

Charge exchange of atoms on multiply charged ions

M. I. Chibisov

I. V. Kurchatov Institute of Atomic Energy

(Submitted 17 October 1978)

Zh. Eksp. Teor. Fiz. 76, 1898–1906 (June 1979)

A new method is proposed for investigation of the asymptotic behavior of the exchange interaction leading to charge exchange of one electron in collision of an atom with a multiply charged ion. The method of determination of the wave function of the electron in the internuclear region is more general than the eikonal method of Landau and Herring. Values of the exchange matrix elements obtained by this method are in good agreement with those obtained by Olson and Salop by a numerical method for charge exchange of the hydrogen atom on bare nuclei.

PACS numbers: 34.70. + e

A study of the interaction of neutral gas atoms with multiply charged ions presents great interest for investigation of the role of these ions at a high temperature. Charge exchange of atoms on multiply charged ions is one of the effective methods of obtaining particles with high excitation energy, which is interesting for creation of a population inversion.¹ At the present time a considerable amount of experimental²⁻¹⁴ and theoretical¹⁵⁻²³ information has been accumulated on the cross sections for charge exchange and ionization of atoms by multiply charged ions. All of the experimental results and part of theoretical ones¹⁷⁻²³ apply to ions of relatively low multiplicity $Z_2 \leq 10$. It is of interest to extend these results to the region of higher Z_2 .

Vinogradov and Sobel'man¹ and also Presnyakov and Ulantsev¹⁵ chose as an approximant a charge-exchange cross-section dependence $\sigma_{\text{ch.ex.}} \propto Z^2$. This dependence is determined by the geometrical size of the electron orbit in the multiply charged ion with a binding energy E_2 of the order of the binding energy of the electron in the atom E_1 , which is of the order of unity (we use atomic units: $e^2 = m_e = \hbar = 1$). All of the theoretical calculations and some of the experimental measurements⁴ show that in charge exchange the deeper lying states of the ion are populated. For this reason the breakup model previously proposed by the author¹⁶ (which is asymptotically exact for $Z_2 \gg 1$) leads to a dependence $\sigma_{\text{ch.ex.}} \propto Z_2 \ln Z_2$ for a relative collision velocity $v \leq 2.2 \times 10^8$ cm/sec. Olson and Salop¹⁷⁻²¹ approximated their own numerical calculations by a dependence $\sigma_{\text{ch.ex.}} \propto Z^{3/2}$.

Up to this time the problem remains of calculating the exchange matrix element responsible for charge exchange. An exception in the case of interaction of a hydrogen atom (or any one-electron ion) with an ion not possessing an electron—the so-called $Z_1 e Z_2$ problem.²⁴ In this case separation of the variables occurs, so that it is possible with a computer to calculate the energy eigenvalues and the exchange matrix elements.²⁴

The purpose of the present work is to calculate the exchange matrix element for the general case of interaction of an arbitrary atom and a multiply charged ion which, generally speaking, has many electrons. The investigation carried out below shows that for internuclear distances which are important for charge exchange the asymptotic theory²⁵⁻²⁷ is inapplicable. The exchange matrix element obtained in this work turns out to be directly proportional to the quasiclassical transmission of

the barrier separating the atom and the ion along the internuclear axis.

EXPANSION OF THE ELECTRON WAVE FUNCTION AT LARGE INTERATOMIC DISTANCES

In calculation of the term splitting in quasicrossings it is necessary to determine the wave function of the electron in the region between the nuclei. Here the interaction with the foreign nucleus is not small and cannot be considered as a perturbation.

In the internuclear region the interaction of the electron with each atomic core can be assumed to be Coulomb, and therefore the Schrödinger equation has the form

$$\left(-\frac{\Delta}{2} - \frac{Z_1}{r_1} - \frac{Z_2}{|r_1 - R|} - E \right) \psi_i = 0, \quad (1)$$

where r_1 is the radius vector of the electron with respect to atom 1, R is the internuclear distance, and Z_1, Z_2 are the charges of the atomic cores in the field of which the electron is moving.

We seek the solution of this equation in the form

$$\psi_i = \frac{q_l(r_1)}{r_1} Y_{l,m}(\theta, \varphi), \quad (2)$$

where l and m are the angular momentum of the electron in an isolated atom and its projection, $Y_{l,m}$ is a spherical harmonic, and $q_l(r_1)$ is a new unknown function. We assume that the distances between the nuclei are large, so that near the atom the wave function coincides with that of the unperturbed atom. This gives a boundary condition: for $r_1 \ll R$, $q_l(r_1)$ approaches the asymptote of the unperturbed atomic function $q_l^{(0)}$, i.e.,

$$q_l \rightarrow q_l^{(0)} \sim a_l r_1^{n_l} e^{-r_1/n_l}, \quad (3)$$

$$2n_l \ll r_1 \ll R, \quad n_l = (2|E_1|)^{-1/2}$$

(E_1 is the binding energy of the electron in atom 1). To satisfy Eq. (3) it is necessary that the internuclear distance be much greater than that at which the potential barrier disappears along the axis between the nuclei, i.e.,

$$R \gg R_0 = (2\sqrt{Z_1 Z_2 + Z_1}) / |E_1|. \quad (4)$$

When this condition is satisfied the polarization energy shift of the electron is small in comparison with E_1 .

For $Z_1 \sim Z_2$ we have $R_0 \sim Z / |E_1|$; the condition (4) then

means that the internuclear distance must be greater than the size of the orbits at both centers with energy $\sim E_1$. However, if $Z_2 \gg Z_1$ the condition (4) permits approach of the atoms to distances of the order of the size of the electron orbit with energy E in the multiply charged ion ($Z_2 \gg 1$). It is just this last case which we intend to study, whereas in the first case ($Z_1 \sim Z_2$) the asymptotic theory²⁴⁻²⁶ is applicable. The exchange matrix elements for those quasicrossings which can be calculated by means of the asymptotic theory ($R \gg Z_2/|E|$) turn out for large $Z_2 \gg Z_1$ to be so small that they do not result in charge exchange.

Let us substitute Eq. (2) into Eq. (1):

$$Y_{l,m} \left[\frac{d^2 q_l}{dr_i^2} + 2 \left(E + \frac{Z_1}{r_i} + \frac{Z_2}{|r_i - R|} \right) q_l \right] + Y_{l,m} \left[\frac{\Delta_{\theta,\varphi} q_l}{r_i} - \frac{l(l+1)}{r_i^2} q_l \right] + \frac{2}{r_i^2} \nabla Y \nabla q_l = 0, \quad (5)$$

where $\Delta_{\theta,\varphi}$ is the angular part of the Laplacian. We retain in this equation in the region $r_1 \sim R$ quantities of order unity and R^{-1} and we neglect quantities of order R^{-2} . The angular dependence of the function $q_l(r_1)$ is not sharp and has the form $q_l(r_1, |r_1 - R|)$. Therefore $r_1^{-2} \nabla_{\theta,\varphi} q_l \sim R^{-2} q_l$ for $r_1 \sim R$. Then we obtain

$$\frac{d^2 q_l}{dr_i^2} + 2 \left(E + \frac{Z_1}{r_i} + \frac{Z_2}{|r_i - R|} \right) q_l = 0, \quad (6)$$

$$E = E_1 - Z_2/R + \dots, \quad r_i \sim R. \quad (7)$$

This equation is one-dimensional and the angular dependence is parametric. Near atom 1 when condition (4) is satisfied it goes over to the radial Schrödinger equation of an isolated atom 1.

In the transition to the one-dimensional equation (6) it is impossible, unfortunately, to retain the term with the centrifugal energy $l(l+1)/r_i^2$, since it is of order R^{-2} , like the term $r_1^{-2} \nabla Y \nabla q_l$. Inclusion of these terms would lead to an equation in partial derivatives.

We shall write Eq. (6) with the help of Eq. (7) in the form

$$\frac{d^2 q_l}{dr_i^2} + 2 \left(E_1 + \frac{Z_1}{r_i} + W_1 \right) q_l = 0, \quad (8)$$

$$W_1 = Z_2 \left(\frac{1}{|r_i - R|} - \frac{1}{R} \right). \quad (9)$$

In the region of distances r_1 where the perturbation W_1 is much less than the total energy E_1 , the solution of Eq. (8) can be sought in the form $q_l = q_l^{(0)} \chi_l$, neglecting the second derivatives of the function χ_l . This turns out to be possible since this function,²⁸ which is equal to

$$\chi_l = \exp \left[-n_l \int_0^{r_1} W_1(r_i') dr_i' \right], \quad (10)$$

depends on the ratio r_1/R and each subsequent derivative is R times less than the preceding one. Thus, the method of Landau²⁵ and Herring²⁶ (which also consists of use of the function (10) is an approximation of the eikonal, which is valid in the region where $W_1 \ll E_1$. Here we can have $W_1 \sim Z_1/r_1$, and χ_l differs from unity by several times.

The Landau-Herring method is suitable for asymptotic interatomic distances $R \gg Z_2/E_1$ where there is a wide region of r_1 values for which $W_1 \ll E_1$. For interaction of

atoms with multiply charged ions distances R are also of interest at which the region where $W_1 \ll E_1$ is significantly smaller than the region of sub-barrier motion of the electron between the two turning points

$$x_{1,2} = \frac{1}{2} \left(R - \frac{Z_2 - Z_1}{|E|} \right) \pm \frac{1}{2} \left[\left(R - \frac{Z_2 - Z_1}{|E|} \right)^2 - \frac{4Z_1 R}{|E|} \right]^{1/2}; \quad (11)$$

here x is the distance along the internuclear axis, measured from atom 1. For example, for $Z_2 \gg R \gg Z_1^{1/2}$ (Ref. 16) the barrier is formed mainly by an approximately uniform electric field:

$$W_1 \approx -Z_2 \frac{r_1 R}{R^3} \quad (12)$$

and has a shape close to triangular. It is clear from geometrical considerations that here the region where $W_1 \ll E_1$ is significantly narrower than $|x_2 - x_1|$.

Thus, for the substantially asymmetric case $Z_2 \gg Z_1$ there is interest in that solution of Eq. (6) which is valid also for $W_1 \sim E_1$.

For the further discussion it is necessary to investigate the solution of Eq. (6) near the internuclear axis. We shall use for this purpose the expansion

$$\frac{p^2(r_i)}{2} = |E| - \frac{Z_1}{r_i} - \frac{Z_2}{|r_i - R|} \approx |E| - \frac{Z_1}{x} - \frac{Z_2}{R - x} = \frac{p^2(x)}{2} + O\left(\frac{\rho^2}{R^2}\right), \quad (13)$$

$$r_i \approx x + \rho^2/2x + \dots, \quad \rho \ll R, \quad x \sim R,$$

where ρ is the distance from the internuclear axis. Obviously $dr_i = d(\rho^2/2x)$ for $x = \text{const}$, and then the solution of Eq. (6) near the internuclear axis can be written in the form

$$q_l(r_i) = q_l(x) \exp(-\rho^2 p(x)/2x), \quad \rho \ll R \sim x, \quad (14)$$

where the function $q_l(x)$ is the solution of the equation

$$\frac{d^2 q_l}{dx^2} + 2 \left(|E| - \frac{Z_1}{x} - \frac{Z_2}{R - x} \right) q_l = 0. \quad (15)$$

The function (14) dies out exponentially at distances from the axis $\rho \sim x^{1/2} \ll R$, and therefore the exponential of this function can be retained in unexpanded form.

The solution of Eq. (15) in the quasiclassical approximation satisfying the boundary condition (3) has the form

$$q_l = \frac{a_l}{p^{1/2}(x)} \left(\frac{Z_1 n_1^2}{2e} \right)^{n_1 x_1} \exp \left[- \int_{x_1}^x p(x') dx' \right], \quad x \sim R. \quad (16)$$

When condition (4) is fulfilled the potential barrier satisfies the quasiclassical condition, so that Eq. (16) is valid for the sub-barrier region. This follows from the fact that in the region between the two turning points (11) the quasimomentum is $p(x) \leq n_1^{-1} \sim 1$, and the force is $\partial U/\partial x \ll 1$.

For the case of interaction of a negative ion with a positive one ($Z_1 = 0, Z_2 \neq 0$) Eq. (15) can be reduced to the Whittaker equation,²⁹ the general solution of which for $Z_1 = 0$ is

$$q_l(\xi) = C_1 M_{n_2, 2n_2 - 1/2}(\xi) + C_2 W_{n_2, 2n_2 - 1/2}(\xi); \quad (17)$$

$$\xi = 2(R - x)/n_2, \quad n_2 = (2|E|)^{-1/2}.$$

The function $q_l(\xi)$ with appropriate choice of the constants $C_{1,2}$ coincides with accuracy to quantities of order R^{-1} with the corresponding Green's function for the Cou-

lomb field of the ion, and consequently the wave function (17) coincides with the function obtained by the method of singular potentials.³⁰⁻³²

Kereselidze and Chibisov³¹ pointed out the difference of the wave functions and of the exchange matrix elements for interaction of a negative ion with a positive ion obtained by the Landau-Herring method³³ and by the singular-potential method.³⁰⁻³² As is clear from what has been said here, this difference is explained by the inapplicability of the Landau-Herring method for non-asymptotic interatomic distances, which are important in the present case. The singular-potential method gives a correct result because it permits correction inclusion of the change of the electron energy below the barrier. Only for asymptotically large R do the results of the two methods coincide.

The solutions of Eqs. (6), (8), and (15) obviously are not expressed in terms of elementary functions or known special functions. However, strictly speaking, it is sufficient to use for calculations only the quasiclassical solution (16), since the criterion for its validity coincides with the criterion for validity of Eq. (6) itself. Use of the exact solutions of this equation would represent excessive accuracy (except for the case of interaction of a negative ion with a positive one).

SEPARATION OF TERMS AT PSEUDOCROSSINGS

In the zero approximation of the atomic term (the electron is in the field of the atomic core Z_1 with energy E_1) crosses the ionic terms (the electron is in the field of the ion Z_2 with energy E_{2n}) at interatomic distances

$$R_n = (Z_2 - Z_1) / (E_1 - E_{2n}). \quad (18)$$

We shall calculate the separation of the terms on these pseudocrossings, using the Firsov surface integral³⁴

$$\Delta E_n = \oint_S [\psi_1 \nabla \psi_2 - \psi_2 \nabla \psi_1] \cdot dS, \quad (19)$$

where the plane S is perpendicular to the internuclear axis and intersects it between the turning points (11). Substituting here the wave functions found above (differentiating only $q_{1,2}(x)$), we obtain

$$\Delta E_n = D_n(R) (2n_1 R)^{-m-1} \left[\frac{(2l_1+1)(2l_2+1)(l_1+m)!(l_2+m)!}{(m!)^2(l_1-m)!(l_2-m)!} \right], \quad (20)$$

$$D_n(R) = q_1(x)q_{2n}'(x) - q_1'(x)q_{2n}(x) = \text{const}(x) \approx e^{-R/n}, \quad (21)$$

where l_1 , l_2 , and m are the "spherical" quantum numbers of the crossing states. The Wronskian $D_n(R)$ is a constant (it does not depend on x) since the functions $q_{1,2n}$ are solutions of the same equation (15). This also leads to the result that the exponential part of ΔE_n does not depend on the specific location of the plane S between the points x_1 and x_2 . An undesirable dependence of ΔE_n on the location of the plane S in the entire segment $x_1 \leq x \leq x_2$ nevertheless remains, but in the preexponential factor: on substitution of the function (14) into Eq. (19) and carrying out the integration over $\rho d\rho$, the splitting ΔE_n turns out to be proportional to $|p(x)|^{-1/2}$. If we shift the plane S closer to atom 1 (closer to the point x_1) where $|u(x)| \ll |E_1|$, then here $p(x) \approx n_1$ and the dependence of ΔE_n on S discussed above disappears. We chose

the plane S in just this way in obtaining Eqs. (20) and (21).¹ We note that use of the Landau-Herring functions would lead to such a dependence in the argument of the exponential.

The same dependence would also be obtained by including in Eq. (6) the centrifugal potentials. In fact, for states in the atom and in the ion with different angular momenta the electron at any point of space has different quasiclassical energies, since the quasimomenta are different.

Substituting the quasiclassical solution (16) into Eqs. (20) and (21), we finally obtain³⁵

$$\Delta E_n = \frac{a_1 a_2 B_{l_1, l_2 m}}{n_2 n_1^2} \left(\frac{n_1^2 Z_1}{2e} \right)^{n_1 z_1} \left(\frac{n_2^2 Z_2}{2e} \right)^{n_2 z_2} \frac{1}{R^{|m|+1}} \exp \left[- \int_{x_1}^{x_2} |p(x)| dx \right], \quad (22)$$

$$p(x) = \left[2|E| - \frac{2Z_1}{x} - \frac{2Z_2}{R-x} \right]^{1/2}, \quad (23)$$

$$B_{l_1, l_2 m} = \frac{(2n_1)^{-m}}{m!} \left[\frac{(2l_1+1)(2l_2+1)(l_1+m)!(l_2+m)!}{(l_1-m)!(l_2-m)!} \right]^{1/2}; \quad (24)$$

here $e = 2.718\dots$

Thus, we have expressed the separation of the terms in terms of the quasiclassical transmission of the barrier separating the atoms. This result is a three-dimensional generalization of the well known one-dimensional result.²⁵ The relation between the exchange matrix element $H_{12} = (1/2)\Delta E$ and the barrier transmission is natural, since we are dealing with a case in which the exchange—transfer of an electron from the atom to the ion—occurs below the barrier.

We note that Eq. (22) involves the transmission of the one-dimensional barrier—along the internuclear axis, although the problem as a whole is three-dimensional. This occurred because the barrier transmission along a path deviating substantially from the internuclear axis is exponentially less likely than along the axis. The barrier in the direction from the nucleus of the atom to the nucleus of the ion is the most penetrable for the electron.

Let us apply Eq. (22) to the case of interaction of the hydrogen atom in its ground state with multiply charged ions which have no electrons (with bare nuclei). In this case the states in the ion are degenerate. The exchange matrix element H_{12} is nonvanishing only for the one of the degenerate states with a given energy which has parabolic quantum numbers^{24, 35}: $\nu_2 = m = 0$, $\nu_1 = \nu - 1$ (the energy of the level is $E_\nu = -Z^2/2\nu^2$, $\nu = 1, 2, 3, \dots$). Equation (22) takes the form

$$\Delta E = \frac{B(Z, \nu)}{R} \exp \left[- \int_{x_1}^{x_2} \left(1 - \frac{2}{x} - \frac{2Z}{R-x} \right)^{1/2} dx \right] \quad (25)$$

$$B(Z, \nu) = Z^\nu \frac{\nu^\nu e^{-\nu-1}}{\nu! \nu} \xrightarrow{\nu \gg 1} \frac{(Z/\nu)^\nu}{e(2\pi)^\nu}. \quad (26)$$

Salop and Olson¹⁹ found that the results of calculations of the energy according to Power's program³⁶ lie satisfactorily on a straight line; specifically, $\log(Z^{1/2}H_{12})$ is approximately a straight line as a function of R/\sqrt{Z} —see the figure—for $1 \leq RZ^{-1/2} \leq 6$. In the figure we have plotted also the results of our calculations according to Eq. (25) and the values of H_{12} given by the asymptotic theory,

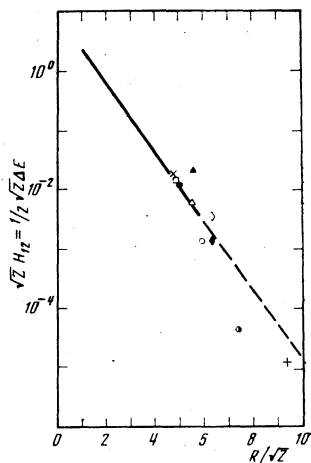


FIG. 1. The exchange matrix element H_{12} , multiplied by \sqrt{Z} , as a function of R/\sqrt{Z} (R is the internuclear distance) for interaction of the hydrogen ion with a bare nucleus of charge Z . The solid line is an approximation in accordance with Ref. 19 of the exact numerical results; the dashed line is the extrapolation of this approximation. The results obtained with Eq. (25) are as follows: $+ - C^{6+} (\nu = 5)$, $\diamond - O^{8+} (\nu = 6)$, $\Delta - Ne^{10+} (\nu = 7)$, $\square - Si^{14+} (\nu = 9)$, $\times - Ar^{18+} (\nu = 11)$, $\bullet - Fe^{26+} (\nu = 15)$, $\circ - Fe^{26+} (\nu = 16)$, $\ominus - Fe^{26+} (\nu = 17)$. The asymptotic results in accordance with Eq. (27) (cf. Ref. 26) are as follows: $\diamond - O^{8+} (\nu = 6)$, $\blacktriangle - Ne^{10+} (\nu = 7)$ (all quantities are measured in atomic units).

which for this case are

$$2H_{12} = \Delta E = \left(\frac{2}{e^{\nu}}\right)^{z+\nu z} \frac{Z^{\nu+1/2}}{\nu^{\nu} \nu!} R^{\nu} \times \exp\left[-\frac{R}{2}\left(1 + \frac{Z}{\nu}\right)\right]. \quad (27)$$

As can be seen from the figure, the quasiclassical approximation (25) is in good agreement with the results of the exact calculations in this case. For $RZ^{-1/2} > 6$ a deviation from the straight line is observed. The approximation used by us, like the asymptotic theory of Ref. 27, cannot give results for this case in the region $RZ^{-1/2} < 4$ in view of the violation here of the condition (4): $R_0 Z^{-1/2} \geq 4$ (and also as $R \rightarrow R_0$ we have $x_1 \rightarrow x_2$). The asymptotic result (27) is larger by two to three times than the exact and quasiclassical results.

Let us compare the result (22) with the asymptotic result²⁵ for the case of interaction of a proton with a hydrogen atom. The asymptotic result for this case is $\Delta E = 4Re^{-R-1}$,²⁵ and Eq. (25) takes the form ($Z = \nu = 1$)

$$\Delta E_{H_1} = R^{-1} \exp\left[-2 - \int_{x_1}^{x_2} \left(1 - \frac{2}{x} - \frac{2}{R-x}\right)^{1/2} dx\right]. \quad (28)$$

In the table the results of a numerical calculation on the basis of Eq. (28) are compared with the asymptotic result. It is evident that the agreement is more than satisfactory, which must be considered a coincidence. In the asymmetric case—an atom and an ion of different types—the disagreement of the results is substantial, as was evident above.

For interaction of a negative ion with a positive one ($Z_1 = 0$, $m = 0$) the integral in Eq. (22) is calculated analytically and we obtain (we use the model of the δ potential for the negative ion: $x_1 = 0$, $x_2 = R - Z_2/|E|$)

TABLE I. Comparison of splitting of terms for the interaction $H^+ + H(1s)$ calculated with Eq. (25), and the asymptotic expression $\Delta E = 4Re^{-R-1}$ (Ref. 24)*.

R	$10^3 \Delta E$, atomic units		
	Eq. (25)	Asymptotic expression	Exact numerical calculation ³⁷
7	9.57	9.38	9.32
8	4.00	3.94	3.96
9	1.65	1.63	1.65
10	0.870	0.867	0.678
11	0.270	0.270	
15	$6.72 \cdot 10^{-3}$	$6.76 \cdot 10^{-6}$	$6.86 \cdot 10^{-3}$
20	$6.02 \cdot 10^{-5}$	$6.07 \cdot 10^{-5}$	$6.17 \cdot 10^{-5}$

*The value of R_0 defined by Eq. (4) is in this case $R_0 = 6$.

$$\Delta E = \frac{a_1 a_2 (2l_2 + 1)^{1/2}}{n_2 n_1^2} \left(\frac{1 + n_2/n_1}{2e^{1/2}}\right)^{2n_2} R^{n_1 + n_2 - 1} \exp[-R(2|E_-|)^{1/2}],$$

$$n_1 = (2|E_-|)^{-1/2}, \quad n_2 = (2|E_-| + 2Z_2/R)^{-1/2}. \quad (29)$$

In Eq. (29) the argument of the exponential involves only the binding energy of the negative ion E_- : $\exp[-R(2|E_-|)^{1/2}]$, which corresponds to the physical picture of a sub-barrier transfer of the electron. A power of the internuclear distance, $R^{n_1 + n_2 - 1}$, is present in Eq. (29) because of Coulomb shape of the barrier. Use of the exact Coulomb Green's function for interaction of an ion A^- with a bare nucleus³⁰⁻³² with use of the δ -potential model for A^- should, of course, provide a more accurate result. The previous analytical results³⁰⁻³³ were obtained either with an asymptotic expansion of the Green's function³⁰⁻³² or with use of the Landau-Herring method.³³ These results are valid therefore for remote, asymptotic crossings of the terms, for which $E_- \approx E_2$. However, Eq. (29) is applicable also at smaller distances: it is necessary that the barrier width be greater than the size of the negative ion, which is of the order n_1 ; therefore Eq. (29) is valid for $R > n_1$.

¹In this region the Landau-Herring approximation is sufficient for correction of the wave function of atom 1 for interaction with the ion. However, this approximation is inadequate in this region for the ion function.

¹A. V. Vinogradov and I. I. Sobel'man, Zh. Eksp. Teor. Fiz. **63**, 2113 (1972) [Sov. Phys. JETP **36**, 1115 (1973)].

²H. Klinger, A. Müller, and E. Salzborn, J. Phys. **B8**, 230 (1975).

³A. Müller, H. Klinger, and E. Salzborn, Phys. Lett. **55A**, 11 (1975).

⁴V. V. Afrosimov, A. A. Basalae, M. P. Panov, and G. A. Leiko, Pis'ma Zh. Eksp. Teor. Fiz. **26**, 699 (1977) [JETP Lett. **26**, 537 (1977)].

⁵G. N. Ogurtsov and I. P. Flaks, Zh. Eksp. Teor. Fiz. **42**, 721 (1962) [Sov. Phys. JETP **15**, 502 (1962)].

⁶D. H. Crandall, Phys. Rev. **A16**, 958 (1977).

⁷E. J. Shipsey, J. C. Browne, and R. E. Olson, Phys. Rev. **A15**, 2166 (1977).

⁸H. Winter, E. Bloemen, and F. J. de Heer, J. Phys. **B10**, L453 (1977).

⁹R. A. Phaneuf, F. W. Meyer, R. H. McKnight, R. E. Olson, and A. Salop, J. Phys. **B10**, L425 (1977).

¹⁰I. S. Dmitriev, Yu. A. Tashae, V. S. Nikolaev, Ya. A. Teplova, and B. M. Popov, Zh. Eksp. Teor. Fiz. **73**, 1684 (1977)

- [Sov. Phys. JETP **46**, 884 (1977)].
- ¹¹J. A. Guffey, L. D. Ellsworth, and J. R. Macdonald, Phys. Rev. **A15**, 1863 (1977).
- ¹²L. D. Gardner, J. E. Bayfield, P. M. Koch, H. J. Kim, and P. H. Stelson, Phys. Rev. **A16**, 1415 (1977).
- ¹³I. P. Flaks and E. S. Solov'ev, Zh. Tekh. Fiz. **28**, 612 (1958) [Sov. Phys. Tech. Phys. **3**, 564 (1958)].
- ¹⁴D. H. Crandall, M. L. Mallory, and D. C. Kocher, Phys. Rev. **A15**, 61 (1977).
- ¹⁵L. P. Presnyakov and A. D. Ulantsev, Kvantovaya Electron. (Moscow) **1**, 2377 (1974) [Sov. J. Quantum Electron. **4**, 1320 (1974)].
- ¹⁶M. I. Chibisov, Pis'ma Zh. Eksp. Teor. Fiz. **24**, 56 (1976) [JETP Lett. **24**, 46 (1976)].
- ¹⁷A. Salop and R. E. Olson, Phys. Rev. **A13**, 1312 (1976).
- ¹⁸A. Salop, Phys. Rev. **A13**, 1321 (1976).
- ¹⁹R. E. Olson and A. Salop, Phys. Rev. **A14**, 579 (1976).
- ²⁰R. E. Olson and A. Salop, Phys. Rev. **A16**, 531 (1977).
- ²¹A. Salop and R. E. Olson, Phys. Rev. **A16**, 1811 (1977).
- ²²J. Vaaben and J. S. Briggs, J. Phys. **B10**, L521 (1977).
- ²³V. A. Abramov, F. F. Baryshnikov, and V. S. Lisitsa, Zh. Eksp. Teor. Fiz. **74**, 897 (1978) [Sov. Phys. JETP **47**, 469 (1978)].
- ²⁴I. V. Komarov, L. I. Ponomarev, and S. Yu. Slavyanov, Sferoidal'nye i kulonovskie sferoidal'nye funktsii (Spheroidal and Coulomb Spheroidal Functions), Moscow, 1976.
- ²⁵L. D. Landau and E. M. Lifshits, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, Moscow, 1963).
- ²⁶C. Herring, Rev. Mod. Phys. **34**, 631 (1962).
- ²⁷B. M. Smirnov, Atomnye stolknoveniya i élementarnye protsessy v plazme (Atomic Collisions and Elementary Processes in Plasma), Moscow, p. 18, 1968.
- ²⁸M. I. Chibisov, Zh. Eksp. Teor. Fiz. **69**, 457 (1975) [Sov. Phys. JETP **42**, 232 (1975)].
- ²⁹E. Jahnke, F. Emde, and F. Lösch, Tables of Higher Functions, McGraw-Hill, 1960. Russ. transl., Moscow, 1964, p. 81.
- ³⁰I. V. Komarov, P. V. Pogorelyĭ, and A. S. Tibilov, Opt. Spektrosk. **27**, 198 (1969) [Opt. Spectrosc. (USSR) **27**, 105 (1969)].
- ³¹T. M. Kereselidze and M. I. Chibisov, Zh. Eksp. Teor. Fiz. **68**, 12 (1975) [Sov. Phys. JETP **41**, 6 (1975)].
- ³²Yu. N. Demkov and V. N. Ostrovskii, Metod singulyarnykh potentsialov v atomnoi fizike (The Method of Singular Potentials in Atomic Physics), Leningrad State University Press, Leningrad, 1975, p. 151.
- ³³B. M. Smirnov, Dokl. Akad. Nauk SSSR **161**, 92 (1965) [Sov. Phys. Dokl. **10**, 218 (1965)].
- ³⁴O. B. Firsov, Zh. Eksp. Teor. Fiz. **21**, 1001 (1951).
- ³⁵M. I. Chibisov, Dissertatsiya (Dissertation), Institute of Atomic Energy, 1976.
- ³⁶J. D. Power, Phil. Trans. Roy. Soc. London **274**, 663 (1973).
- ³⁷D. R. Bates and R. H. Reid, Adv. Atom. and Mol. Phys. **4**, 13 (1968).

Translated by Clark S. Robinson

Threshold features of the excitation and ionization of atoms by high-intensity electromagnetic radiation

A. I. Andryushin, A. E. Kazakov, and M. V. Fedorov

P. N. Lebedev Institute of Physics, Academy of Sciences of the USSR

(Submitted 30 October 1978)

Zh. Eksp. Teor. Fiz. **76**, 1907-1918 (June 1979)

The step-by-step transition from the resonance excitation of the levels of a discrete spectrum by an external electromagnetic field to the ionization of the atom is studied on the basis of a unified theoretical approach. It is shown that in the intermediate region, where the interaction encompasses a large number of levels, the excitation process is on the whole irreversible, but retains to some extent the properties of the transitions between isolated discrete levels: the excitation probability depends nonmonotonically on the time. The nonexponential decay of the bound state in the near-threshold region is investigated. A quasistationary regime characterized by a constant mean probability for finding the atom in the ground state is found to exist in some interval of time. The threshold for the excitation and ionization decay processes is found to be depressed by an amount determined in a weak field by the parameter $t^{-2/3}$ and in a strong field by the parameter $F^{4/3}$, where t and F are the pulse length and amplitude of the radiation intensity.

PACS numbers: 32.80.Fb, 31.50.+w

1. INTRODUCTION

The probability, w , for a direct single-photon ionization of an atom, which depends linearly on the time t in the initial phase of the process, is at large t usually described by the formula^{1,2}

$$w = 1 - e^{-\Gamma t}, \quad (1)$$

which corresponds to a simple exponential decay of the ground state. Here Γ is the ionization width:

$$\Gamma = 2\pi |\langle \psi_1 | V | \psi_{E_1+\omega} \rangle|^2, \quad (2)$$

$V = \frac{1}{2} \mathbf{d} \cdot \mathbf{F}$ is the atom-field interaction operator; \mathbf{d} is the dipole moment; \mathbf{F} is the intensity amplitude of the alternating electric field, $\mathbf{F}(t) = \text{Re}(\mathbf{F}e^{-i\omega t})$, of frequency ω ; ψ_1 and E_1 are the wave function and energy of the ground state; $\psi_{E_1+\omega}$ is the wave function of the continuous spectrum with energy $E = E_1 + \omega$. Here and below we use the atomic system of units. The ionization width Γ is a slowly varying function of the energy $E = E_1 + \omega$, and tends to a constant limit as $E_1 + \omega \rightarrow 0$, in accord with the threshold property of the cross section for the photoelectric effect in neutral atoms.³ In view of the slowness