Tunnel ionization of complex atoms and of atomic ions in an alternating electromagnetic field

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An expression is derived for the probability of tunnel ionization, in an alternating field, of a complex atom and of an atomic ion that are in an arbitrary state. The expression for the tunnel-ionization probability is obtained in the quasiclassical approximation $n^* \gg 1$.
Expressions are also obtained for states with arbitrary values of l at arbitrary ellipticity of the radiation. A quasiclassical approximation yields results up to values $n^* \approx 1$, with accuracy up to several percent.

1. INTRODUCTION

The theoretical description of tunnel ionization of atoms in an alternating field has long attracted attention.[1] In a certain sense this task is more promising than that of ionization in the opposite multiphoton case. First, only the initial and final states of the electron are significant in tunneling, while the intermediate states place no rule. Second, when the conditions $\hbar\omega \ll E$ and $\mathscr{E} \ll \mathscr{E}_{at}$ ($\hbar\omega$ is the emitted-photon energy, E is the energy of the considered state of the electron in the atom, and $\mathscr{E}_{at}$ the atomic field strength) permit the use of a quasiclassical approximation. Third, the results for an alternating field are easily obtained from those for a constant field by substituting $\mathscr{E} \to \mathscr{E} \cos \omega t$ and integrating over the period T of the field. All this permits analytic expressions to be obtained for the tunnel-ionization probability. So far, however, expressions for the tunnel-ionization probability in an alternating field were obtained only for arbitrary states of the hydrogen atoms.[1,2]

In this situation it is expedient to derive an equation for the probability of tunnel ionization of complex atoms or atomic ions, and in arbitrary states. To this end it is necessary, starting from the equation obtained in Ref. 2 for the ionization probability for states of the hydrogen atoms, to obtain the sought-for equation, in which the states of the complex atom are characterized by effective principal and orbital quantum number n^* and l^* that take into account the quantum effects, and for the states of the atomic ions also the degree of ionization Z.

2. DETERMINATION OF THE CONSTANT $C_{n^*l^*}$ FOR ATOMS AND IONS IN THE QUASICLASSICAL APPROXIMATION ($n^* \gg 1$)

Assuming that the external electromagnetic field is linearly polarized, the probability of ionization per unit time from a state with energy E, orbital quantum number l, and its projection m, is described by the expression[2]

$$w = C_{n^*l^*}^2 \left(\frac{3\mathscr{E}}{\pi \mathscr{E}_0}\right)^{1/2} E \frac{(2l+1)(l+|m|)!}{2^{|m|}(|m|)!(l-|m|)!} \left(\frac{2\mathscr{E}_0}{\mathscr{E}}\right)^{2n^*-|m|-1}$$
$$\times \exp\left(-\frac{2\mathscr{E}_0}{3\mathscr{E}}\right). \qquad (1)$$

Here

$$n^* = Z(2E)^{-1/2} \quad \mathscr{E}_0 = (2E)^{3/2}, \qquad (2)$$

Z is the charge of the atomic residue. We use the atomic system of units, $\hbar = m_e = e = 1$.

The quantity $C_{n^*l^*}$ in (1) is determined from the following considerations[2]: in the distance region $(2E)^{-1/2} \ll r \ll 2E/\mathscr{E}$ the atomic-residue field is already weak, but the external field can still be neglected. The wave function Ψ_{n^*lm} coincides therefore in this region with the asymptotic wave function of the free electron at $r \gg (2E)^{-1/2}$:

$$\Psi_{n^*lm}(r) = C_{n^*l^*} \left(\frac{Z}{n^*}\right)^{1/2} \left(\frac{Z}{n^*}\right)^{n^*-1} \exp\left(-\frac{Zr}{n^*}\right) Y_{lm}\left(\frac{\mathbf{r}}{r}\right). \qquad (3)$$

An analytic expression for the constant $C_{n^*l^*}$ is known[3] only for arbitrary states of the hydrogen atom. The values of $C_{n^*l^*}$ obtained from numerical calculations for the ground states of complex atoms and single ions are tabulated in Ref. 4. Here we calculate $C_{n^*l^*}$ for an arbitrary state of an atom or an atomic ion in the quasiclassical approximation.

Consider an atom (ion) in the absence of an external field in the quasiclassical approximation, which is valid when the condition $n^* \gg 1$ is satisfied. In the classically allowed region $r_1 < r < r_2$ are the classical turning points) the quasiclassical radial wave function of an electron with principal quantum number n and with orbital quantum number l is of the form (see Ref. 3, §46)

$$R_{nl}(r) = \frac{a_{nl}}{r p_{nl}^{1/2}} \cos\left(\int_{r_1}^{r} p_{nl}\, dr - \frac{\pi}{4}\right), \qquad (4)$$

where

$$p_{nl} = [2(-Z^2/(2n^{*2}) + Z/r - V)]^{1/2}, \quad n^* = n - \delta_l,$$

V is a small non-Coulomb increment to the potential of the interaction between the electron and the atomic residue, δ_l is the quantum effect and a_{nl} is a normalization factor. Consider the case $l \ll n$. The centrifugal potential in the momentum p_{nl} can then be neglected. We determine the coefficient a_{nl} by using the Bohr-Sommerfeld quantization rule

$$\int_{r_1}^{r_2} p_{nl}\, dr = (n+\tfrac{1}{2})\pi. \tag{5}$$

We differentiate (5) with respect to n, assuming δ_l to be independent of n:

$$\frac{2Z^2}{n^{*3}} \int_{r_1}^{r_2} \frac{dr}{2p_{nl}} = \pi. \tag{6}$$

We also use the condition for quasiclassical normalization of a radial function:

$$a_{nl}^2 \int_{r_1}^{r_2} \frac{dr}{2p_{nl}} = 1. \tag{7}$$

From (6) and (7) we obtain the value of a_{nl}:

$$a_{nl} = Z(2/\pi n^{*3})^{1/2}. \tag{8}$$

In the forbidden region $r > r_2$ the radial wave function of the electron is (see Ref. 3, §46)

$$R_{nl} = \frac{a_{nl}}{2r p_{nl}^{1/2}} \exp\left(-\int_{r_2} |p_{nl}|\, dr\right). \tag{9}$$

Equation (9) should coincide with the asymptotic form of the wave function (3) when $r \gg (2E)^{-1/2}$. Simplifying (9) with this condition satisfied, we get

$$R_{nl} = \left(\frac{Z}{2\pi}\right)^{1/2} \frac{1}{n^* r} \exp\left(-\frac{Zr}{n^*}\right)\left(\frac{2Zre}{n^*}\right)^{n^*}. \tag{10}$$

A comparison of (3) with (10) yields

$$C_{n^* l^*} = \left(\frac{2e}{n^*}\right)^{n^*} \frac{1}{(2\pi n^*)^{1/2}}. \tag{11}$$

It must be pointed here that at $l \ll n$ the coefficient $C_{n^* l^*}$ depends only on the quantity $n^* = n - \delta_l$.

3. PROBABILITY OF ATOM OR ION IONIZATION IN THE CASE $l \ll n$

Using expression (11) for $C_{n^* l^*}$, we rewrite expression (1):

$$w = \left(\frac{3\mathscr{E}n^{*3}}{\pi Z^3}\right)^{1/2} \frac{Z^2}{2n^{*2}} \left(\frac{2e}{n^*}\right)^{2n^*} \frac{1}{2\pi n^*} \frac{(2l+1)(l+|m|)!}{2^{|m|}(|m|)!(l-|m|)!}$$
$$\times \left(\frac{2Z^3}{\mathscr{E}n^{*3}}\right)^{2n^*-|m|-1} \exp\left(-\frac{2Z^3}{3n^{*3}\mathscr{E}}\right). \tag{12}$$

Putting next $l = 1$ in (12), we obtain the probability of tunnel ionization of an atom or an ion in the form

$$w_{m=0} = \left(\frac{3e}{\pi}\right)^{1/2} \frac{Z^2}{n^{*4,5}} \left(\frac{4eZ^3}{\mathscr{E}n^{*4}}\right)^{2n^*-1,5} \exp\left(-\frac{2Z^3}{3n^{*3}\mathscr{E}}\right), \tag{13a}$$

$$w_{|m|=1} = \left(\frac{3e}{\pi}\right)^{1/2} \frac{2eZ^2}{n^{*5,5}} \left(\frac{4eZ^3}{\mathscr{E}n^{*4}}\right)^{2n^*-2,5} \exp\left(-\frac{2Z^3}{3n^{*3}\mathscr{E}}\right). \tag{13b}$$

It is important that in these expressions the principal change of the ionization probability as a function of the field $\mathscr{E}$ is determined not by the exponential, but by the factor $(Z^3/\mathscr{E}u^{*4})^{2n^*}$. In addition, it must be noted that the relation

$$w_{m=0}/w_{|m|=1} = 2Z^3/\mathscr{E}n^{*3} = 2\mathscr{E}_0/\mathscr{E} \gg 1, \tag{14}$$

i.e., the probability of detachment of an electron with magnetic quantum number $m = 0$ exceeds substantially the probability of detachment of an electron with $|m| = 1$

A tunnel-ionization probability on the order of unity is reached, according to (13), at an electric field strength $\mathscr{E} \sim Z^3/n^{*4}$, in agreement with earlier classically obtained results.[5]

It is of interest to compare the expression obtained for the tunnel-ionization probability (13a) with the δ-potential probability w_δ of tunneling caused by a linearly polarized field[2]:

$$w_\delta = \frac{Z^2}{2n^{*2}} \left(\frac{3\mathscr{E}n^{*3}}{\pi Z^3}\right)^{1/2} \exp\left(-\frac{2Z^3}{3n^{*3}\mathscr{E}}\right). \tag{15}$$

Simple algebra leads the ratio of the probabilities of tunnel ionization from a Coulomb potential (13a) and a δ potential (15), in the form

$$\frac{w}{w_\delta} = \frac{3e}{\pi n^{*2}} \left(\frac{4eZ^3}{\mathscr{E}n^{*4}}\right)^{2n^*-1}. \tag{16}$$

It can be seen that $w/w_\delta \gg 1$ for all n^* and Z and for all field strengths up to atomic.

TABLE I. Experimental[7] and theoretical [from Eq. (13a)] values of the laser intensity I for two values of the ionization probability w.

Atom or ion	$w=0,01\tau^{-1}$		$w=0,1\tau^{-1}$		Atom or ion	$w=0,01\tau^{-1}$		$w=0,1\tau^{-1}$	
	I_{exp}, 10^{14} W/cm^2	I_{theor}, 10^{14} W/cm^2	I_{exp}, 10^{14} W/cm^2	I_{theor}, 10^{14} W/cm^2		I_{exp}, 10^{14} W/cm^2	I_{theor}, 10^{14} W/cm^2	I_{exp}, 10^{14} W/cm^2	I_{theor}, 10^{14} W/cm^2
He	1.70	1.74	2.10	2.13	Ar$^+$	1.30	1.41	1.35	1.64
Ne	1.22	1.24	1.30	1.25	Xe	0.16	0.16	0.17	0.18
Kr	0.20	0.24	0.30	0.29	Xe$^+$	0.40	0.56	0.70	0.66
Kr$^+$	0.80	0.92	1.15	1.08	Xe^{++}	–	1.59	1.50	1.81
Ar	0.40	0.36	0.45	0.44					

Note. The experimental dependences of the relative number of recorded ions on the laser intensity were compared with the analytic expression (13a) for the tunnel ionization probability under the assumption that the region of the ion-signal saturation the ionization is the reciprocal of the laser-pulse duration τ ($\tau = 1.1$ ns, Ref. 7).

TABLE II. Comparison of the coefficients C_{n*l*} obtained by numerical methods[4] and from the analytic equation (11).

Atom or ion	$n*$	Value of coefficients C_{n*l*}		Atom or ion	$n*$	Value of coefficients C_{n*l*}	
		$A(Z/n*)^{n*-0.5}$ (A–from handbook[4])	From Eq. (11)			$A(Z/n*)^{n*-0.5}$ (A–from handbook[4])	From Eq. (11)
He	0.74	1.99±0.007	2.03	Kr	0.99	2.17±0.03	2.16
Ne	0.79	1.31±0.07	2.06	Kr+	1.44	2.30=0.12	2.26
Ne+	1.15	1.37±0.08	2.22	Xe	1.06	2.27±0.09	2.19
Ar	0.93	1.90±0.04	2.13	Xe+	1.60	2.24±0.14	2.23
Ar+	1.40	1.73±0.15	2.25				

Note. The factor $(Z/n)^{n*-0.5}$ was introduced because the definition of the coefficients C_{n*l*} in Eq. (3) differs from the coefficients of A in the handbook.[4]

Note that (13a) agrees well with the experimental data[6,7] on tunnel ionization of atoms and atomic ions of noble gases in a large interval of electron binding energies and in a wide intensity range of the field in which the ionization took place[8] (see Table I).

4. TUNNEL-IONIZATION PROBABILITY FOR AN ARBITRARY ORBITAL QUANTUM NUMBER l

In the case of an arbitrary quantum number l and for $n \neq n*$ we must use the effective value $l*$ of the orbital number, defined as[9]

$$l* = n_0* - 1. \tag{17}$$

Here n_0* is the effective principal quantum number of the ground state. To determine the constant C_{n*l*} for arbitrary $l* \lesssim n*$ we use the asymptotic form of the radial wave function of an electron in a Coulomb potential[3]:

$$R_{nl} = \frac{2^n Z^{1/2}(Zr)^{n-1}}{n^{n+1}((n+l)!(n-l-1)!)^{1/2}} \exp\left(-\frac{Zr}{n}\right). \tag{18}$$

Using the definition (3) of C_{n*l*} and replacing the principal and orbital quantum numbers n and l by the effective $n*$ and $l*$ we get

$$C_{n*l*}^2 = \frac{2^{2n*}}{n*\Gamma(n*+l*+1)\Gamma(n*-l*)}. \tag{19}$$

Using Stirling's factorial formula, we get from (19)

$$C_{n*l*}^2 = \left(\frac{4e}{n*^2-l*^2}\right)^{n*} \left(\frac{n*+l*}{n*-l*}\right)^{l*+1/2} \frac{1}{2\pi n*}. \tag{20}$$

If $l* \ll n*$, Eq. (20) goes over into the equation obtained for C_{n*l*}^2 in the quasiclassical approximation [see (11)].

We substitute (20) in Eq. (1) for the tunnel ionization probability:

$$w = \left(\frac{3}{\pi^3}\right)^{1/2} \frac{(2l+1)(l+|m|)!}{(|m|)!(l-|m|)!}$$

$$\times \left(\frac{e}{(n*^2-l*^2)^{1/2}}\right)^{|m|+1/2} \left(\frac{n*+l*}{n*-l*}\right)^{l*+1/2}$$

$$\times \frac{Z^2}{n*^3} \left(\frac{4eZ^3}{\mathscr{E}n*^3(n*^2-l*^2)^{1/2}}\right)^{2n*-|m|-1/2} \exp\left(-\frac{2Z^3}{3\mathscr{E}n*^4}\right). \tag{21}$$

This expression is the probability of tunnel ionization of a state with arbitrary value of the orbital quantum number l.

5. TUNNEL IONIZATION IN AN ELLIPTICALLY POLARIZED ELECTROMAGNETIC FIELD

We have considered so far a linearly polarized electromagnetic wave field. The dependence of the tunnel ionization probability on the degree of field ellipticity was studied in detail in Ref. 2. The field of an elliptical-polarization wave is given by

$$\mathscr{E}(t) = \mathscr{E}(e_x \cos \omega t \pm \varepsilon e_y \sin \omega t), \quad 0 \leqslant \varepsilon \leqslant 1. \tag{22}$$

The probability of ionization in an elliptically polarized alternating field is connected with the probability of ionization in a constant field by the relation[2]

$$w = \left(\frac{\varepsilon(1+\varepsilon)}{2}\right)^{-1/2} a\left(\frac{1-\varepsilon}{3\varepsilon} \frac{Z^3}{n*^3\mathscr{E}}\right) w_{\text{stat}}. \tag{23}$$

Here

$$a(x) = e^{-x}I_0(x), \tag{24}$$

$I_0(x)$ is a Bessel function of imaginary argument and w_{stat} is the ionization probability in a static field. If the wave polarization is circular, we have $w_{\text{circ}} = w_{\text{stat}}$ and the ionization probability takes in the quasiclassical approximation [see (13a)]

$$w_{\text{circ}}(l=1, m=0) = \frac{3e}{2\pi} \frac{Z^2}{n*^4} \left(\frac{4eZ^3}{n*^4\mathscr{E}}\right)^{2n*-1} \exp\left(-\frac{2Z^3}{3n*^3\mathscr{E}}\right). \tag{25}$$

If the field polarization is not too close to circular, we have[2]

$$w \approx \frac{1}{1-\varepsilon^2} w_{\text{lin}}, \tag{26}$$

where w_{lin} is the ionization probability in a linearly polarized field. We have a ratio

$$w_{\text{circ}}/w_{\text{lin}} = (\pi Z^3/\mathscr{E}n*^3)^{1/2} \gg 1 \tag{27}$$

since the field $\mathscr{E}$ is weak compared with the atomic field.

6. CONCLUSION

It must be noted that the coefficients C_{n*l*} calculated in the quasiclassical approximation ($n* \gg 1$) using Eq. (11) for atoms and ions in the ground state ($n* \approx 1$) are in good

agreement[8] with the numerical calculations[4] of these coefficients (see Table II). This agreement confirms the fact that, for numerical reasons, the quasiclassical approximation is highly accurate up to principal quantum numbers of order unity.[10] This was corroborated many times by numerical calculations (see Ref. 11, §8.4.1).

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