by hydrogen atoms in hydrogen and helium, and by He^+ ions in hydrogen, coincided with the results corresponding to the calculations of Bates and

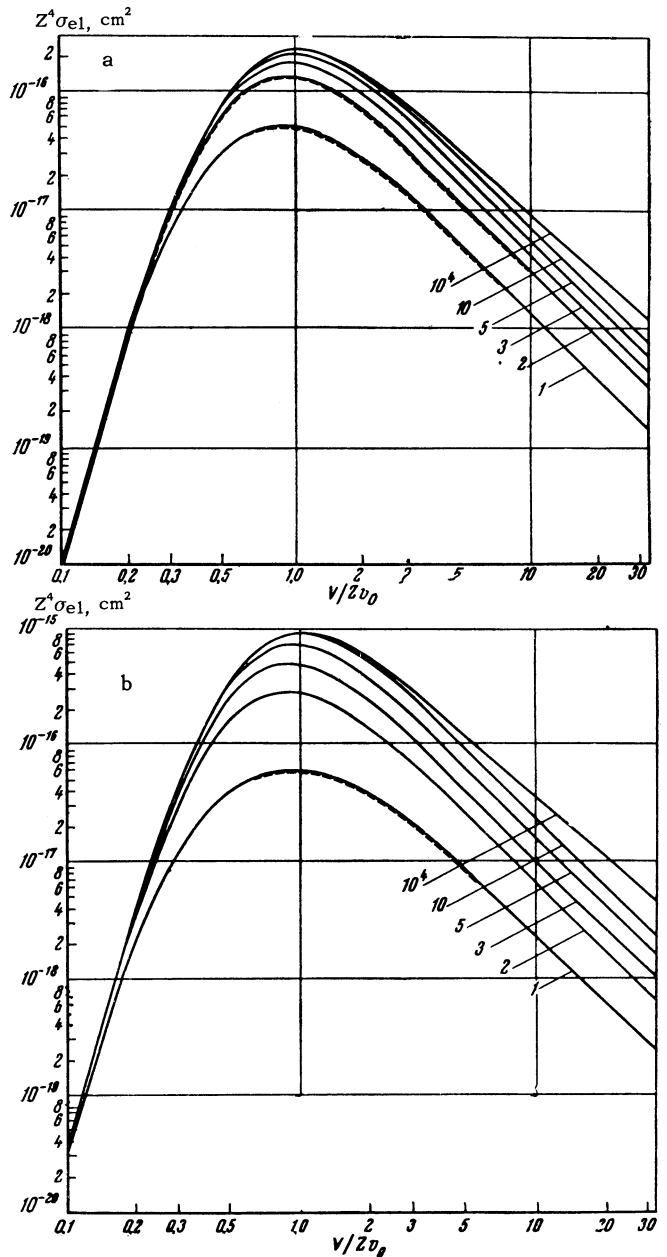


FIG. 1. $\sigma_{el}Z^4$ vs. $v = V/Zv_0$: a - in hydrogen, b - in helium. The values of Z are marked on the curves. Dashed curves - result of calculations from^[1-3].

Griffing^[1], Boyd, Moiseiwitsch and Stewart^[2], and Bates and Williams^[3].

The upper curve of each figure pertains to the ions with large values of Z , for which $F = 0$. The values of σ_{e1} given by these curves are therefore also the cross sections for the ionization of the hydrogen-like ions in collisions with unscreened nuclei, and coincide with the cross sections calculated earlier by Bates and Griffing^[1] and Merzbacher and Stewart^[5] for the knocking out of a K electron by fast atomic nuclei. In the region $v < 1$, these cross sections coincide within 15% with the values of σ given by the approximate formula of Henneberg^[4].

The screening of the Coulomb field of the nuclei of the atoms of the medium by the atomic electrons, which is accounted for by the value of F , leads to a noticeable decrease in the electron-loss cross sections if $v > Z/4Z_S^*$, when $(1 - F)^2$ becomes appreciably smaller than unity for $q_{\min} = 1/2v$.¹⁾ It is seen from the figures that the role of the screening does not weaken with increasing velocity. In the region $v < Z/4Z_S^*$, the value of σ_{e1} for collisions of the ion with the atoms of hydrogen and helium turns out to be the same as for collisions with the hydrogen and helium nuclei, which have no electron shell.

The dependence of σ_{e1} on the ion velocity is determined by the general character of the function $\epsilon_{k,q}^2$ and by the range of q and k over which the integration in (7) is carried out in accordance with the laws of energy and momentum conservation. At fixed values of q , the value of $\epsilon_{k,q}^2$ reaches a maximum at $k \sim 1/2$ if $q \lesssim 1/2$ and at $k \approx q$ if $q \gtrsim 1$, after which it decreases rapidly with further increase in k . Therefore, when the maximum is included in the integration region, the value of the integral

$$J = \int_0^{k_{\max}} \epsilon_{k,q}^2 dk$$

depends little on the upper limit and is close to its limiting value J_∞ at $k_{\max} = \infty$, namely, $J_\infty = 0.28q^2$ when $q \ll 1$ and $J_\infty = 1$ when $q \gg 1$. On the other hand, if the maximum of the integrand is outside the integration limits, then $J \ll J_\infty$.

When $v \ll 1$, so that the maximum of $\epsilon_{k,q}^2$ remains outside the integration region, the main contribution to σ_{e1} is made by collisions with $q \approx 1/2v \gg 1$ and $k \approx 0$. In this case $\epsilon_{k,q}^2 = 256q^{-8}k$ and

$$\sigma_y = \frac{1}{45} 2^{10} \pi a_0^2 (Z_c/Z^2)^2 v^{-8}. \quad (8)$$

¹⁾The quantity $(1 - F)^2$ differs little from unity when $q > 2Z_S^*/Z$, and is close to $(Z^2q^2/2Z_S^{*2})^2$ when $q < Z_S^*/Z$.

This expression coincides with the previously obtained^[1,5] limiting formulas for the cross sections for K-electron knockout by atomic nuclei. The approximate Henneberg formula with $v \ll 1$ leads to values which are $2/3$ times larger than in (8).

As the velocity v approaches unity and q_{\min} approaches $1/2$, the dependence of $\epsilon_{k,q}^2$ on q in the region $q \sim q_{\min}$ and $k \sim 0$ becomes weaker, and the increase in the cross sections σ_{e1} with increasing v slows down. In the region $v \sim 1$, when the limit of integration reaches the region of the maximum of the function $\epsilon_{k,q}^2$, the values of σ_{e1} are maximal. The change in the ion momentum $\hbar Q_{\min}$ in remote ionizing collisions then constitutes about one-half the average momentum μv_e which must be transferred to the electron to detach it from the ion.

In the region $v \geq 3$, in a sufficiently broad interval of q ($q \approx 5/8v$ to $q \approx 2v$, corresponding to $k_{\max} \approx 1/2$ and $k_{\max} \approx q$), the maximum of the function $\epsilon_{k,q}^2$ lies in the integration region and consequently $J \approx J_\infty$. For values of q outside this interval we have $J \ll J_\infty$. We can therefore write in this case the following approximate expression for σ_{e1} :

$$\sigma_{e1} = 8\pi a_0^2 \left(\frac{Z_s}{Z^2 v} \right)^2 \times \left\{ \int_1^{2v} (1 - F)^2 \frac{dq}{q^3} + 0.28 \int_{5/8v}^q (1 - F)^2 \frac{dq}{q} \right\}. \quad (9)$$

The first term of this expression coincides with the cross section for electron loss in elastic collisions between the electrons and the atoms of the medium, in the free-collision approximation, in which the electron-loss cross section is assumed equal to the cross section for the scattering of a free electron of velocity v by an atom of the medium, with a momentum change $\hbar Q > Z\mu v_0$ (i.e., $q > 1$). The second term corresponds to the so-called resonance effects, i.e., to cases when the electron is lost in remote collisions, with small change of momentum of the colliding particles ($q < 1$).

Recognizing that when $q > 2Z_S^*/Z$ the quantity $(1 - F)^2$ is close to unity, and when $q < Z_S^*/Z$ it is close to 0, we get from (9) that for ions with $Z > 2Z_S^*$ and $v > 3$, accurate to 10%,

$$\sigma_{e1} = 4\pi a_0^2 (Z_s/Z^2 v)^2 \{1 - (2v)^{-2} + 0.56 \ln A\}, \quad (10)$$

where A is the smaller of the quantities $8v/5$ or $Z/2Z_S^*$.

For ions with $Z > 2Z_S^*$, as can be seen from (10), the screening of the Coulomb field of the nuclei of the medium by the atomic electrons limits

the contribution of the resonance collisions to σ_{el} when $v > Z/2Z_S^*$. When $Z < Z_S^*$, the screening becomes so appreciable that resonance effects can be completely neglected. In this case the Born approximation leads to cross sections which coincide with those calculated in the free-collision approximation. The corresponding expressions for σ_{el} are given in our earlier paper^[6].

4. LOSS OF K ELECTRON AND PSEUDOELASTIC COLLISIONS

Calculation of the electron-loss cross sections in collisions accompanied by excitation of the atom of the medium is a more complicated problem than the calculation of σ_{el} , for in this case it is necessary to calculate the probability of the electron loss as the atoms of the medium go over simultaneously into each of the excited final states, and then it is necessary to sum these probabilities. If the summation were not limited by the energy and momentum conservation laws, and extended over all the excited states of the atom of the medium, then we would have in accordance with the sum rule

$$S_{n_s}' |\epsilon(m_s n_s)|^2 = 1 - F^2 \quad (11)$$

and consequently we could write for σ_{inel}

$$\sigma_{inel} = 8\pi a_0^2 \frac{Z_s}{(Z^2 v)^2} \int_{q_{min}}^{\infty} (1 - F^2) \frac{dq}{q^3} \int_0^{k_{max}} \epsilon_{k,q}^2 dk, \quad (12)$$

where $k_{max} = [2qv - 1 - \overline{\Delta E_{n_s}}/I_0 Z^2]^{1/2}$ ($I_0 = \mu v_0^2/2$ is the electron binding energy in the ground state of the hydrogen atom), and q_{min} is determined from the equation $k_{max} = 0$.

Actually, for each pair of values of k and q , the summation in (11) is limited only to those excited states for which

$$\Delta E_{n_s} \leq I_0 Z^2 (2qv - 1 - k^2).$$

It is obvious that if this inequality allows transitions to the levels of the continuous spectrum with $\Delta E_{n_s} = I_s + \hbar^2 K_s^2/2\mu$, where $I_s = u_s^2 I_0$ is the binding energy of the electron in the atoms of the medium ($u_s = 1$ for hydrogen and $u_s = 1.35$ for helium) and K_s is the wave number of the electron emitted from the atom of the medium, then the sum $S_{n_s}' |\epsilon(m_s n_s)|^2$ includes also terms corresponding to transitions to arbitrary discrete levels with $\Delta E_{n_s} < I_s$. In the case when the electron goes over from hydrogen or helium atoms into the continuous spectrum, the expression for $|\epsilon(m_s n_s)|^2$ coincides with the formula for $|\epsilon(mn)|^2$ with the quantities q and k replaced respectively by qZ/Z_S^*

and $k_s Z/Z_S^*$, where $k_s = K_s a_0/Z$. Therefore in the region $q > Z_S^*/Z$, where the plot of ϵ^2 vs. k_s has a sharp maximum at $k_s \approx q$, the main contribution to $S_{n_s}' |\epsilon(m_s n_s)|^2$ is made by the terms corresponding to the transitions of the atomic electron to the states of the continuous spectrum with $k_s \sim q$. Transitions to the states with $k_s > q$ can be neglected. Consequently, if the integration with respect to k_s in $S_{n_s}' |\epsilon(m_s n_s)|^2$ extends to $k_s \gtrsim q$, relation (11) is in practice correct; cases when the upper limit of integration remains smaller than q can be neglected.

In the region $q < Z_S^*/2Z$ we can disregard the contribution made to $S_{n_s}' |\epsilon(m_s n_s)|^2$ by terms corresponding to transitions to the states with $k_s \geq Z_s/Z$. Therefore, if the integration with respect to k_s extends to $k_s > Z_S^*/Z$ in this region of q , then relation (1) is also valid. In this connection, we can use for σ_{inel} at high velocities expression (12) with a modified upper limit for integration with respect to q . For the value of the average excitation energy of the atom of the medium $\overline{\Delta E_{n_s}}$ we have

$$\overline{\Delta E_{n_s}} = I_0 Z^2 (u_s^2/Z^2 + \bar{k}_s^2),$$

and for $q \gtrsim Z_S^*/Z$ it is necessary to assume that the mean value \bar{k}_s is equal to q . Nor will a large error result from assuming that $k_s = q$ when $q < Z_S^*/2Z$, since most collisions that end in a change of the state of the atom of the medium lead, at such small values of q , not to ionization of the atom, but to its excitation, with $\Delta E_{n_s} < I_s$. The values of q_{max} and q_{min} are determined from the equation $k_{max} = 0$, so that when $k_s = q$ we get

$$q_{max, min} = v \pm [v^2 - (1 + u_s^2/Z^2)]^{1/2}.$$

Relation (12) with $k_s = q$ is valid in the region $v \geq [3(1 + u_s^2/Z^2)]^{1/2}$, when k_{max} exceeds q in a sufficiently large interval of values of q , from q_1 to q_2 , such that $q_2/q_1 \geq 3$. In the region of small velocities, formula (12) with $k_s = q$ gives too low a value of σ_{inel} , since no account is taken in this approximation of collisions with those k and q for which the maximum possible value is $k_s < q$, i.e., the maximum possible value $\Delta E_{n_s} < I_0 Z^2 (u_s^2/Z^2 + q^2)$. To calculate σ_{inel} in the region of v from $v = 0.5$ to $v = [3(1 + u_s^2/Z^2)]^{1/2}$ we therefore used formula (12) with the simplest type of expression for ΔE_{n_s} :

$$\overline{\Delta E_{n_s}} = I_0 Z^2 (\alpha u_s^2/Z^2 + \beta).$$

If the coefficients α and β are properly chosen, formula (12) leads to values of σ_{inel} close to those

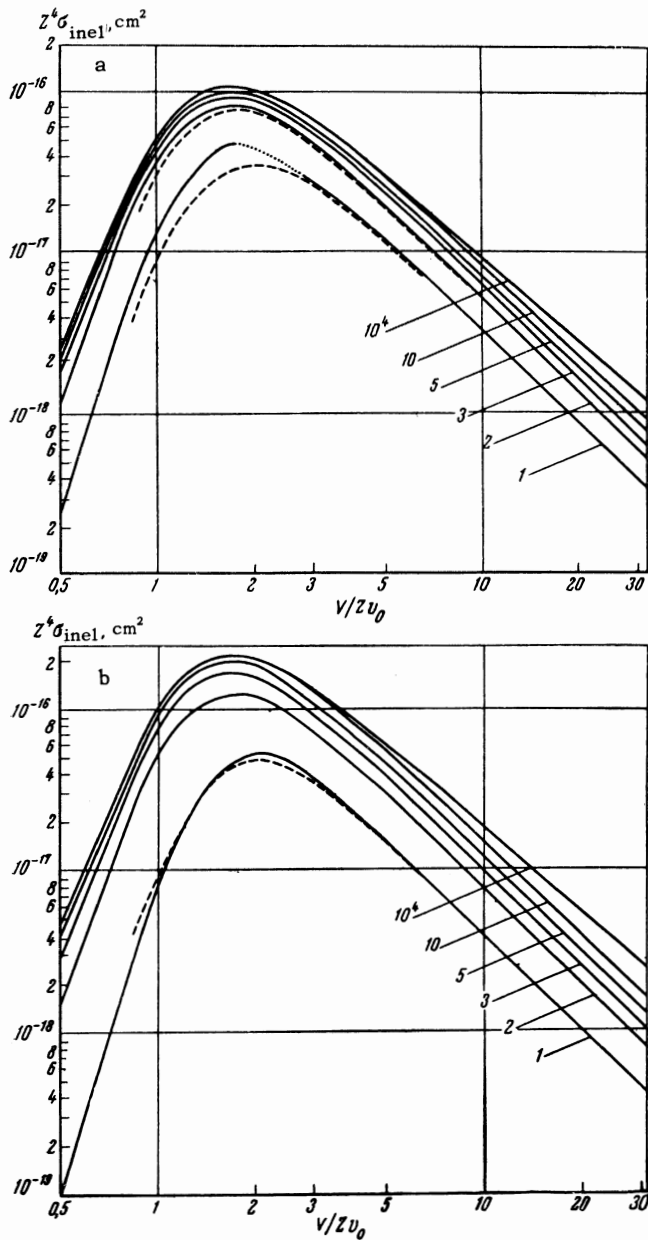


FIG. 2. $\sigma_{inel}Z^4$ vs. $v = V/Zv_0$: a – in hydrogen, b – in helium. The values of Z are indicated next to the curves. Dashed curves – results of calculations from [1-3].

obtained by others [1-3] as a result of more detailed calculations. It turned out that for $\alpha = 0.7$ and $\beta = 1$, the values of σ_{inel} obtained in this manner for the cases of H in He ($u_S^2/Z^2 = 1.76$) and He⁺ in H ($u_S^2/Z^2 = 0.25$) coincide within 10% with the more accurate calculations in this velocity interval, and in the case of electron loss by hydrogen atoms in hydrogen ($u_S^2/Z^2 = 1$) they exceed the exact values by ~ 50%.

The calculation of σ_{inel} in the region $v \ll 1$, from the point of view of obtaining the total cross sections for the electron loss energy, is of no in-

terest, for $\sigma_{inel} \ll \sigma_{el}$ in this velocity region. This is connected with the fact that for $v < 1$ the values of the cross sections decrease rapidly with increasing values of ΔE , which are larger for σ_{inel} than for σ_{el} . The results of calculations of σ_{inel} , obtained by numerical integration of (12) with the indicated values of ΔE_{nS} , are shown in Figs. 2a and b.

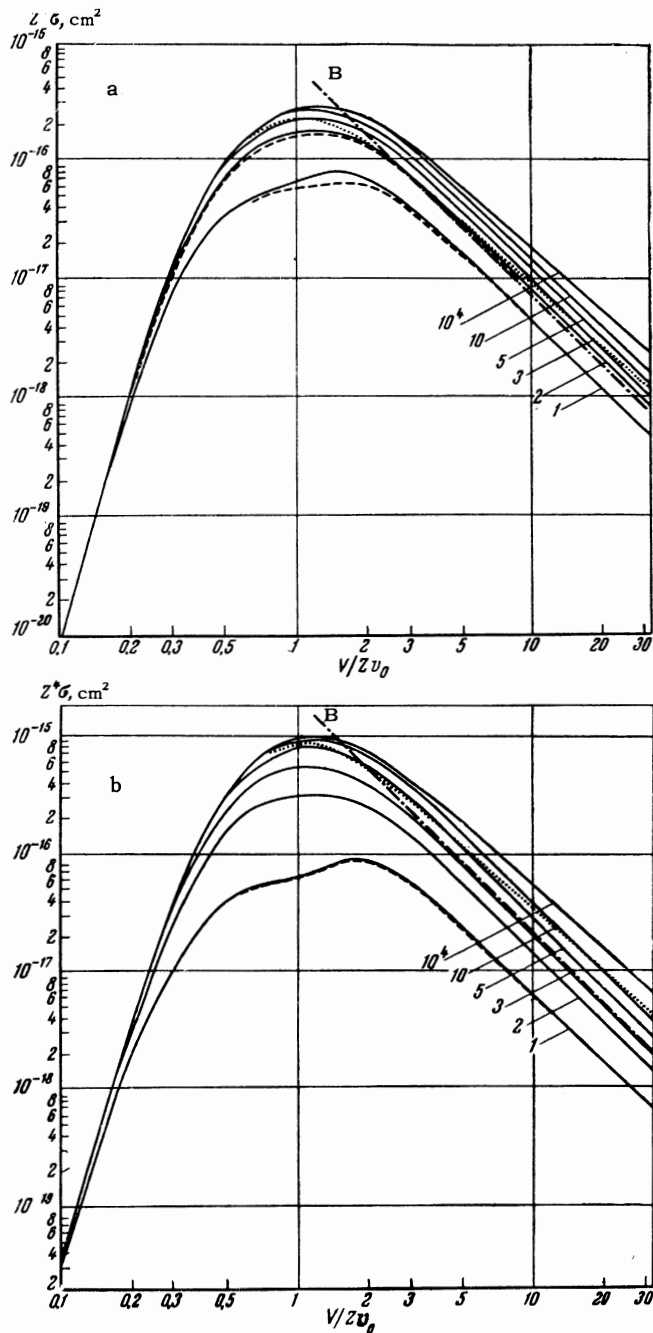


FIG. 3. σZ^4 vs. $v = V/Zv_0$: a – in hydrogen, b – in helium. The values of Z are marked near the curves. Dashed curves – results of calculations from [1-3]; dash-dot curves – values of σZ^4 for collisions between ions and atomic nuclei.

Just as we obtain from (7) the limiting formula (9), we can obtain from (12) the following expression for σ_{inel} in the region of high velocities ($v \geq 3$):

$$\sigma_{inel} = 8\pi a_0^2 \frac{Z_S}{(Z^2 v)^2} \left\{ \int_1^v (1 - F^2) \frac{dq}{q^3} + 0.28 \int_1^q (1 - F^2) \frac{dq}{q} \right\},$$

$$q_{min} = (v^{5/4} + u_s^2/Z^2)/2v. \quad (13)$$

Recognizing that when $q > Z_S^*/Z$ the value of $(1 - F^2)$ is close to unity, and when $q \ll Z_S^*/Z$ it is close to $(Zq/Z_S^*)^2$, i.e., it is much smaller than unity, we obtain from (13), for $Z_S^*/Z < 1$,

$$\sigma_{inel} = 4\pi a_0^2 \frac{Z_c}{(Z^2 v)^2} \left\{ 1 - \frac{1}{v^2} + 0.56 \ln B \right\}, \quad (14)$$

where B is equal to the smaller of the quantities Z/Z_S^* or $1.6v(1 + 0.8u_s^2/Z^2)$. The cross sections calculated with this formula for $v \geq 3$ differ from those given by (13) by not more than 10%.

When $Z_S^*/Z > 1$, the second integral in (13) practically vanishes, and the Born approximation leads to the same result as the free-collision approximation. The expressions for σ_{inel} in this approximation are also given in the earlier paper [6].

5. DISCUSSION

The total cross sections for the loss of a K electron in hydrogen and in helium, obtained by summing σ_{el} and σ_{inel} , are shown in Figs. 3 and 4. In the region $V > Zv_0$, the contributions of σ_{el} and σ_{inel} to the total cross section turn out to be comparable, and as the ion velocity changes the ratio of σ_{el} to σ_{inel} remains practically constant. In the region $V < Zv_0$, the contribution of σ_{inel} to the total cross section decreases rapidly with decreasing velocity, as a result of which, for $V < Zv_0/2$, the total electron-loss cross section is determined actually only by the value of σ_{el} . In this connection, the approximate nature of the calculations of σ_{inel} in the region $V \lesssim Zv_0$ affects little the obtained values of the cross sections. The greatest difference between the cross sections calculated in the present paper and those obtained in [1-3] is observed when $V \sim (1-2)Zv_0$, and does not exceed 5-10%.

As was already indicated in the introduction, in calculations of the cross sections for inelastic collisions between ions and nuclei with charge $Z_S e$, the Born approximation is valid for ions with $Z \lesssim Z_S$ when $V > 2Z_S v_0$ [7,8] and for ions with Z

$\gg Z_S$ when $Z > Zv_0 [ZZ_S \mu / M_0]^{1/4}$ [10]. For the Born approximation to be applicable to the cross sections for electron loss by ions in collisions with neutral atoms, it is necessary in addition that the perturbation of the electron shell of the atoms in these collisions be small or, otherwise, that it exert no noticeable influence on the value of the cross section. This perturbation can be regarded

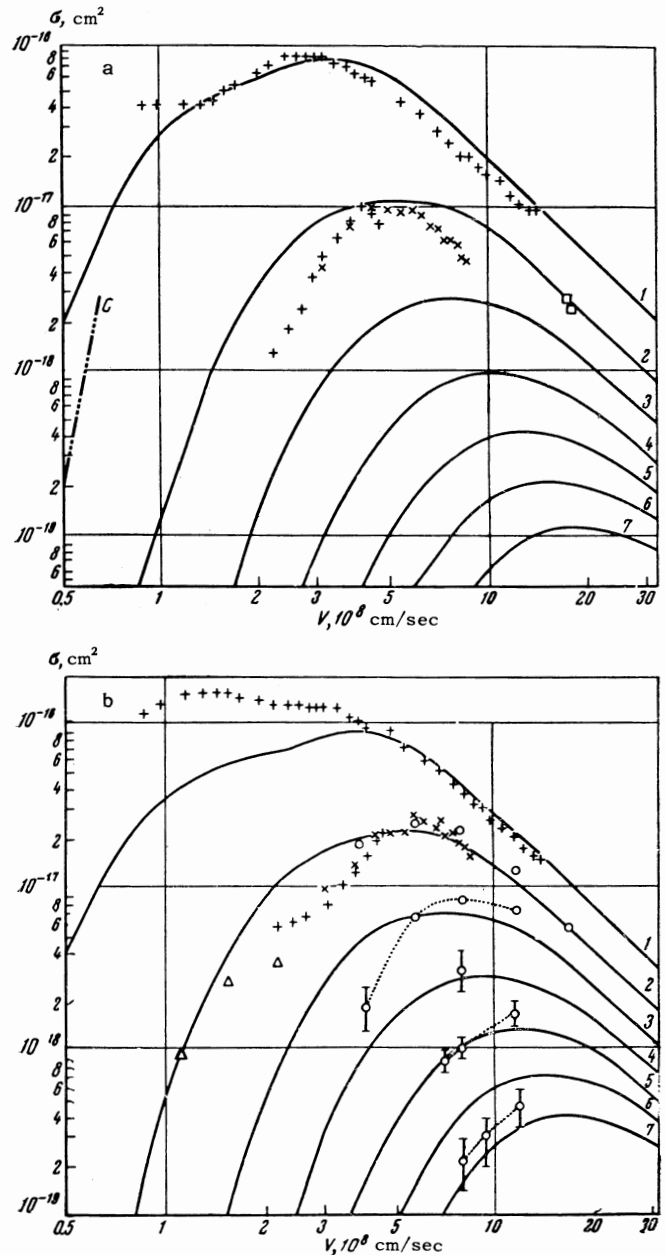


FIG. 4. Total cross section for the loss of a K-electron as a function of V : a — in hydrogen, b — in helium. The values of Z are indicated next to the curves. Experimental data: + — for H and He^+ from [16]; x — for He^+ from [18]; □ — for He^+ (in hydrogen) from [15]; Δ — for He^+ (in helium) from [17]; ○ — for He^+ , Li^+ , Be^+ , Be^{+3} , and N^+ (in helium) from [19]; C — cross section for the ionization of hydrogen atoms by protons, from [10].

as small when $2Zv_0/V < 1$, and therefore in the region $V > 2Zv_0$ the Born approximation is valid for ions with $Z < Z/2v_0$. When $Z > V/2v_0$, the perturbation of the electron shell of the atoms of the medium can turn out to be sufficiently large and change appreciably the atomic form factor F , which enters in expressions (7) and (12) for σ_{el} and σ_{inel} , and the binding energy I_S of the atomic electron, on which σ_{inel} depends. With increasing Z , however, the influence of the values of F and I_S on σ_{el} and σ_{inel} decreases, and therefore the Born approximation should give the correct value of the cross section for ions with sufficiently large Z .

The weakened influence of I_S on the cross section σ_{inel} with increasing Z is connected with the rapid growth of the binding energy of the electron belonging to the ion, and a resultant decrease in the role of I_S in the energy balance of the process under consideration. From the calculations presented it follows that whereas for ions with $Z \sim (1-2)Z_S$ a change by a factor of 2 in the value of I_S leads to a $\sim 30\%$ change in σ_{inel} in the region of V from $2Z_Sv_0$ to $2Zv_0$, and a change of 10–20% in $\sigma_{el} + \sigma_{inel}$, in the case of ions with $Z = 3Z_S$ the same change in I_S changes σ_{inel} and $\sigma_{el} + \sigma_{inel}$ by not more than 10% respectively, and for ions with $Z \geq 4Z_S$ these cross sections are hardly changed.

The value of F ceases to exert a noticeable influence on the cross sections σ_{el} and σ_{inel} at small values of the parameter VZ_S^*/Z^2v_0 , when a short-range collision with transfer of relatively large momentum Q is necessary for the ionization of the particle. According to Secs. 3 and 4, the cross section σ_{el} is practically independent of F when $Z > (4Z_S^*V/v_0)^{1/2}$, and the same holds for σ_{inel} when $Z > (2Z_S^*V/v_0)^{1/2}$.

Thus, in the region $V > 2Z_Sv_0$, the Born approximation should lead to correct ionization cross sections in collisions with neutral atoms for ions with $Z < Z_S/\kappa_S$ and $Z > Z_S(8Z_S^*/Z_S\kappa_S)^{1/2} > Z_S(8/\kappa_S)^{1/2}$, where $\kappa_S = 2Z_Sv_0/V < 1$. We expect the actual cross section to differ from that calculated in the Born approximation only for ions for which $1/\kappa_S > Z/Z_S > (8/\kappa_S)^{1/2}$. It is little likely, however, that these deviations would be large in such a narrow region of values of Z .

A comparison of the calculated results with the presently known experimental cross sections for the loss of a K electron by fast hydrogen-like ions is shown in Figs. 4a and b. It is seen from the figures that in the region $V \geq 2Z_Sv_0$, when $\kappa_S \lesssim 1$, good agreement between the calculated and experimental cross sections is observed for all the ions, including the ions for which $1/\kappa_S > Z/Z_S > (8/\kappa_S)^{1/2}$.

For ions with $Z \sim Z_S$ (He^+ , Li^{+2}), the experimental cross sections are somewhat lower than the calculated ones when $V < Z_Sv_0$. It must be noted that the cross sections for the ionization of hydrogen atoms by protons in the region $V \sim (0.1-0.3)v_0$ (see Fig. 4a), obtained by Smirnov^[10] in the adiabatic approximation, are also lower than those calculated in the Born approximation.

Even in the region of high velocities, the cross sections for K-electron loss are generally speaking greatly different from the values given by the well-known Bohr formula^[8]

$$\sigma = 4\pi a_0^2 (Z_S^2 + Z_S) Z^{-2} (v_0/V)^2. \quad (15)$$

This formula corresponds to the free-collision approximation without account of screening of the Coulomb field of the nuclei of the atoms of the medium by the atomic electrons. As can be seen from Figs. 3a and b, the Bohr formula is applicable in fact only to cases when the electron is lost by ions with $Z \sim 2Z_S$. Only when screening is taken into account for ions with $Z \sim Z_S$ does the approximation of free collisions lead to cross sections which coincide to those calculated in the Born approximation^[6]. From Figs. 3a and b we see that at high electron binding energies the cross section for electron loss in collisions with atoms turned out to be larger than in collisions with the corresponding atomic nuclei. When the lost electrons have lower binding energies, the opposite relation is observed.

We see from the foregoing calculation that the initial state of the lost electron influences the electron-loss cross section through the function $\epsilon_{k,q}^2$ and through the region of values of q and k over which the integration is carried out. For the K electron the function ϵ^2 is such that when $V > v_e$ ($v_e = Zv_0$ is the average orbital velocity of the electron in question) the main contribution to the cross section is made by collisions for which $q \sim k \sim 1$. For the L shell^[21] with $v_e = Zv_0/2$, the function ϵ^2 plotted against $q = Q\hbar/\mu v_e$ and $k = K\hbar/\mu v_e$ has qualitatively the same form as for the K electron, and in the region $q \sim k \sim 1$ the values of ϵ^2 for the K and L electrons differ relatively little. In this connection, in the region $V \gtrsim v_e$ the cross sections for the loss of K and L electrons should be approximately the same for the same values of V and v_e .

Such an agreement between the cross sections is actually obtained^[19,20] and is not limited to ions with only one electron in the K or L shell. According to the experimental data, for positive atomic ions, at fixed values of V and $u = (2I/\mu)^{1/2}$ (where I is the electron binding energy), the cross

sections for the loss of an individual electron from the K and L shell are equal within 20% regardless of the number of electrons in the shell.

Inasmuch as I enters in the equation for the integration limit

$$q_{min} V = 1/2 k^2_{max} v_e + (I + \Delta E_{n_s}) / \mu v_e,$$

the cross section for electron loss should in general depend both on v and on u . For hydrogen-like ions $u = v_e$, but for multi-electron ions the values of u and v_e may not coincide.

The agreement of the cross sections for the loss of an individual electron by different ions, at identical values of V and u , apparently proves that we can neglect the difference between v_e and u when considering the ionization of positive ions.

In connection with this equality of the cross sections for the loss of an electron from different shells, the results of the calculation given above for the hydrogen-like ions can be used also in estimates of the cross sections for the loss of electrons by other ions.

The authors are grateful to O. B. Firsov for valuable advice and remarks in a discussion of the present work.

APPENDIX

All the integrals considered in this paper were calculated by the method of optimal coefficients^[22]. To this end, the initial region where the integrand function was defined mapped on a unit square, and the integral was calculated in accordance with the following quadrature formula:

$$\int_0^1 \int_0^1 f(x, y) dx dy = \frac{1}{N} \sum_{k=1}^N f \left[\tau \left(\frac{ka_1}{N} \right), \tau \left(\frac{ka_2}{N} \right) \right] \tau' \left(\frac{ka_1}{N} \right) \tau' \left(\frac{ka_2}{N} \right) + R,$$

where $\tau(x)$ and $\tau(y)$ are functions which realize the periodization of the integrand, N the number of integration points, a_1 and a_2 the optimal coefficients in modulo N , and R the integration error. In the two-dimensional case we can replace the numbers N , a_1 , and a_2 by ξ_n , 1, and ξ_{n-1} , where ξ_i is the i -th member of the Fibonacci number sequence; then, if $\tau(x)$ and $\tau(y)$ realize full periodization, the error of the approximate integration is equal to

$$R = O(\ln \xi_n / \xi_n^\alpha).$$

Starting from the properties of the given integrands, the integration was carried out over 2,584 points ($\xi_n = 2584$) with fourth-order periodization

($\alpha = 4$). As a result of such a choice of parameters, the average relative error in the calculation of the integrals was 10^{-5} .

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