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"Destruction" of hydrogen atom by collisions with multiply charged ions

E. L. Duman, L. I. Men'shikov, and B. M. Smirnov

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A calculation is reported of the total cross section of "destruction" of a hydrogen atom by collision with a multiply charged ion ($Z \geqslant 1$). The partial cross sections representing charge exchange between a hydrogen atom and a multiply charged ion are calculated using perturbation theory for collision velocities low compared with $e^2/\hbar$ (e is the electron charge and $\hbar$ is the Planck constant). The total charge-exchange cross section is compared with the results of a model in which the number of final states of a multiply charged ion is regarded as infinite. The criterion of validity of this model is determined. The coordinate and time dependences of the argument of the exponential electron wave function are determined for collision velocities low compared with $Z^{1/2}e^2/\hbar$ (Z is the ion charge) using the quasiclassical Keldysh method. The ionization cross section of a hydrogen atom colliding with a multiply charged ion is calculated for collision velocities high compared with $Z^{1/2}e^2/\hbar$. Matching of these cross sections makes it possible to determine the total destruction cross section of a hydrogen atom colliding with a multiply charged ion, which is valid in a wide range of collision velocities.

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The parameters of a thermonuclear (fusion) plasma and the rates of heating and decay of such a plasma are affected considerably by impurities.[1,2] In a fusion plasma the impurities are present in the form of multiply charged ions so that their influence on the plasma properties if manifested in various processes involving such ions. In particular, when a beam of fast hydrogen atoms is injected into a plasma, the processes of "destruction" of hydrogen atoms by collisions with multiply charged ions are important. The present paper is concerned with a calculation of the cross sections of such processes.

The cross sections of inelastic processes in collisions of multiply charged ions with atoms or singly charged ions have been determined in many recent experiments[3-8] and found in many calculations.[9-19] A characteristic of these processes is associated with a large number of possible reaction channels because there are many electron states in the field of a multiply charged ion to which the electron can be transferred. The existing theoretical approaches to the calculation of cross sections of such processes are based on the two-level approximation or on perturbation theory and are designed to determine the partial cross sections of the investigated processes. They require detailed information on the spectrum of multiply charged ions, which can be obtained only after laborious calculations, and the results apply to specific partners and parameters of collisions. Such calculations cannot always be applied to other collision parameters and other partners.

Our aim is to find the total cross section for the process of an inelastic collision between a hydrogen atom and a multiply charged ion. The loss of information on the details of the process makes it possible to combine all the channels that "destroy" the hydrogen atom.

We shall use asymptotic and quasiclassical methods. We shall divide the range of collision velocities arbitrarily into three regions. In the first region the relative collision velocity is small compared with the character-

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istic velocity of an electron in a hydrogen atom, so that the motion of the nuclei does not affect the nature of the transition. In this range the charge-exchange process is regarded as the transfer of an electron in the field of a multiply charged ion, which has many states. This approach[20] has been used earlier.[18,19] We shall concentrate our attention on this approach. It is important to note that an electron is transferred when the distance between the nuclei between the two collision partners is large compared with the size of the hydrogen atom. This makes it possible to consider high collision velocities using an elegant quasiclassical method developed by Keldysh[21,22] to deal with the ionization of a hydrogen atom in an alternating electric field. The essence of the method is to find the argument of the exponential function in the "tail" of an electron wave function. In the range of distances from an electron to the atomic core we can use classical approaches which make it possible to determine also the time dependence of the electron wave function. Since in our case the charge-exchange process involves the transfer of an electron from the wave-function tail, the quasiclassical Keldysh approach is very effective.

As long as the velocity in a collision between a hydrogen atom and a multiply charged ion is low compared with the characteristic electron velocity in the ion field, the "destruction" of the hydrogen atom is due to charge exchange. At higher collision velocities the ionization cross section is much larger than the charge-exchange cross section and, therefore, at high velocities our problem reduces to finding the ionization cross section of the hydrogen atom under the influence of the field of the multiply charged ion.

The final result is obtained by matching the cross sections for different collision velocities, which gives the cross section for the "destruction" of a hydrogen atom colliding with a multiply charged ion in a wide velocity range $1 < v \lesssim Z$, where Z is the charge of the incident ion.[1)]

CHARGE EXCHANGE BETWEEN A HYDROGEN ATOM AND A MULTIPLY CHARGED ION AT LOW COLLISION VELOCITIES $v \ll 1$

We shall consider the process of charge exchange in the limit of low collision velocities when the motion of the nuclei does not affect the nature of the electron transition. We shall introduce $w(R)$, which is the probability of electron transfer per unit time from the field of a proton to that of a multiply charged ion, and we shall regard the electron spectrum of the ion as quasicontinuous for the final electron states. The charge-exchange cross section is then

$$\sigma = \int_0^\infty 2\pi\rho\, d\rho \left[1 - \exp\left(-\int_{-\infty}^{\infty} w(R)\, dt\right)\right], \tag{1}$$

where the brackets contain the probability of charge-exchange when the impact parameter is ρ, the distance between the nuclei is R, and time is t. In view of the strong dependence $w(R)$ in the case of rectilinear trajectories, Eq. (1) can be conveniently rewritten in the form[20]

$$\sigma = \pi R_0^2, \quad \left(\frac{R_0}{\gamma}\right)^{1/4} \frac{w(R_0)}{v} = 0.56. \tag{2}$$

Here, v is the relative velocity in the collision and $\gamma = |(d \ln\omega/dR)_{R=R_0}|$. Thus, the main problem reduces to the calculation of the probabilities of subbarrier electron transfer per unit time $w(R)$ for a distance R between the nuclei.

The simplest method of finding this quantity is to calculate the electron wave function near the axis joining the nuclei of the atom and ion. This makes it possible to calculate the electron flux in the field of the ion. Assuming that the motion of an electron in the field of a multiply charged ion is quasiclassical, we can determine the value of $w(R)$ as the result of a subbarrier transition. This approach is used in Refs. 18 and 19. Here, we shall employ a different approach, which makes is possible to find the range of validity of the above model.

Charge exchange represents a transition between the two systems in question during a collision. In the ground state of the hydrogen atom the electron energy is

$$-\frac{1}{2} - \frac{Z}{R} + O\left(\frac{1}{R^4}\right).$$

The final state has the energy

$$-\frac{Z^2}{2n^2} - \frac{1}{R},$$

where n is the principal quantum number of the state. Splitting of each group of states amounting to[22] $3n(n_1 - n_2)/2ZR^2$ (n, n_1, n_2 are the parabolic quantum numbers of an electron of a multiply charged ion) is small compared with the difference between the energies of the neighboring groups of levels Z^2/n^3 when the distance between the nuclei is large. This is true for

$$R \gg Z^{1/2},$$

when the ranges of the proton and multiply charged ion fields can be separated. We shall confine our discussion to distances between the nuclei

$$4Z^{1/2} < R < 2Z, \tag{3}$$

for which the action of a multiply charged ion on an electron can be replaced by the action of an electric field of intensity $E = Z/R^2$, which is created by the multiply charged ion, at the point of location of the proton.

We shall use perturbation theory to find the probability of charge exchange in collisions between atoms. The amplitude of the probability of a transition to one of the levels deduced from perturbation theory is

$$C_i = \int_{-\infty}^{\infty} \frac{\Delta_i}{2} \exp\left\{i \int_{-\infty}^{t} \omega_n\, dt'\right\},$$

where Δ_i is the potential of the exchange interaction between the states in question, ω_n is the difference between their energies which, to within the splitting in the same group of levels, is given by

$$\omega_n = \frac{Z-1}{R} + \frac{1}{2} - \frac{Z^2}{2n^2}. \tag{4}$$

The process under consideration occurs when the distance R between the nuclei, defined by Eq. (3), is large. In the region where the transition takes place the exchange interaction potential $\Delta_i(R)$ decreases steeply on

increase of R, and the width of the transition region is small compared with the distance between the nuclei. Therefore, in the region of the transition ($R-\rho \ll \rho$) we can rewrite the law of free relative motion ($R^2=\rho^2+v^2t^2$) in the form $R \approx \rho + v^2t^2/2\rho$, and express the difference between the energies of the initial and final states (4) in a time-independent form:

$$\omega_n = \frac{Z-1}{\rho} + \frac{1}{2} - \frac{Z^2}{2n^2} \tag{4a}$$

and-finally-to write the exchange interaction energy as $\Delta_i(R) = \Delta_i(\rho)\exp[-\alpha(R-\rho)]$, where $\alpha = |(d\ln\Delta_i/dR)_\rho|$. In this way we obtain

$$C_i = \Delta_i(\rho)\frac{1}{v}\left(\frac{2\pi\rho}{\alpha}\right)^{1/2}\exp\left[-\frac{\omega_n^2\rho}{2v^2\alpha}\right],$$

where ρ is the impact parameter of the collision and v is the relative velocity. Consequently, the transition probability is

$$W(\rho) = \sum_i \Delta_i^2(\rho)\frac{2\pi\rho}{v^2\alpha}\sum_n \exp\left[-\frac{\omega_n^2\rho}{\alpha v^2}\right]. \tag{5}$$

The above expression is derived using the fact that the exchange interaction potential is governed by the symmetry of the terms and depends weakly on their energy. Therefore, the index i applies to states with the same values of n.

We shall replace the summation over n with integration. This is valid if

$$\frac{\omega_n}{v}\left(\frac{\rho}{\alpha}\right)^{1/2} \ll 1, \tag{6}$$

where ω is defined by Eq. (4a) for the distance of closest approach of the particles and the series of the nearest values of n. The condition (6) is the Massey criterion for the collisions in question. This operation gives the following expression for the transition probability

$$W(\rho) = \frac{2\pi}{v}\left(\frac{\pi\rho}{\alpha}\right)^{1/2}\sum_i \Delta_i^2(\rho)\frac{n_0^3}{Z^2}, \tag{7}$$

where

$$\omega(n_0) = \frac{Z-1}{\rho} + \frac{1}{2} - \frac{Z^2}{2n_0^2} = 0.$$

We shall now calculate the exchange interaction potential, which is given by[23]

$$\Delta_i(R) = \int_S (\Psi_H \nabla\Psi_i - \Psi_i\nabla\Psi_H)\,dS, \tag{8}$$

where Ψ_H and Ψ_i are the wave functions centered on the proton and multiply charged ion, respectively; S is the surface intersecting the axis joining the two nuclei. Since the projection of the electron momentum along the axis is zero, the electron wave functions are real and independent of the azimuthal angle. It is also worth noting another point: the quantity $\sum_i \Delta_i^2$ of interest to us depends quadratically on the wave functions. We should start with parabolic quantum numbers. However, if we transform the expansion of the wave function from the parabolic to the spherical quantum numbers, the quantity $\sum_i \Delta_i^2$ retains the same form in the new representation. It will be convenient to use the spherical quantum numbers because higher values of the orbital momentum l create a greater centripetal barrier, so that $\sum_i \Delta_i^2$ is governed only by the small values $l \ll n$.

We shall calculate the integral (8) using the fact that this integral converges rapidly near the axis joining the nuclei. We shall select as the surface S the plane perpendicular to the axis joining the nuclei and separated by the distance R_1 from the proton and by R_2 from the multiply charged ion ($R_1+R_2=R$). Then, using the fact that the integral (8) is determined by the stronger of the exponential dependences of the wave functions on the distance given by $\Psi_H \propto e^{-\beta_H r_1}$ and $\Psi_i \propto e^{-\beta_i r_2}$, we can reduce the integral (8) to the form

$$\Delta_i(R) = \frac{2\pi(\beta_H+\beta_i)}{\beta_H/R_1+\beta_i/R_2}\Psi_H(R_1)\Psi_i(R_2).$$

The plane S can be drawn conveniently near the top of the potential barrier at $R_1 = R/(1+Z^{1/2})$ where the range of divergence of the integral (8) in the transverse direction is minimal. Moreover, the quasiclassical description of both wave functions is valid here and this makes it possible to determine easily the arguments of the exponential functions:

$$\beta_H = \left(1 - \frac{2}{R_1} - \frac{2ZR_1}{R(R-R_1)}\right)^{1/2}, \quad \beta_i = \left(\frac{Z^2}{n^2} - \frac{2Z}{R_2} - \frac{2}{R_1}\right)^{1/2}.$$

If we bear in mind that the energy difference (4) between the states of the transition involved is small, we obtain the following expression for the exchange interaction potential ($\beta_H = \beta_i \approx 1$):

$$\Delta_i(R) = \frac{4\pi RZ^{1/2}}{(1+Z^{1/2})^2}\Psi_H\left(\frac{R}{Z^{1/2}+1}\right)\Psi_i\left(\frac{RZ^{1/2}}{Z^{1/2}+1}\right). \tag{9}$$

The structure of the above formula is a generalization of the existing expressions for the potential of the exchange interaction between an ion and an atom[23] when the projection of the electron momentum on the axis joining the nuclei is zero.[2)] In the $Z=1$ case this formula reduces to those already available.

We can find the wave functions Ψ_H and Ψ_i using the quasiclassical approach[23,24] and representing these functions in the form

$$\Psi_H = \varphi_H\chi_H, \quad \Psi_i = \varphi_i\chi_i,$$

where φ_H and φ_i are the wave functions of an electron in an isolated hydrogen atom and in an isolated multiply charged ion. In calculation of the wave functions χ_H and χ_i we must bear in mind that the main exponential dependence is contained in the atomic wave functions. This gives[23,24]

$$\varphi_H(R_1) = \pi^{-1/2}e^{-R_1} = \pi^{-1/2}\exp\left(-\frac{R}{Z^{1/2}+1}\right),$$

$$\chi_H(R_1) = \left(\frac{R}{R_2}\right)^z\exp\left(-\frac{ZR_1}{R}\right) = \frac{1}{e^{1/2}}.$$

In determining the wave functions φ_i and χ_i we shall consider only the limiting case $R \ll Z$. The condition of smallness of the energy difference (4) for the states involved in the transition under consideration is then $n = (ZR/2)^{1/2}$ and the quasiclassical expressions for the wave functions become

$$\varphi_i(R_2) = \frac{(Z/n)^{1/2}}{2^{1/2}\pi RZ^{1/2}}\exp\left(-\frac{R^2}{3Z} + \frac{R}{Z^{1/2}} + \frac{1}{2}\right),$$

$$\chi_i(R_2) = 2R/Z^{1/2}, \quad 4Z^{1/2} < R < 2Z.$$

Substituting the expression for the wave functions in Eq. (8), we obtain the exchange interaction potential

$$\Delta_{n0} = 2\left(\frac{2}{\pi}\right)^{1/2}\frac{R}{n^{3/2}}\exp\left(-\frac{R^2}{3Z}\right), \quad 4Z^{1/2} < R < 2Z. \tag{10}$$

The expression for the potential (10) for the interaction between a hydrogen atom and a multiply charged ion is valid for an s state of an electron in a multiply charged ion. We shall extend this result to the case when the electron momentum l of the multiply charged ion differs from zero so that the electron wave function is

$$\Psi_i=(2l+1)^{1/2}P_l(\cos\theta_2)\varphi_{il}(r_2)\chi_i(r_2),$$

where r_2 and θ_2 are the spherical coordinates of the electron of the multiply charged ion. We shall assume that the main contribution to the integral (8) is made by the angular range $l^2\theta^2\ll 1$, where the angular dependence of the wave function can be neglected, i.e., where we can replace the Legendre polynomial with unity. Since $\theta^2 \propto \rho^2/R^2$ and $\rho \propto R_1 \propto R/Z^{1/2}$ [ρ is the characteristic distance of the electron to the axis, which governs the value of the integral (8)], this is justified if

$$l^2\ll Z. \tag{11}$$

In this case the main dependence of the exchange interaction potential on the momentum is due to the dependence of the radial wave function on the orbital momentum. In the case of small values of the latter the quasiclassical expression for the radial wave function can be represented in the form

$$\varphi_{il}(r)=\varphi_{0i}(r)\exp\left\{\int_{r\geq 1}^{r}\left[\left(\frac{Z^2}{n^2}-\frac{2Z}{r}\right)^{1/2}-\left(\frac{Z^2}{n^2}-\frac{2Z}{r}+\frac{l(l+1)}{r^2}\right)^{1/2}\right]dr\right\},$$

where φ_{0i} corresponds to zero orbital momentum. If $l^2\ll Z$, we obtain the exchange interaction potential (9) in the form

$$\Delta_{nl}(R)=(2l+1)!!\exp\left(-l(l+1)/2Z\right)\Delta_{n0}(R), \quad 4Z^{1/2}<R<2Z, \tag{12}$$

where $\Delta_{n0}(R)$ is the exchange interaction potential (10) for zero orbital momentum.

We shall employ Eq. (7) for the charge-exchange probability, which has the following form for $\rho\ll Z$ ($\alpha=2\rho/3Z$, $n_0^2\approx Z\rho/2$):

$$W(\rho)=\pi\left(\frac{\pi}{3}\right)^{1/2}\frac{1}{Zv}\sum_l \Delta_{nl}^2(\rho).$$

Replacing the summation over l by integration, and using Eqs. (12) and (10), we find that the charge-exchange probability is

$$W(\rho)=\pi\left(\frac{\pi}{3}\right)^{1/2}\frac{1}{v}\Delta_{n0}^2(\rho)=4\left(\frac{3\pi}{2Z}\right)^{1/2}\frac{\rho^2}{v}\exp\left(-\frac{2}{3}\frac{\rho^2}{Z}\right). \tag{13}$$

We shall now compare the result obtained for the total cross section of charge exchange between a hydrogen atom and a multiply charged ion with the result of the model approach[18,19] in which it is assumed that the electron spectrum in the field of a multiply charged ion is continuous. In the limiting case when the electron transition occurs mainly at distances between the nuclei $R\ll Z$, such a transition can be regarded as occurring under the action of the electric field $E=Z/R^2$ of the multiply charged ion. The probability of this transition per unit time is[23]

$$w=\frac{4}{E}e^{-\frac{2}{3}/E},$$

so that the total probability of charge exchange during a transit along a rectilinear trajectory ($R^2=\rho^2+v^2t^2$) for a given impact parameter is

$$W(\rho)=\int_{-\infty}^{\infty}w(R)\,dt=w(\rho)\int_{-\infty}^{\infty}\exp\left(-\frac{2}{3}\frac{v^2t^2}{Z}\right)dt$$
$$=4\left(\frac{3\pi}{2Z}\right)^{1/2}\frac{\rho^2}{v}\exp\left(-\frac{2}{3}\frac{\rho^2}{Z}\right).$$

We have made use of the assumption $W\ll 1$, used to derive Eq. (24) within the perturbation theory framework.

We can see that the results of both approaches are identical and were obtained under the same assumptions. The model based on the hypothesis of a continuous electron spectrum in the field of a multiply charged ion yields Eq. (1) for the charge-exchange probability [$W=1-\exp(-\int w\,dt)$]. We can use it to determine the partial cross sections for charge exchange to a given state nl of a multiply charged ion if we go beyond the perturbation theory framework. For this cross section it follows from Eq. (5) that

$$\sigma_{nl}=\int_0^{\infty}2\pi\rho\,d\rho\,\Delta_{nl}^2(\rho)\frac{2\pi\rho}{v^2\alpha}\exp\left(-\frac{\omega^2\rho}{\alpha v^2}\right)$$
$$\times\left[1-\exp\left(-\int_{-\infty}^{\infty}w(R)\,dt\right)\right]\left[\int_{-\infty}^{\infty}w(R)\,dt\right]^{-1}.$$

Hence, we find that in the case of partial charge-exchange cross sections in the limit of high values of Z

$$\sigma_{n=\nu,l}=\sigma_{nl}\exp\left(-\frac{3}{2}\frac{Z^3v^2}{n_0^6v^2}\right), \quad \nu=0,1,2,\ldots,i, \quad n_0\approx\left(\frac{ZR_0}{2}\right)^{1/2}, \tag{14}$$

where

$$\sigma_{nl}=2(2l+1)\exp\left(-\frac{l(l+1)}{Z}\right)\frac{Z^{3/4}}{vn_0^3}\left(\frac{3}{2\pi}\right)^{1/2}\sigma_{\text{ch-ex}}, \tag{15a}$$

$$\sigma_{\text{ch-ex}}=\pi R_0^2, \quad W(R_0)=4\left(\frac{3\pi}{2Z}\right)^{1/2}\frac{R_0^2}{v}\exp\left(-\frac{2}{3}\frac{R_0^2}{Z}\right)=0.56. \tag{15b}$$

It follows from Eqs. (14) and (15) for the partial cross sections that in the velocity range $v<Z^{1/2}$ the charge-exchange process terminates mainly at the ion levels characterized by the quantum numbers n_0 and l, which are given by $n_0\approx 2^{1/2}Z^{3/4}$ and $l\lesssim Z^{1/2}$.

CHARGE EXCHANGE BETWEEN A HYDROGEN ATOM AND A MULTIPLY CHARGED ION AT MODERATE COLLISION VELOCITIES

In considering charge exchange between a hydrogen atom and a multiply charged ion we can ignore the influence of the ion motion on the nature of the transition as long as $v\ll(d\ln w/dR)^{-1}$, where w is the probability of a transition per unit time. In the limiting cases this condition has the following form:

$$v\ll Z^{1/2}, \ R\ll Z; \quad v\ll 1, \ R\gg Z.$$

When the conditions are no longer obeyed, the time-dependent change in the height of a barrier penetrated by an electron affects the electron transition to the same extent as the shape of the barrier. Nevertheless, we can find the solution of the problem also in the range of higher velocities if we bear in mind that the electron transition takes place from the wave-function tail where we can apply the quasiclassical description of an electron. Then, using quasiclassical methods, we can determine the electron wave function far from its nucleus allowing for its time dependence and this can be done with exponential precision. For moderate collision velocities,

when an electron transition occurs mainly from the wave-function tail, this can be used to determine the charge-exchange cross section. In this respect, our problem is fully equivalent to that of the "destruction" of an atom in a harmonic electric field solved by Keldysh.[22] The only difference is in the nature of the variations of the electric field in space and time. Therefore, we shall follow exactly the quasiclassical Keldysh method applying it to the conditions of our problem.

We shall discuss the limiting case $\rho \ll Z$. In this case a hydrogen atom is in an electric field of intensity $\mathbf{E}=Z\mathbf{n}/(\rho^2+v^2t^2)$, where $\mathbf{n}$ is a unit vector along the axis joining the proton to the nucleus of the multiply charged ion. The electron Hamiltonian in the coordinate system linked to the proton is

$$H=\frac{1}{2}\left(i\frac{\partial}{\partial x}-\frac{A_x}{c}\right)^2+\frac{1}{2}\left(i\frac{\partial}{\partial y}-\frac{A_y}{c}\right)^2,$$

where the components of the vector potential are

$$\frac{A_x}{c}=-\int_{-\infty}^{t}E_x dt=-\frac{Z}{v(\rho^2+v^2t^2)^{1/2}},$$

$$\frac{A_y}{c}=-\int_{-\infty}^{t}E_y dt=\frac{Z}{\rho v}\left(\frac{vt}{(\rho^2+v^2t^2)^{1/2}}+1\right).$$

The x axis coincides with the direction of the ion velocity and the y axis with the direction of the vector of the impact parameter ρ; the scalar potential is assumed to be zero.

We shall introduce new variables:

$$\tau=\frac{1}{2}t,\quad \Omega=\frac{2v}{\rho},\quad F=\frac{2Z}{\rho^2}. \tag{16}$$

Substitution of the variables from Eq. (16), reduces the Schrödinger equation to

$$i\frac{\partial\Psi}{\partial\tau}=\left[\left(i\frac{\partial}{\partial x}+\frac{F}{\Omega(1+\Omega^2\tau^2)^{1/2}}\right)^2+\left(i\frac{\partial}{\partial y}-\frac{F}{\Omega}\left(\frac{\Omega\tau}{(1+\Omega^2\tau^2)^{1/2}}+1\right)\right)^2\right]\Psi. \tag{17}$$

With exponential precision we now have $\Psi=\exp(iS)$, where S is the classical action. The boundary condition for S is $S\to\tau$ for $y\to 0$ and $x\to 0$. In the quasiclassical approximation, S obeys the Hamilton–Jacobi equation, which is obtained by substituting Ψ in Eq. (17) and ignoring the terms with the second derivatives of S with respect to the coordinates:

$$\frac{\partial S}{\partial\tau}=-\left(\frac{\partial S}{\partial x}-\frac{F}{\Omega(1+\Omega^2\tau^2)^{1/2}}\right)^2-\left(\frac{\partial S}{\partial y}+\frac{F}{\Omega}\left(\frac{\Omega\tau}{(1+\Omega^2\tau^2)^{1/2}}+1\right)\right)^2.$$

This equation can be separated as follows:

$$S=p_x x+p_y y+A+\int_{\tau}^{\tau_0}H(p_x,p_y;\tau')d\tau',$$

$$H(p_x,p_y;\tau)=\left(p_x-\frac{F}{\Omega(1+\Omega^2\tau^2)^{1/2}}\right)^2+\left(p_y+\frac{F}{\Omega}\left(\frac{\Omega\tau}{(1+\Omega^2\tau^2)^{1/2}}+1\right)\right)^2,$$

where $\tau=\tau_0$ corresponds to $x=y=0$. Hence, using the boundary condition for S, we obtain $A=\tau_0$. The equations of motion $\partial S/\partial p_x=\partial S/\partial p_y=0$, $\partial S/\partial\tau_0=0$ are then

$$\left.\begin{aligned}x+\int_{\tau}^{\tau_0}\frac{\partial H}{\partial p_x}d\tau'=0,\quad y+\int_{\tau}^{\tau_0}\frac{\partial H}{\partial p_y}d\tau'=0,\\ 1+H(\tau_0)=0.\end{aligned}\right\} \tag{18}$$

The electron flux from the proton field can be expressed in terms of the electron wave function in the classically accessible range of its motion. In this range, we obtain

$$\left(\frac{\partial\,\mathrm{Im}\,S}{\partial x}\right)_\tau=\left(\frac{\partial\,\mathrm{Im}\,S}{\partial y}\right)_\tau=0.$$

Hence, $\mathrm{Im}p_x=\mathrm{Im}p_y=0$. We shall determine the momentum $\mathbf{p}=(p_x,p_y)$ which, under initial conditions $x(\tau_0)=y(\tau_0)=0$ brings us at a moment τ to a point (x,y) lying in the classically accessible range. For that, we shall take the imaginary parts of the system (18). We shall introduce new notation:

$$\frac{\Omega}{F}p_x=p,\quad \frac{\Omega}{F}\left(p_y+\frac{F}{\Omega}\right)=P,\quad \Omega\tau_0=\eta,\quad \frac{\Omega}{F}=\frac{\rho v}{Z}=\xi.$$

In this way we obtain the following system of equations:

$$\left.\begin{aligned}P\,\mathrm{Im}\,\eta+\mathrm{Im}\,(1+\eta^2)^{1/2}=0,\\ p\,\mathrm{Im}\,\eta-\mathrm{Im}\,\mathrm{Arsh}\,\eta=0,\\ (\xi^2+P^2+p^2+1)(1+\eta^2)^{1/2}-2p+2P\eta=0.\end{aligned}\right\} \tag{19}$$

Taking the imaginary part of the third equation and comparing it with the first equation, we find that $\mathrm{Im}(1+\eta^2)^{1/2}=0$ and $P=0$. This makes it possible to represent η in the form $\eta=i\sin\varphi$ so that the system (19) becomes

$$p\sin\varphi=\varphi,\quad (\xi^2+p^2+1)\cos\varphi=2p. \tag{20}$$

The probability of loss of an electron from the proton field (i.e., the total probability of charge exchange and ionization of the hydrogen atom) is given, with exponential precision, by the following expression

$$W(\rho)\propto\exp(-2\,\mathrm{Im}\,S)=\exp\left(-2\,\mathrm{Im}\,\tau_0-2\,\mathrm{Im}\int_{\tau}^{\tau_0}H\,d\tau'\right)$$

$$=\exp\left\{-\frac{2F^2}{\Omega^3}\left(1+\frac{\Omega^2}{F^2}-p^2\right)\sin\varphi\right\}=\exp\left\{-\frac{2\rho^2}{3Z}g\left(\frac{\rho v}{Z}\right)\right\}, \tag{21}$$

where $g(\xi)=\frac{3}{2}\xi^{-1}(1-p^2+\xi^2)\sin\varphi$; p and φ are expressed in terms of ξ on the basis of the system (20). The limiting expressions for the function $g(\xi)$ are

$$g(\xi)=\begin{cases}1-{}^4/_{15}\xi^2, & \xi\ll 1,\\ {}^3/_2\xi^{-1}, & \xi\gg 1,\end{cases}$$

and its intermediate values are given in the table below:

ξ:	0.1	0.2	0.3	0.5	0.7	1.0	1.5
$g(\xi)$:	0.997	0.989	0.976	0.940	0.893	0.814	0.688
ξ:	1.8	2.0	2.2	2.5	3.0	5.0	10.0
$g(\xi)$:	0.623	0.584	0.549	0.503	0.438	0.284	0.148

Thus, Eq. (21) allows us to reconstruct the exponential variation of the probability of "destruction" of the hydrogen atom by collision with a multiply charged ion in the case of large impact parameters. In the limit of low collision velocities this formula describes charge exchange, whereas at high velocities it describes ionization of the hydrogen atom. We shall now use it to find the cross section of "destruction" of the hydrogen atom by a multiply charged ion.

IONIZATION OF A HYDROGEN ATOM BY COLLISION WITH A MULTIPLY CHARGED ION

At high collision velocities the "destruction" of a hydrogen atom by a multiply charged ion is due to the ionization of the former. We shall consider this process on the basis of perturbation theory since the "destruction" occurs mainly at large distances between the nuclei, compared with the size of the hydrogen atom, i.e., the cross section of the ionization process exceeds the cross-sectional area of the hydrogen atom. Then, the perturbation operator is $V=Z\mathbf{r}\cdot\mathbf{n}/R^2$, where $\mathbf{r}$ is the electron coordinate and $\mathbf{R}$ is the distance between the

nuclei. The amplitude of the transition probability is[25]

$$C_k=-i\int_{-\infty}^{\infty}V_{0k}e^{i\omega_k t}dt=\frac{2Z}{v^2}\omega_k\left[y_{0k}K_0\left(\frac{\omega_k\rho}{v}\right)+x_{0k}K_1\left(\frac{\omega_k\rho}{v}\right)\right]. \quad (22)$$

Here, k is one of the states in the continuous spectrum; ω_k is the excitation energy of this state; ρ is the impact parameter (it is assumed that the nuclei move along rectilinear classical trajectories); x and y are the projections of the electron radius vector onto the directions of $\boldsymbol{\rho}$ and $\mathbf{v}$, respectively; K_0 and K_1 are the Macdonald functions.

Having averaged the ionization probability over the projections of the momentum of the final state ($\overline{y_{0k}^2}=\overline{x_{0k}^2}=\frac{1}{3}r_{0k}^2$), we obtain the following expression for the probability of ionization of an atom for a given value of the impact parameter

$$W_{\text{ion}}(\rho)=\frac{4Z^2}{3v^4}\sum_k\omega_k^2r_{0k}^2\left[K_0^2\left(\frac{\omega_k\rho}{v}\right)+K_1^2\left(\frac{\omega_k\rho}{v}\right)\right], \quad (23)$$

where the summation is carried out over the states in the continuous spectrum.

We shall calculate the ionization cross section in the usual way.[26] We shall introduce the impact parameter $\rho_{\min}$ for which the total probability of excitation and ionization is unity ($\rho_{\min}=2Z/v$). We shall represent the ionization cross section in the form

$$\sigma_{\text{ion}}=\pi\rho_{\min}^2\xi+\int_{\rho_{\min}}^{\infty}W_{\text{ion}}(\rho)2\pi\rho\,d\rho.$$

Here,

$$\xi=\sum_k\frac{r_{0k}^2}{\langle r\rangle^2}=0.283$$

is the probability that the transition terminates in a state in the continuous spectrum; the summation in the above expression is carried out only over the states in the continuous spectrum and the expression (23) for the ionization probability found from perturbation theory is used in the second term. Calculating the required integral in the limit $Z^{1/2}/v\ll1$, we finally obtain

$$\sigma_{\text{ion}}=7.2\frac{Z^2}{v^2}\ln\left[\frac{av^2}{Z}\right], \quad (24)$$

where—in agreement with the properties of the hydrogen atom ($\xi=0.283$)—the numerical factor in the logarithm is $a=1.51$.

This method cannot be used in the range $\rho\approx\rho_{\min}$, because perturbation theory no longer applies ($\rho>\rho_{\min}$) or because we cannot replace the ionization probability with unity ($\rho<\rho_{\min}$). Since this range of impact parameters is narrow, the factor in question has little effect on the results of calculations. For example, the use of the second order of perturbation theory within this framework gives the parameter $a=1.43$, which has little effect on the cross section in this range of velocities.

We shall now analyze the general pattern of "destruction" of the hydrogen atom by a multiply charged ion. At low collision velocities this process involves charge exchange between the atom and ion and the cross section of this process is obtained in our paper[19] on the assumption that the electron spectrum is continuous in the field of a multiply charged ion. At high collision velocities the process of "destruction" of the hydrogen atom is due to its ionization so that the cross section, apart from the factor in the logarithm, is given by Eq. (24). Moreover, we have the probability of the loss of an electron from the wave-function tail found using the quasiclassical Keldysh method. This result includes both charge exchange and ionization but it makes it possible to obtain only the exponential variation of the probability of "destruction" of the atom per unit time. The probability of ionization in the case of large impact parameters is, according to Eq. (23),

$$W(\rho)=1.14\frac{Z^2}{v^2\rho^2}e^{-\rho/v}. \quad (25)$$

Matching Eqs. (13) and (25) for the probability of "destruction" by means of Eq. (21), which has the correct exponential dependence, we link these two limiting cases and obtain a general expression for the probability of "destruction" of a hydrogen atom in the case of large impact parameters within the perturbation theory framework ($W\ll1$):

$$W(\rho,v)=C(\rho,v)\exp\left[-\frac{2\rho^2}{3Z}g\left(\frac{\rho v}{Z}\right)\right], \quad (26)$$

where

$$C(\rho,v)=\begin{cases}8.7\rho^2/vZ^{1/3}, & \rho v/Z\leqslant1,\\ 1.14Z^2/\rho^2v^2, & \rho v/Z\geqslant1.\end{cases}$$

This makes it possible to obtain a general expression for the cross section of "destruction" of a hydrogen atom by collision with a multiply charged ion:

$$\sigma=\int_0^{\infty}\{1-\exp[-W(\rho)]\}2\pi\rho\,d\rho=Zf(v/Z^{1/3}). \quad (27)$$

The transition probability used above is based on correct expressions of this quantity in those cases when perturbation theory is invalid. The values of the universal function $f(x)$ are given below:

x:	0.002	0.004	0.008	0.01	0.02	0.04	0.08	0.1
$f(x)$:	55.7	52.1	48.5	47.3	43.7	40.2	37.0	36.2
x:	0.2	0.4	0.8	1	2	4	8	10
$f(x)$:	35.2	19.4	6.6	4.8	2.1	1.0	0.5	0.36

We shall now analyze the result obtained. It is based on the assumption that the action of a multiply charged ion can be represented by an equivalent electric field. This is justified as high velocities when "destruction" of a hydrogen atom is due to ionization in the electric field of a multiply charged ion. This assumption allows us to use the quasiclassical Keldysh method for moderate velocities. At low collision velocities, when the "destruction" of a hydrogen atom is due to charge exchange, the process is solved in a more general form in Ref. 19. We shall now compare the charge-exchange cross sections $\sigma_{\text{ch-ex}}$ at low collision velocities[19] with the cross section $\sigma^0_{\text{ch-ex}}$ found from Eqs. (1) and (2) and corresponding to the replacement of the action of the field of a multiply charged ion by an effective electric field. The ratio $\sigma_{\text{ch-ex}}/\sigma^0_{\text{ch-ex}}$ is as follows:

Z:	4	6	8	10	12	15
$\sigma_{\text{ch-ex}}/\sigma^0_{\text{ch-ex}}$	1.22	1.13	1.06	1.03	1.01	1.00

This ratio allows us to judge the precision of the results obtained for various values of Z. At high values of Z the approach employed is asymptotically correct.

The above approach can be extended, by renormalization of the formulas, to the case of "destruction" of order atoms or small-charge ions colliding with multiply charged ions.

[1)]Here, v is the relative velocity of colliding particles; we shall use the atomic system of units: $\hbar = m = e = 1$.

[2)]We shall not consider the relationship between the exchange matrix element and the quasiclassical barrier permeability. This relationship is analyzed in Chibisov's thesis.[27]

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Characteristics of electron and photon spectra associated with interaction between quasistationary terms

A. Z. Devdariani, V. N. Ostrovskiĭ, and Yu. N. Sebyakin

A. A. Zhdanov State University, Leningrad

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An analysis is made of the energy spectra of electrons or photons emitted as a result of decay of two quasistationary terms which interact with one another in accordance with the Demkov or Nikitin models. General expressions are obtained for describing the lines of isolated atoms and of the background corresponding to decay of a quasimolecular state. The profiles of atomic lines, their satellites, far wings, etc., are investigated. The general problem of the interaction of discrete states with degenerate continua, corresponding to different directions of electron or photon emission and different decay channels, is considered. The interaction of discrete levels via a continuum is related to interference in the final states. It is shown that each model of the interaction of quasidiscrete levels predicts a variety of spectra which differ in respect of the nature of interference.

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§1. INTRODUCTION

Ionization in $A + B \to A + B^+ + e$ atomic collisions at velocities lower than the characteristic electron value can conveniently be described in terms of formation and decay of the corresponding autoionizing states of a quasimolecule. In contrast to the usual discrete levels, such states are characterized not only by the dependences,

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