Ionization and charge exchange in atom collision with multicharged ion

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Single-electron ionization and charge exchange are considered in collisions of an atom with an ion of charge $Z \geqslant 3$ and at velocities $v > Z^{-1/3}$. The approach is based on the Keldysh quasiclassical method. The ionization and charge exchange processes are described within the framework of a single formalism. Effects of rotation and translation are taken into account. The calculated total and partial cross sections agree well with the available experimental data.

1. INTRODUCTION

The single-electron charge-exchange and ionization processes

$$A^{+z}+B \to A^{+(z-1)*}+B^{+}, \tag{1a}$$

$$A^{+z}+B \to A^{+z}+B^{+}+e \tag{1b}$$

play a dominant role in the stripping of atoms in collisions with multicharged ions. At low relative velocities, the most effective is the charge exchange (1a), which leads to predominant population of the ion excited states having cross sections that increase approximately linearly with the ion charge Z and depend little on the velocity at $v \ll Z^{1/2}$. With increasing velocity, the charge exchange cross section decreases rapidly, and the ionization cross section begins to increase sharply. Theoretical models have by now been developed for a sufficiently accurate analysis of charge exchange at $v \ll Z^{1/2}$ (Refs. 1–9; for more details see the review[10]), as well as of both processes (1a) and (1b) in the region $v \gg Z^{1/2}$ where the Born perturbation theory is valid.[10–15]

In the intermediate region $v \sim Z^{1/2}$ the charge-exchange and ionization processes must be considered within the framework of a single collision mechanism. The best for this purpose is the approach formulated by Keldysh[16] and subsequently developed in Refs. 17–22 (see also the monograph[23]) for ionization of an atom in an electromagnetic field. The physical basis of this approach is the determination of the passage of an atomic electron through a time-variable barrier. The first to use a modification of the Keldysh method[24] to determine the quasiclassical argument of the exponential in an estimate of the cross section for stripping a hydrogen atom by a multicharged ion were Duman *et al.*[5] In their approach, however, it is impossible to investigate ionization in the region from the adiabatic threshold of the reaction to the maximum of the cross section.

We propose in this paper for the ion-atom collision problem a natural generalization of the Keldysh method.[16] It permits a study of each of the reactions (1a) and (1b) in the entire parameter range where relativistic effects can be neglected. The processes (1a) and (1b) are distinguished by projecting an approximate solution of the nonstationary Schrödinger equation on the states of the discrete and continuous spectrum in the output channel, and the projection itself is carried out with a limiting transition to classical mechanics.

In accord with the foregoing, we present in Sec. 2 a general formulation of the proposed method. Section 3 contains the analytic results for the quantum part of the problem. Section 4 contains numerical calculations of the cross sections for processes (1a) and (1b), as well as their comparison with the available experimental data and calculations by others.

2. FORMULATION OF APPROACH, DERIVATION OF FUNDAMENTAL EQUATIONS

To describe single-electron charge exchange and ionization we use the nonstationary Schrödinger equation

$$\left[i\frac{\partial}{\partial t}+\frac{1}{2}\Delta_{\mathbf{r}}+\frac{Z}{|\mathbf{R}(t)-\mathbf{r}|}-V(\mathbf{r}) \right] \Psi(\mathbf{r},t)=0, \tag{2}$$

with initial condition

$$\lim_{t \to -\infty} \Psi(\mathbf{r},t)=\psi_{\varkappa l}(r)\,Y_{lm}(\mathbf{r}/r)\,e^{-i\varkappa^2 t/2}=\psi_0(\mathbf{r},t). \tag{3}$$

Here Z is the ion charge, $V(r)$ is the potential of the atomic core, and $\psi_{\varkappa l}$ and Y_{lm} are the radial and angular part of the wave function of the initial bound state of an electron and an atom of energy $\varepsilon = -\varkappa^2/2$. The trajectory of the internuclear motion will be assumed to be a straight line: $\mathbf{R}(t) = \boldsymbol{\rho} + \mathbf{v}t$. The change of variables $\mathbf{r}' = \varkappa\mathbf{r}$, $t' = \varkappa^2 t$, $Z' = \varkappa^{-1}Z$ leads to Eqs. (2) and (3) with $\varkappa = 1$ in the argument of the exponential in (3). We replace the ion potential by the potential of the uniform electric field produced by the ion in the center of the atom, i.e., we use the expansion

$$\frac{Z}{|\mathbf{R}(t)-\mathbf{r}|} \approx \frac{Z}{R(t)}+\mathbf{r}\mathbf{F}(t), \quad \mathbf{F}(t)=-\frac{Z\mathbf{R}(t)}{R^3(t)}, \tag{4}$$

in which the first term in the right-hand side can be omitted, for when substituted in (2) it leads to an insignificant change of the phase of the wave function. The admissibility of the approximation (4) was discussed in a number of papers. For example, in a solution of the charge-exchange problem at low velocities it was shown[5] that the error due to this approximation does not exceed several percent for ions with charge $Z \geqslant 10$. With increasing velocity, the time and the effective length of the trajectory of the below-barrier transition decrease and the role of the region of the configuration space described by the linear approximation (4) increases. Following Keldysh,[16] we seek the amplitudes of transitions to final states with definite values of the momentum $\mathbf{p}$. We use the

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equation of motion of a free electron in the field of the dipole potential (4)

$$i\frac{\partial}{\partial t}\Phi_{\mathbf{p}}(\mathbf{r},t)=-\frac{1}{2}\Delta_{\mathbf{r}}\Phi_{\mathbf{p}}(\mathbf{r},t)-\mathbf{r}\mathbf{F}(t)\Phi_{\mathbf{p}}(\mathbf{r},t), \tag{5}$$

the exact solution of which is

$$\Phi_{\mathbf{p}}=(2\pi)^{-3/2}\exp\left[i\mathbf{k}(t)\mathbf{r}-\frac{i}{2}\int_0^t k^2(t')\,dt'\right] \tag{6}$$

$$\mathbf{k}(t)=\mathbf{p}-\mathbf{A}(t),\quad \mathbf{A}(t)=-\int_0^t \mathbf{F}(t')\,dt'. \tag{7}$$

In the amplitude of the transition

$$a_{\mathbf{p}}(t)=\int_{-\infty}^{t}dt'\int d\mathbf{r}\Phi_{\mathbf{p}}^{*}(\mathbf{r},t)V(\mathbf{r})\Psi_i(\mathbf{r},t), \tag{8}$$

$$a(\mathbf{p})=\lim a_{\mathbf{p}}(t) \tag{8a}$$

the function $\Psi_i(\mathbf{r},t)$ is an exact solution of Eq. (2) with initial condition (3), and $V(r)$ is an atomic potential not taken into account in (5). The error of (8) is determined by the contribution of the higher multipoles that appear in the expansion of the Coulomb potential (4) and should, strictly speaking, be taken into account together with the potential $V(r)$. This contribution, however, is of order of smallness $Z^{-1/2}$ compared with the integral (8). The approximation used by us for the function $\Psi_i(\mathbf{r},t)$ and the method of calculating the integral (8a) are given in Sec. 3. The wave function of the electron detached from the atom can be represented in the form

$$\Psi_f(\mathbf{r},t)=\int d\mathbf{p}a_{\mathbf{p}}(t)\Phi_{\mathbf{p}}(\mathbf{r},t)$$

$$=\int d\mathbf{p}G(\mathbf{p},t)\exp[i\mathbf{k}(t)\mathbf{r}-\Omega_1(\mathbf{p})+i\Omega_2(\mathbf{p},t)]. \tag{9}$$

The wave function (9) is correct near the atom, at $r\ll R\sim Z^{1/2}$, where the expansion (4) is valid. To determine the partial cross sections for the processes (1a) and (1b) we use the quasiclassical character of the electron motion in the finite channel. The small parameter of this approximation is the quantity Z^{-1} obtained from an estimate of the value of the action in a finite channel. It is instructive that electron capture by an ion is to levels with principal quantum number $n\sim Z/2$. We set the wave packet (9) in correspondence with motion of a stream of noninteracting particles, in accord with the statistical interpretation of the limiting transition from the quantum to the classical description. Their source is the region near the atom, where a below-barrier transition takes place [see Eqs. (10)–(13) below], and where expression (9) for the wave function is valid. The further motion of the particles is along classical Coulomb trajectories ion the field of an ion moving with constant velocity $\mathbf{v}$. The flow characteristics such as the coordinate, momentum, and density at the running instant $t_0(\mathbf{p})$ are specified by the integrands of (9) as functions of the quantity $\mathbf{p}$, which serves as a parameter:

$$\mathbf{r}(\mathbf{p})=-\nabla_{\mathbf{p}}\Omega_2(\mathbf{p},t),$$

$$\mathbf{q}(\mathbf{p})=\mathbf{k}(t), \tag{11}$$

$$\nu(\mathbf{p})=|a(\mathbf{p})|^2=|G(\mathbf{p})|^2\exp[-2\Omega_1(\mathbf{p})],\quad G(\mathbf{p})=\lim_{t\to\infty}G_{\mathbf{p}}(t). \tag{12}$$

The quality $t_0(\mathbf{p})$ is determined by the stationary-phase $t_s(\mathbf{p})$ of the integral (8a):

$$k^2(t_s)+1=0,\quad t_0(\mathbf{p})=\mathrm{Re}\,t_s(\mathbf{p}). \tag{13}$$

Such a description corresponds to the matching of the wave function (9) to a nonstationary quasiclassical function of the type $A(\mathbf{r},t)\exp[iS(\mathbf{r},t)]$ with respect to the value of the amplitude A and the momentum ∇S on three-dimensional surface (10), (13) in the space $\{t,\mathbf{r}\}$. The total probability of detaching the electron is determined by the total flux through a closed surface around the atom, enclosing the region of the below-barrier motion, and is equal according to (12) to $\int d\mathbf{p}|a(\mathbf{p})|^2$, which coincides with the amplitude of the wave function (9) at large values of t. To determine the cross sections of interest to us we change over to the following variables: M and M_x are the modulus and projection of the angular momentum on the ion coordinate-system axis directed along the relative-velocity vector $\mathbf{v}$ of the colliding particles. The quantities E, M, and M_x are expressed in elementary fashion through $\mathbf{r}_0$, $\mathbf{q}_0$, and t_0, which depend on $\mathbf{p}$ in accord with (10), (11), and (13). The flux density ν_E in the space (E, M, M_x) is connected with $\nu(\mathbf{p})$ via

$$\nu_E=\left|\frac{\partial(E,M,M_x)}{\partial(p_x,p_y,p_z)}\right|^{-1}\nu(\mathbf{p}). \tag{14}$$

To determine the partial probabilities $W_1=W_{nl}$ and the total ones

$$W_2=\sum_{nl}W_{nl}$$

of the charge exchange, and also the ionization probability W_3, we must subdivide the entire space (E, M, M_x) into regions $\Lambda_1, \Lambda^2=\sum_{nl}\Lambda_1$ and Λ_3 corresponding to the indicated reaction channels, and determine the number of particles that enter the stream in each Λ region. These probabilities are

$$W_\alpha=\int_{\Lambda_\alpha}\nu_E dE dM dM_x=\int_{\Lambda_\alpha'}\nu(\mathbf{p})\,d\mathbf{p},\quad \alpha=1,2,3, \tag{15}$$

where Λ_α' denotes the region of integration after changing the variables in (15). The charge-exchange and ionization processes are then uniquely determined by the conditions $E<0$ (bound states) and $E>0$ (continuous spectrum), in accord with which the values of the Λ regions are specified.

The following conditions must also be satisfied; none of the stream particles lands in a state with incorrect quantum numbers, e.g., $l\geqslant n$; no region $\Lambda_1=\Lambda_{nl}$ lands in an "empty" part of the space (E, M, M_x), e.g., $M_x>M$; the statistical weights corresponding to volumes Λ_1 must be proportional to $(2l+1)$. In accord with these requirements, we assign a particle to the region Λ_1 under the condition

$$n-1<(2Z^2/|E|)^{1/2}<n;\quad n-l-1<(2Z^2/|E|)^{1/2}-M<n-l. \tag{16}$$

The cross sections in the different channels are expressed in the form

$$\sigma_\alpha = \int_0^\infty d\rho \int_{\Lambda_\alpha'} d\mathbf{p} 2\pi\rho v(\mathbf{p}), \quad \alpha = 1, 2, 3. \tag{17}$$

In the approach presented, the solution of the problem can be arbitrarily divided into two parts. The first consists of determining the state of the electron detached from the atom, a state specified by the quantum-mechanical description (8a). The second part is to determine that part of the particle flux with known parameters, which lands in a definite region of configuration space; this part is solved by classical-mechanics methods. Its solution on the basis of Eqs. (10)–(12), (16), (17) can be obtained by simple numerical methods.

3. SOLUTION OF QUANTUM PROBLEM

To clarify the physical meaning of the foregoing calculations and the ensuing regularities, we represent the solution of the initial equation (2) in the form

$$\Psi_i(\mathbf{r}, t) = \psi_{i0}(\mathbf{r}, t) b_0(t) + \Psi_f(\mathbf{r}, t), \quad b_0 = \exp\left[-\int_{-\infty}^{t} \Gamma(\tau) d\tau\right]. \tag{18}$$

Here Ψ_f is determined by Eq. (9), and the function ψ_{i0} pertains to the initial atom state distorted by the external field at arbitrary finite values of t. In the case of slow collisions $v \ll Z^{1/2}$, the explicit form of the functions $\psi_{i0}(\mathbf{r}, t)$ of the atom in the ion field has been thoroughly investigated.[25] In the opposite limiting case $v \gg Z$ (Born perturbation theory), ψ_{i0} coincides with the initial condition (3). It is known[19] that in the calculation of the detachment (8) of an electron from a short-range potential the use of the initial condition (3) for ψ_{i0} is valid at all parameter values, and the presence of the Coulomb field of the neutral-atom core leads to an additional pre-exponential factor in (8); this factor results, strictly speaking, from the distortion of the wave function of the initial state of the atom in the interaction region. The Coulomb factor was first introduced by Keldysh,[16] and a corroboration of this procedure and a calculation for multiphonon ionization of the atom by an electromagnetic field is contained in Refs. 18, 20, and 21. In the present paper the difference between the long-range potential of the atomic core from the short-wave one is taken into account in similar fashion, i.e., via the Coulomb factor.

The evolution of the amplitude $b_0(t)$ of the initial states ψ_{i0} in the interaction of a bound electron with a multicharged ion in accord with the decay given by (18) was corroborated later[8,9] by a consistent quantum approach. We shall impose here any special restrictions on the real quantity $\Gamma(t)$, and calculate it from the condition for the normalization of the wave function (18). This yields

$$\exp\left[-2\int_{-\infty}^{t} \Gamma(t') dt'\right] + \int d\mathbf{p} |a_p(t)|^2 = 1. \tag{19}$$

In the derivation of (19) we neglected the nonorthogonality integrals $\langle \psi_{i0} | \Psi_f \rangle$ whose contribution can be easily verified to be small and to be zero at $t \to \infty$. Another approximation we used was to retain only the first term in the right-hand side of (18) on substitution of Ψ_i in the integral (8). This approximation is not mandatory in this approach, but preservation of the second term of Ψ_f corresponds to the return of the particles from the multicharged ion to the core of the atom. This process has low probability in charge exchange and ionization of atoms by multicharged ions at velocities $v > Z^{-1/2}$, as confirmed by our calculations. The indicated restriction on the relative velocity means smallness of the characteristic time of flight in comparison with the classical time of revolution of the electron in the bound orbit of the ion.

We note that by substituting $b_0(t)\psi_0$ in the right-hand side of (8) and taking into account the equation for the coordinate part of ψ_0

$$[{}^1/_2\Delta_r - V_B(r) - {}^1/_2]\psi_{\varkappa lm}(\mathbf{r}) = 0, \tag{20}$$

we obtain the relation

$$a_p(t) = -\int_{-\infty}^{t} dt' \cdot \frac{1}{2}[k^2(t') + 1]\chi(\mathbf{k}) \times \exp\left[\frac{i}{2}t' + \frac{i}{2}\int_0^{t'} k^2(\tau) d\tau - \int_{-\infty}^{t'} \Gamma(\tau) d\tau\right], \tag{21}$$

$$\chi(\mathbf{k}) = (2\pi)^{-3/2} \int \exp[-i\mathbf{k}(t)\mathbf{r}]\psi_{\varkappa lm}(\mathbf{r}) d\mathbf{r}, \tag{21a}$$

which connects, alongside with (19), the quantities $a_p(t)$ and $\Gamma(t)$. The integral (21) is determined mainly in the vicinity of the stationary-phase point (13). By taking outside the integral sign at this point the exponential that contains $\Gamma(t)$ we obtain

$$a_p(t) = \exp\left[-\int_{-\infty}^{t_0(\mathbf{p})} \Gamma(\tau) d\tau\right] h_p(t), \tag{22}$$

$$|h_p(t)| = \left| \int_{-\infty}^{t} dt' \cdot \frac{1}{2}[k^2(t') + 1] \times \exp\left[\frac{i}{2}t' + \frac{i}{2}\int_0^{t'} k^2(\tau) d\tau\right] \chi(\mathbf{k}) \right| \approx \theta[t - t_0(\mathbf{p})] |h(\mathbf{p})|, \tag{23}$$

$$h(\mathbf{p}) = \lim_{t \to \infty} h_p(t),$$

$$\theta(x) = 1, \quad x > 0; \quad \theta(x) = 0, \quad x < 0, \tag{24}$$

and by using (24) we obtain the sought connection of the rate of decay of the initial atomic state per unit time with the quantity $h(p)$:

$$\Gamma(t) = \frac{1}{2} \int d\mathbf{p} |h(\mathbf{p})|^2 \delta[t - t_0(\mathbf{p})], \tag{25}$$

which yields, taking (22)–(24) into account,

$$a(\mathbf{p}) = \lim_{t \to \infty} a_p(t) = h(\mathbf{p}) \exp\left[-\frac{1}{2}\int_A d\mathbf{p}' |h(\mathbf{p}')|^2\right], \tag{26}$$

$$\int d\mathbf{p} |a(\mathbf{p})|^2 = 1 - \exp\left[-\int d\mathbf{p} |h(\mathbf{p})|^2\right]. \tag{27}$$

$$A = \{t_0(\mathbf{p}') < t_0(\mathbf{p})\}$$

Equations (25)–(27) demonstrate the unitarity of the partial and total probabilities of detaching an electron from an atom

and reduce the solution of the charge-exchange and ionization problem to a calculation of the quantity $h(\mathbf{p})$ which, according to (23) and (24), is equal to

$$h(\mathbf{p})=\int_{-\infty}^{\infty}dt\cdot\frac{1}{2}[k^2(t)+1]\chi(\mathbf{k})\exp\left\{\frac{i}{2}\int_0^t[k^2(\tau)+1]d\tau\right\}, \tag{28}$$

and has the physical meaning of the probability amplitude of detaching an electron on a nonstationary field of an ion from an atomic state that is "nondecaying" in the course of the collision. The rate $\Gamma(t)$ of decay of this state is also expressed in terms of $h(\mathbf{p})$ via (25).

It is interesting to note that after integrating by parts Eq. (28) is transformed into an expression that contains the external-field potential $\mathbf{r}\cdot\mathbf{F}(t)$ as a perturbation

$$h(\mathbf{p})=\int_{-\infty}^{\infty}dt\,\langle\Phi_{\mathbf{p}}(r,t)\,|\mathbf{r}\mathbf{F}(t)\,|\psi_0(\mathbf{r},t)\rangle$$

$$=\int_{-\infty}^{\infty}dt\,\lambda(\mathbf{k},t)\exp\left\{\frac{i}{2}\int_0^t[k^2(\tau)+1]d\tau\right\}, \tag{29}$$

$$\lambda(\mathbf{k},t)=(2\pi)^{-3/2}\int d\mathbf{r}\,\psi_{\varkappa lm}(\mathbf{r})\mathbf{r}\mathbf{F}(t)\exp[-i\mathbf{k}(t)\mathbf{r}],$$

where the functions ψ_0, Φ_p, and $\nu_{\varkappa lm}$ are defined respectively through (3), (6), and (20). In Keldysh's paper[16] an integral similar to (28) was written directly in the form (29), but Eq. (28) is more convenient for practical calculations. The fact that (28) and (29) are identical at an arbitrary potential V_B in (20) eliminates, in our approach, one of the basic difficulties in the description of asymmetric charge exchange at medium and high velocities, a difficulty connected with the prior- and post-representations for the electron-capture matrix elements. From (29) follows directly the first order of perturbation theory for the problem of atom ionization at $v\gg Z^{1/2}$, $\mathbf{k}(t)\to\mathbf{p}$. In the quasistationary limiting case, $v\ll Z^{1/2}$, expressions (28) and (29) also lead to asymptotically exact results.

It was already noted above that in this approach, just as in multiphoton ionization problems, it is advantageous to perform all the calculations with the wave function of an electron bound by a short-range potential, and to take into account the effects of the long-range action of the atomic core by using the Coulomb factor. In the particular case of a δ-function potential, the function ψ_{0i} is equal to

$$\psi_{0i}(\mathbf{r},\,t)=(2\pi)^{-3/2}r^{-1}e^{-r-it^3/2}, \tag{30}$$

and the integral (28) can be calculated exactly

$$h(\mathbf{p})=\frac{i}{\omega\pi}\frac{\exp[c(\pi/2+i)]}{(\eta^2-\mu^2)^{1/2}}\left\{\mu K_{1+ic}[(\eta^2-\mu^2)^{1/2}]\right. \tag{31}$$
$$\left.+\left(\frac{\eta-\mu}{\eta+\mu}\right)^{1/2}icK_{ic}[(\eta^2-\mu^2)^{1/2}]\right\};$$

$$c=\frac{1}{\omega\gamma}\left(p_x+\frac{1}{\gamma}\right),\quad \eta=\frac{1}{2\omega}\left(p^2+\frac{2p_x}{\gamma}+\frac{1}{\gamma^2}+1\right),\quad \mu=\frac{p_y}{\omega\gamma}, \tag{31a}$$

$$\omega=v/\rho,\quad \gamma=v\rho/Z, \tag{32}$$

where K is a Macdonald function.

In the quasistationary limiting case, $v\ll Z^{1/2}$, Eqs. (31) and (25) yield

$$\Gamma(t)=\frac{Z}{4R^2}\exp\left(-\frac{2}{3}\frac{R^2}{Z}\right),\quad R=(\rho^2+v^2t^2)^{1/2}. \tag{33}$$

In the perturbation theory limit, $v\gg Z^{1/2}$, $c\to 0$, $\mu/\eta\to 0$, expression (31) obviously coincides with the known result of the dipole approximation.

Of greatest interest is the intermediate region, in which it is advantageous to calculate the integral (28) with a more general wave function having a coordinate-part asymptotic form

$$\psi_{\varkappa lm}(\mathbf{r})\sim C_{\varkappa l}r^{-1}e^{-r}Y_{lm}(\mathbf{r}/r),\quad r\gg 1. \tag{34}$$

The coefficient $C_{\varkappa l}$ depends on the concrete form of the binding potential. The stationary-phase point $t_s(\mathbf{p})$ in the integral (28) is determined from Eq. (13), which is reducible to a quadratic one:

$$\left(\sum_{n=1}^{3}p_n^2+1\right)(\xi_s^2+1)^{1/2}+2p_2\xi_s-2p_3=0,\quad \xi_s=\omega t_s, \tag{35}$$
$$p_1=\gamma^2(p_z^2+1),\quad p_2=\gamma p_y,\quad p_3=\gamma p_x+1.$$

At the stationary point $k_s^2=-1$ the pre-exponential expression is regular and is equal to

$$\lim_{t\to t_s}{}^1/_2[k^2(t)+1]\chi(\mathbf{k})=i(2\pi)^{-1/2}C_{\varkappa l}Y_{lm}(-i\mathbf{k}_s). \tag{36}$$

It can be seen from (36) that to determine the behavior of the preexponential function in the vicinity of the stationary point t_s it suffices to know only the asymptotic form of the wave function (34). Recognizing that

$$\frac{d}{dt}[k^2(t)+1]\,|_{t=t_s}=2\mathbf{k}(t_s)\mathbf{F}(t_s)=2\mathbf{k}_s\mathbf{F}_s, \tag{37}$$

we obtain for the integral (28)

$$h(\mathbf{p})=G(\mathbf{p})\exp[iS(\mathbf{p})],\quad S(\mathbf{p})=\frac{1}{2}\int_0^{t_s(\mathbf{p})}[k^2(t)+1]dt, \tag{38}$$
$$G(\mathbf{p})=C_{\varkappa l}(1/i\mathbf{k}_s\mathbf{F}_s)^{1/2}Y_{lm}(-i\mathbf{k}_s).$$

As can be seen from (38) that the function $h(\mathbf{p})$ has at $\mathbf{p}=\mathbf{p}_0$ a sharp maximum which can be determined from the equation

$$\nabla_{\mathbf{p}}\,\mathrm{Im}\,S(\mathbf{p})\,|_{\mathbf{p}=\mathbf{p}_0}=\mathrm{Im}\int_0^{t_s(\mathbf{p}_0)}\mathbf{k}(t)\,dt=0, \tag{39}$$

so that the slowly varying pre-exponential factor $G(\mathbf{p})$ in (38) can be set equal to the constant $G(\mathbf{p}_0)$. To determine the Coulomb factor we use the results of calculations performed in Ref. 18 for a harmonic field. The main contribution to the transition probability is made by the point $\mathbf{p}_0$. It follows from (25) and (38) that $t_0(\mathbf{p}_0)=0$, i.e., the time closest to $t=0$, where the distance between nuclei is a minimum, determines the probability of detaching the atomic electron. The ion field (4) is in this vicinity, accurate to 0 (v^2t^2), a circularly

polarized field of frequency ω. In the case (4) one can therefore use the Coulomb factor obtained in Refs. 16 and 18 for a circularly polarized field whose parameter $\tilde{\gamma}$ we shall determine from the condition that $t_{so} = t_s(\mathbf{p}_0)$ be equal to the analogous quantity $\tilde{t}_{s0}$ for a harmonic field; this yields

$$\tilde{\gamma}=2\vartheta^{-1}\operatorname{sh}\vartheta\operatorname{ch}\vartheta-\vartheta^{-2}\operatorname{sh}^2\vartheta-1,$$
$$\vartheta=\vartheta(\gamma)=t_{s0}/i\omega^{-1}, \quad \operatorname{Re} t_{s9}=0. \tag{40}$$

In the quasistationary limiting case $\gamma \ll 1$ the quantities γ and $\tilde{\gamma}$ are equal to within $o(\gamma^2)$. We thus obtain for the Coulomb factor

$$f_k=[2\tilde{\gamma}/\omega(1+\tilde{\gamma}^2)^{1/2}]^{\lambda}, \quad \lambda=1/\varkappa. \tag{41}$$

The quantity λ has the meaning of an effective principal quantum number (λ coincides with the principal quantum number of $V_B = r^{-1}$) and is contained in the asymptotic form of the wave function of the atom

$$\psi_{\varkappa lm}\sim C_{\varkappa l}r^{-\lambda-1}e^{-r}Y_{lm}(\mathbf{r}/r), \quad r\gg 1. \tag{42}$$

Calculations have shown that a change of f_k^2 by a factor of 2 compared with (41) changes the cross sections by about 10%, so that the requirements on the accuracy of (41) are not stringent in the present paper.

Equation (38) takes the form

$$h(\mathbf{p})=G_{\lambda}\exp[iS(\mathbf{p})],$$
$$G_{\lambda}=C_{\varkappa l}[2\tilde{\gamma}/\omega(1+\tilde{\gamma}^2)^{1/2}]^{\lambda}(1/i\mathbf{k}_{s0}\mathbf{F}_{s0})^{l/2}Y_{lm}(-i\mathbf{k}_{s0}), \tag{43}$$
$$\mathbf{k}_{s0}=\mathbf{k}_s, \quad \mathbf{F}_{s0}=\mathbf{F}_s \quad \text{at} \quad \mathbf{p}=\mathbf{p}_0.$$

Equation (43) at $\lambda = 0$ corresponds to (38) when (42) coincides with (34) and the Coulomb factor is $f_k = 1$.

For the electron coordinate and for the flux density ν, which are defined by (10) and (12), we obtain from (43)

$$\mathbf{r}(\mathbf{p})=\operatorname{Re}\int_{t_s(\mathbf{p})}^{t_0(\mathbf{p})}\mathbf{k}(t')\,dt', \tag{44a}$$

$$\nu(\mathbf{p})=|G_{\lambda}|^2\exp\left[-2\operatorname{Im}S(\mathbf{p})-2\int_{-\infty}^{t_0(\mathbf{p})}\Gamma(\tau)\,d\tau\right], \tag{44b}$$

where $\Gamma(t)$ is determined from (25).

We now factor out the dependences on the components of the momentum $\mathbf{p}$ in (44b). We use here the fact that the function $h(\mathbf{p})$ is not small only in a narrow vicinity of the momentum $\mathbf{p}_0$, where Im S can be expanded in a Taylor series up to second order. We recognize that

$$\frac{\partial^2 S(\mathbf{p})}{\partial p_x\,\partial p_z}=0, \quad \frac{\partial t_0(\mathbf{p})}{\partial p_x}=\frac{\partial t_0(\mathbf{p})}{\partial p_z}=0 \quad \text{at} \quad \mathbf{p}=\mathbf{p}_0. \tag{45}$$

We introduce the notation

$$\xi_i=\frac{\partial^2 \operatorname{Im}S(\mathbf{p})}{\partial p_i^2} \quad \text{at} \quad \mathbf{p}=\mathbf{p}_0, \quad i=\{x,y,z\}. \tag{46}$$

The p_y-dependent value of p_x at which

$$\frac{\partial \operatorname{Im}S(\mathbf{p})}{\partial p_x}=\frac{\partial \operatorname{Im}S(\mathbf{p})}{\partial p_z}=0, \tag{47}$$

will be designated $p_x(p_y)$. The condition (47) is satisfied by $p_z = 0$. The quantities analogous to (46) and defined at the point $\mathbf{p} = \{p_x(p_y), p_y, p_z = 0\}$, will be designated $\xi_x(p_y)$ and $\xi_z(p_y)$. Accurate to the quadratic terms $o(|\mathbf{p}-\mathbf{p}_0|^2)$ we have

$$\nu(\mathbf{p})=W_{\rho}w_y(p_y)\,w_x(p_y,\,p_x)\,w_z(p_y,\,p_z), \tag{48}$$

$$W_{\rho}=1-e^{-\Delta}, \quad \Delta=\pi^{3/2}|G_{\lambda}|^2(\xi_x\xi_y\xi_z)^{1/2}e^{-2\operatorname{Im}S_0}, \quad S_0=S(\mathbf{p}_0), \tag{49}$$

$$w_y=\frac{\Delta}{\pi^{1/2}}\exp\left\{-\xi_y p_y^2-\frac{\Delta}{2}[1+\operatorname{erf}(-\xi_y^{1/2}p_y)]\right\}, \tag{50}$$

$$w_x=\left[\frac{\pi}{\xi_x(p_y)}\right]^{1/2}\exp\{-\xi_x(p_y)[p_x(p_y)-p_x]^2\}, \tag{51}$$

$$w_z=\left[\frac{\pi}{\xi_z(p_y)}\right]^{1/2}\exp[-\xi_z(p_y)p_z^2], \tag{52}$$

$$\operatorname{erf}(x)=2\pi^{-1/2}\int_0^x e^{-y^2}\,dy.$$

The functions $w_{x,y,z}$ in (48) are normalized to unity. To calculate (17) with the aid of (48)–(52) we used the so-called statistical trials (Monte Carlo) method. A value ρ is chosen from the interval $(0,\infty)$ with probability proportional to a quantity ρw_{ρ} specified through (49). The probability distributions (50), (51), and (52) are used next to select p_y, p_x, and p_z. The obtained values of ρ and $\mathbf{p}$ specify uniquely the quantities E and M. In the case of realization of the charge exchange ($E < 0$), Eqs. (16) are used to determine the values of n and l. As a result of N_T repetitions ($N_T \sim 10^4$) there are calculated N_{α} ($\alpha = 1, 2, 4$) realizations of each partial channel of the reaction. The cross sections are defined as

$$\sigma_{\alpha}=\sigma_T N_{\alpha}/N_T, \tag{53}$$

$$\sigma_T=\int_0^{\infty}2\pi\rho W_{\rho}\,d\rho. \tag{54}$$

The total cross section σ_T is calculated as a single integral in accord with (49) and (54).

4. ANALYSIS OF RESULTS, COMPARISON WITH EXPERIMENT

The calculated ionization and charge-exchange cross sections and their sums, for the collision of a hydrogen atom H with a completely stripped ion, are shown in Figs. 1–4. A detailed comparison with the available experimental data 26–29 and with other theories[2,5,30–32] is given in Figs. 1, 2, and 3.

The calculated values of the cross sections are in good agreement with experiment in the entire range of energy variation. It can be seen from the measurement results plotted in Figs. 1–3 that the presence of an electron core in the atom influence the cross section only insignificantly. The reason is that in the considered velocity region the main contribution is made by large impact parameters $\rho \sim Z^{1/2}$, where the atom "feels" only the Coulomb field of the ion. At the same time, as shown by our calculations, introduction of an effective charge[32] makes the agreement between theory and

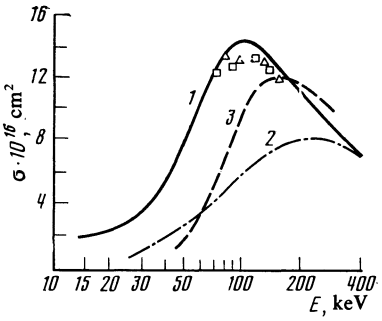

FIG. 1. Cross section of the ionization reaction $H + X^{5+} \rightarrow H^+ + X^{5+} + e$ incident-ion energy divided by the atomic weight. Curve 1—calculation, Eqs. (17); 2—Glauber approximation 31; 3—MCT[32]. Points—experiment (Refs. 27, 28, 29), △ – N^{5+}, □ – O^{5+}.

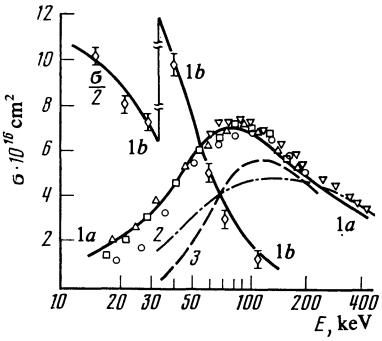

FIG. 3. Cross sections of the reactions $H + X^{3+} \rightarrow H^+ + X^{3+} + e$ (curve 1*a*), and $H + X^{3+} \rightarrow H^+ + X^{3+} + e$ (curve 1*b*). The notation is that of Fig. 1; ◇, ○ – C^{3+}, □ – O^{3+}, △ – N^{3+}, ▽ – Li^{3+}.

experiment only worse. In the velocity region $v \sim Z$ the charge-exchange cross section is negligibly small compared with the ionization cross section, and the results of various calculations based on the Born approximation agree well with the measurement results.

To describe the experimental data on ionization at large velocities, it is expedient to use approximation formulas. Using the dipole approximation for transitions into the continuous spectrum of the atom[12]

$$\sigma = 8\pi (Z\lambda_i/v)^2 \ln (v^2\zeta/\omega_i\lambda_i Z); \quad Z^{1/2} < v < Z, \quad \omega_i = \varkappa^2/2, \tag{55}$$

and the high-energy Born aproximation[33,12-14]

$$\sigma = 4\pi (Z^2/v^2)(\lambda_i^2 \ln v^2 + c_i); \quad v > Z, \tag{56}$$

we obtain the approximation formula

$$\sigma = 8\pi (Z\lambda_i/v)^2 \ln [v^2/(c_1 Z + c_2 v)]; \quad v > Z^{1/2}, \tag{57}$$
$$c_1 = \omega_i\lambda_i/\zeta, \quad c_2 = \exp(-c_i/2\lambda_i^2).$$

The constants λ_i and c_i are expressed in terms of the target-atom wave functions,[14] and for the collisions of an ion with a hydrogen atom we have $\lambda_i^2 = 0.283$. $c_i = 1.26$. A comparison with experiment yields for the constant in (55) a value 1.32 (values 0.322 and 1.42 are cited in Refs. 5 and 12). At velocities $v > Z$, when the approximation (55) is not applicable and account must be taken of the regions $R < r$ (Refs. 33 and 34), Eq. (57) goes over into the correct Born approximation (56). For lower velocities we obtain from (57) expression (55), which is based on the approximation (4), which is valid for these velocities.

Since the method of classical trajectories (MCT) is widely used to calculate the cross sections of various processes, it is important to determine the limits of applicability of the MCT so as to indicate possible sources of its errors. Analysis of the presented experimental and theoretical data shows that the MCT underestimates the results systematically. The reason is that the electron density distribution in a single-electron atom, calculated by classical mechanics,[35] is cut off at a distance $r \sim 1$ from the nucleus, whereas the quantum-mechanical distribution is attenuated at much larger distances. More importantly, the MCT does not take into account the tunnel-transition effect, which makes the main contribution to the probability of the ionization and charge exchange at low velocities.

The results of the calculations of the cross sections for charge exchange (1a), ionization (1b) and their sum (1a) + (1b), for charges $Z = 4$–26 are shown in Fig. 4. The

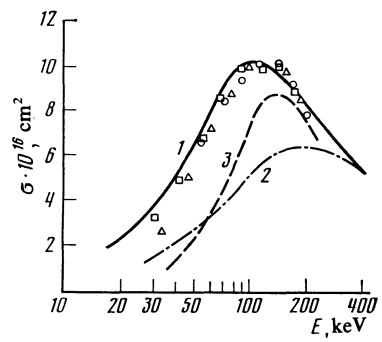

FIG. 2. Cross section of the reaction $H + X^{4+} \rightarrow H^+ + X^{4+} + e$. The notation is given in the caption of Fig. 1; ○ – C^{4+}, □ – O^{4+}, △ – N^{4+}.

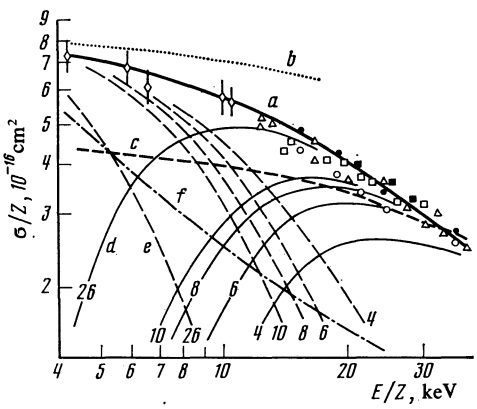

FIG. 4. Ionization and charge-exchange cross sections and the total cross section for stripping of a hydrogen atom colliding with an ion XZ^+. The energy of the incident ion is referred to one atomic mass unit, and the parametrization of the coordinates corresponds to Eq. (59). Stripping cross section: *a*—Eqs. (48), (59); *b*—decay model 2; *c*—MCT approximation[30]; *f*—quasiclassical exponential approximation 5; ● – He^{2+}, ■ – Li^{2+}, △ – C^{q+} ($q = 2, 3, 4$), □ – Ne^{q+} ($q = 2 - 5$), ○ – O^{q+} ($q = 2 - 5$), experiment.[26,27,28] Sets of curves *e* and *d*—calculation of the ionization and charge exchange cross sections for $Z = 4$, 6, 8, 10 and 26 (the charge is marked on the curves). The points ◇ were obtained from the charge-exchange cross section[29] and from the calculated ionization cross sections for C^{3+} and C^{4+}.

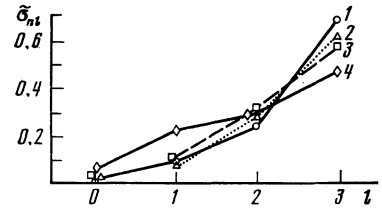

FIG. 5. Partial cross sections $\tilde{\sigma}_{nl}=\sigma_{nl}/(\Sigma_l \sigma_{nl})$ of the reaction $H+C^{6+}\to H^{+}+C^{5+}(nl)$ for a velocity $v=1$ a.u. and $n=4$. Points: 1—calculation (17), 2—MCT[38]; 3—tight-binding method for 33 states[37]; 4—rotational "shakeup" approximation,[7] Eq. (61).

cross section σ_m for ionization at the maximum and the corresponding value E_m are well approximated by the power-law dependence

$$\sigma_m \approx 1.6Z^{1,3}\ (\text{cm}^2\cdot 10^{-16}),$$
$$E_m \approx 39Z^{0.65}\ (\text{keV/a·m·u}). \tag{58}$$

The charge exchange cross section can be approximately represented in the parametrized form $\sigma_{ex}\sim ZQ_{ex}(EZ^{-1/2})$, which agrees with the known theoretical and experimental data.[10] The results shown in Fig. 4 demonstrate the degree of accuracy of the different theoretical methods, compared with experiment, for the total cross section of single-electron stripping. The difference between curves *a* and *b* shows the influence of the fact that the barrier is not stationary.

The choice of the parametrized coordinates in Fig. 4 is connected with a question of very great importance for a large number of applications,[28] viz., the scaling law for the total cross section for atom stripping. A consequence of the approximation (4) is that the probability [of the form (27)] of the process (1a) + (1b) depends only on two parameters ω and γ, which are determined in (32). The cross section is parametrized then in the form

$$\sigma=\int_0^\infty 2\pi\rho\, d\rho\, W_\rho = 2\pi\int_0^\infty \left(\frac{Z\gamma}{\omega}\right)^{1/2} W(\omega,\gamma)\, d\left(\frac{Z\gamma}{\omega}\right)^{1/2} = ZQ\left(\frac{E}{Z}\right). \tag{59}$$

The energy E here is per unit atomic mass, and Q is a universal function. This parametrization law was obtained empirically in Ref. 30 and was later confirmed in experiment.[26–28]

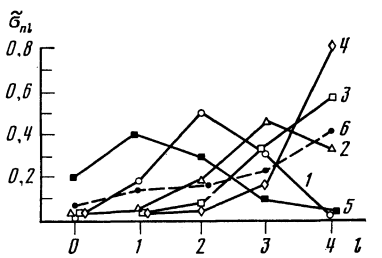

FIG. 6. Dependence of the partial cross sections $\tilde{\sigma}_{nl}=\sigma_{nl}/(\Sigma_l \sigma_{nl})$ of the reaction $H+O^{8+}\to H^{+}+O^{7+}(nl)$ on the collision velocity for $n=5$. The set of points 1, 2, 3, and 4 corresponds to $x=0.5, 0.75, 1.0$ and 1.5 a.u. Curve 5—limiting case of $v\ll 1$ a.u., Eq. (60). 6—"rotational-shake-up" approximation,[7] Eq. (61).

We emphasize that the form (59) is the consequence of the approximation (4) alone. The high-velocity limit of (59), as follows from (57), can be estimated at $v\sim c_1 Z/c_2\sim 2Z$. This agrees qualitatively with the experimental results.[28] At low velocities the limit of the validity of (59) is connected with the applicability of the decay approximation and, as shown in Ref. 8, is of the order of $Z^{-1/2}$ for systems having Coulomb symmetry. In the case when this symmetry is broken, the decay model describes also the lower-velocity region $v<Z^{-1/2}$. We note that the processes (1a) and (1b), in contrast to their sum, do not conform to the scaling law (59).

The partial cross section σ_{nl} are no less of interest for the solution of applied problems than the total cross sections.[36] The cross-section distributions in the principal quantum numbers n, obtained within the frameworks of various approaches, are in satisfactory agreement with one another[10,8] and are determined at low velocities, $v<1$ a.u., by the splittings of the molecular terms of the ion + atom system at their quasicrossing points. On the contrary, the cross-section distributions in the orbital quantum numbers vary greatly, depending on the models assumed. For example, at low velocities in the rotating-axis approximation, the distribution is given by squares of Clebsch-Gordan coefficients for the expansion of the parabolic state $n_1=0$, $n_2=n-1$, $m=0$ in spherical functions

$$\sigma_{nl}=\sigma_n(2l+1)\frac{[(n-1)!]^2}{(n+l)!\,(n-l-1)!}. \tag{60}$$

The distribution (60) has a maximum at small $l\sim(n/2)^{1/2}$. Allowance for the interaction of the degenerate states in the final channel of the reaction yields in the "shakeup" approximation[6]

$$\sigma_{nl}=\sigma_n\sum_{\substack{i_1\neq j\\ i_2\neq j}} |C^{lm}_{ji_1,ji_2}|^2 \binom{2j}{j-i_1}\binom{2j}{j-i_2}(2^{4j}-1)^{-1}; \qquad j=(n-1)/2,\quad Z^{-1/4}<v<1. \tag{61}$$

The maximum of (61) takes place at $l=n-1$. A numerical calculation 37 at a velocity $v=10^7$ cm/sec yielded a nonmonotonic dependence of nl on l. The results of our calculations of the partial cross sections for velocities $v>Z^{-1/2}$ are shown in Figs. 5 and 6.

Comparison with other theories shows that all the approaches yield at $v>1$ a.u. a maximum of the distribution at $l=n-1$ and fall off differently with decreasing l (Fig. 5).

[1] A. A. Radtsig and B. M. Smirnov, Zh. Eksp. Teor. Fiz. **60**, 521 (1970) [Sov. Phys. JETP **33**, 282 (1970)].
[2] M. I. Chibisov, Pis'ma Zh. Eksp. Teor. Fiz. **24**, 56 (1976) [JETP Lett. **24**, 46 (1976)].
[3] A. Salop and R. E. Olson, Phys. Rev. **A14**, 579 (1976).
[4] E. L. Duman and B. M. Smirnov, Fiz. Plazmy **5**, 1161 (1978) [*sic*].
[5] E. L. Duman, L. I. Men'shikov, and B. M. Smirnov, Zh. Eksp. Teor. Fiz. **76**, 516 (1979) [Sov. Phys. JETP **49**, 260 (1979)].

[6]V. A. Abramov, F. F. Baryshnikov, and V. S. Lisitsa, *ibid.* **74**, 897 (1978) [**47**, 469 (1978)].
[7]V. A. Abramov, F. F. Baryshnikov, and V. S. Lisitsa, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 494 (1978) [JETP Lett. **27**, 464 (1978)].
[8]L. P. Presnyakov, D. B. Uskov, and R. K. Yanev, Zh. Eksp. Teor. Fiz. **83**, 933 (1982) [Sov. Phys. JETP **56**, 525 (1982)].
[9]L. P. Presnyakov, D. B. Uskov, and R. K. Janev, Phys. Lett. **84A**, 243 (1981).
[10]R. K. Nayev and L. P. Presnyakov, Phys. Reports **70**, 1 (1980).
[11]L. P. Presnyakov, Trudy FIAN **119**, 52 (1980).
[12]R. K. Yanev and L. P. Resnyakov, J. Phys. **B13**, 4233 (1980).
[13]M. Inokuti, Rev. Mod. Phys. **43**, 397 (1971).
[14]G. H. Gillepsie, Phys. Lett. **72A**, 329 (1979).
[15]G. H. Gillepsie, J. Phys. **B5**, 729 (1982).
[16]L. V. Keldysh, Zh. Eksp. Teor. Fiz. **47**, 1945 (1964) [Sov. Phys. JETP **20**, 1307 (1965)].
[17]A. I. Nikishov and V. I. Ritus, *ibid.* **50**, 255 (1966) [**23**, 168 (1966)].
[18]A. I. Nikishov and V. I. Ritus, *ibid.* **52**, 223 (1967) [**25**, 145 (1968)].
[19]A. M. Presnyakov, V. S. Popov, and M. V. Terent'ev, *ibid.* **50**, 1393 (1966) [**23**, 924 (1966)].
[20]A. M. Perelomov, V. S. Popov, and M. V. Terent'ev, *ibid.* **51**, 309 (1966) [**24**, 207 (1967)].
[21]A. M. Perelomov and V. S. Popov, *ibid.* **52**, 514 (1967) [**25**, 336 (1967)].
[22]V. S. Popov, V. P. Kuznetsov, and A. M. Perelomov, *ibid.* **53**, 331 (1965) [**26**, 222 (1968)].
[23]L. P. Rapoport, B. A. Zon, and N. L. Manakov, Theory of Multiphoton Processes in Atoms [in Russian], Atomizdat, 1978, Chap. 5.
[24]L. D. Landau and E. M. Lifshitz. Quantum Mechanics, Nauka, 1974, pp. 344, 345 [Engl. Transl. Pergamon, 1977].
[25]V. M. Galitskiĭ, E. E. Nikitin, and B. M. Smirnov, Teoriya stolknoveniĭ atomnykh chastits [Theory of Collision of Atomic Particles), Nauka, 1981, §1.2.
[26]M. B. Shah and H. B. Gilbody, J. Phys. **B14**, 2631 (1981).
[27]M. B. Shah and H. B. Gilbody, *ibid.* p. 2831.
[28]M. B. Shah and H. B. Gilbody, *ibid.* **15**, 413 (1982).
[29]T. V. Goffe, M. B. Shah, and H. B. Gilbody, J. Phys. **B12**, 3763 (1979).
[30]K. H. Berkner, W. G. Grahm, R. V. Pyle, A. S. Schlachter, J. W. Stearns, and R. E. Olson, Phys. Rev. Lett. **41**, 163 (1978).
[31]J. H. McGuire, Phys. Rev. **A26**, 143 (1982).
[32]R. E. Olson and A. Salop, *ibid.* **A16**, 521 (1977).
[33]L. A. Vainshtein and A. V. Vinogradov, J. Phys. **B3**, 1090 (1970).
[34]V. P. Shevelko, A. M. Urnov, and A. V. Vinogradov, J. Phys. **B9**, 1 (1976).
[35]R. Arbines and I. C. Percival, Proc. Phys. Soc. London **88**, 861 (1966).
[36]V. S. Lisitsa and V. I. Kogan, Itogi nauki i tekhniki, ser. Fiz. Plazmy **3**, 5 (1982).
[37]T. A. Green, E. L. Shipsey, and J. C. Browne, Phys. Rev. **A25**, 1364 (1983).
[38]A. Salop, J. Phys. **B12**, 919 (1979).

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