Effect of a magnetic field on the ionization of atoms

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The ionization probability of an atomic s state under the action of static electric and magnetic fields is calculated taking into account the Coulomb interaction between the escaping electron and the atomic core. The structure of the perturbation series for the energy of the level is investigated and the asymptotic behavior of the higher orders of the perturbation theory is found. © *1996 American Institute of Physics.* [S0021-3640(96)00306-4]

1. Problems associated with the ionization of atoms and ions in strong fields have become especially topical after the advent of lasers. A quasiclassical theory of ionization in an electric field $\mathscr{E}$ was developed in the 1960s, and both the case of neutral atoms[1–3] and the case of negative ions[4] of the type H^-, I^-, and so on were studied. The first of these problems is more complicated because the Coulomb interaction between the electron and the atomic core in the tunneling process must be taken into account.

The effect of a magnetic field $\mathscr{H}$ on the level width, i.e., on the ionization probability $w(\mathscr{E},\mathscr{H})$, was studied in Refs. 5–8, but in these works only the case of negative ions was considered. Both the exponential factor[5] in the probability w and the pre-exponential factor[6–8] were calculated (granted, the latter factor was calculated, only in several particular cases).

As is well known, taking into account the Coulomb interaction in problems of this type presents great difficulties and, for example, this has still not been done in the theory of multiphoton ionization of atoms[9–12] (we have in mind analytical formulas and not numerical calculations). For the problem of the ionization of an atomic level under the action of constant and uniform fields $\mathscr{E}$ and $\mathscr{H}$ such a calculation can be performed completely in an analytical form. The basic results are presented below.

2. Let $E=-\kappa^2/2$ be the energy of the atomic level $(l=0)$, and let ϵ and h be the ''reduced'' values of the external fields:

$$\epsilon=\mathscr{E}/\kappa^3\mathscr{E}_a, \quad h=\mathscr{H}/\kappa^2\mathscr{H}_a, \tag{1}$$

where $\mathscr{E}_a=m_e^2e^5/\hbar^4=5.14\cdot 10^9$ V/cm and $\mathscr{H}_a=m_e^2ce^3/\hbar^3=2.35\cdot 10^9$ G are the atomic units for the field intensities (here and below $\hbar=e=m_e=1$); the ratio $\mathscr{H}/\mathscr{E}$ and the angle θ between the fields can be arbitrary. We note that for the ground state $\kappa\approx 1$ ($\kappa=1$, 1.344, and 1.259 for hydrogen, helium, and neon atoms, respectively), but for the

Rydberg states this parameter can also be less than 1 (in the hydrogen atom $\kappa=1/n$ for the ns levels). In this case the values $\epsilon, h\sim 1$ are reached for fields much weaker than atomic fields.

We shall employ the imaginary time method (ITM) to calculate the ionization probability. The subbarrier electron trajectory satisfies the classical equations of motion but with an imaginary ''time.'' The imaginary part of the truncated action function W calculated along the trajectory determines the probability of tunneling, i.e. (in the present case), the ionization probability of the atom:[10,11]

$$w(\mathscr{E},\mathscr{H})\propto \exp\left\{-\frac{2}{\hbar}\,\mathrm{Im}\,W(0,t_0)\right\}, \tag{2}$$

where t_0 is the initial (complex) time of the subbarrier motion and $t=0$ is the time at which the electron emerges from under the barrier. In the case of a δ-function potential (i.e., $Z=0$, where Z is the charge of the atomic fragment) the subbarrier trajectories can be found analytically. We give an expression for the extremal trajectory minimizing Im W and determining the most likely tunneling path of the particle:

$$x=i\frac{\mathscr{E}}{\omega_L^2}\left(\tau-\tau_0\frac{\sinh\tau}{\sinh\tau_0}\right)\sin\theta,\quad y=\frac{\mathscr{E}}{\omega_L^2}(\cosh\tau-\cosh\tau_0)\frac{\tau_0}{\sinh\tau_0}\sin\theta,$$

$$z=\frac{\mathscr{E}}{2\omega_L^2}(\tau_0^2-\tau^2)\cos\theta, \tag{3}$$

where $\tau=i\omega_L t$ $(-\tau_0\leqslant\tau\leqslant 0)$, ω_L is the Larmor frequency, and the initial time of the subbarrier motion is determined from the equation

$$\tau_0^2-\sin^2\theta(\tau_0\coth\tau_0-1)^2=\gamma^2, \tag{4}$$

and $\gamma=\kappa\mathscr{H}/c\mathscr{E}=h/\epsilon$ (the notation is the same as in Ref. 5). Substituting expressions (3) into Eq. (2) gives[a)]

$$w_{short}(\mathscr{E},\mathscr{H})=\omega_0 P(\gamma,\theta)\epsilon\exp\left\{-\frac{2}{3\epsilon}g(\gamma,\theta)\right\},$$

$$g(\gamma,\theta)=\frac{3\tau_0}{2\gamma}\left[1-\frac{1}{\gamma}\left(\frac{\tau_0^2}{\gamma^2}-1\right)^{1/2}\sin\theta-\frac{\tau_0^2}{3\gamma^2}\cos^2\theta\right],\quad \omega_0=\frac{\kappa^2}{2}, \tag{5}$$

where the subscript *short* means that the formula refers to the ionization of the s level, bound by a short-range $(Z=0)$ potential (see Fig. 1), and P is a pre-exponential factor (calculated in Refs. 6–8 for the two cases $\theta=0$ and $\theta=\pi/2$, $\gamma\ll 1$); in the case of a δ-function potential $P(0,\theta)=1$.

We employ the matching procedure[1] to calculate the Coulomb interaction. We introduce a matching point r_1 such that $\kappa^{-1}\ll r_1<r_0\ll b$, where $b\sim\kappa^2/2\mathscr{E}$ is the barrier width and $r_0=\sqrt{Z/\mathscr{E}}$ is the distance at which the Coulomb field of the atomic core (charge Z) is equal in magnitude to the external field. For $r>r_1$ the Coulomb interaction distorts the subbarrier trajectory very little, and for $r<r_1$ the wave function of the elec-

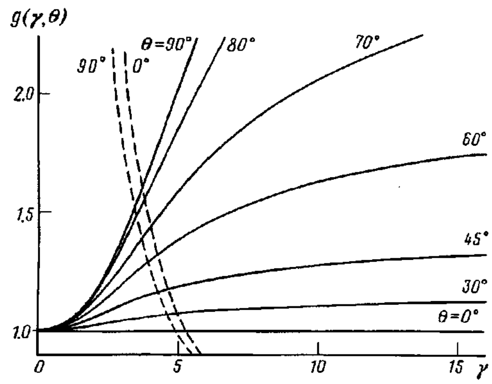

FIG. 1. $g(\gamma,\ \theta)$ as a function of the parameter γ. The values of the angle θ between the electric and magnetic fields are indicated on the curves. The dashed curves correspond to the complex solution $g_c(\gamma,\theta)$.

tron is practically identical to that in the free atom. Therefore the change produced in the action function by the Coulomb potential $\delta V(r)=-Z/r$ can be calculated from a perturbation theory formula on the basis of the IMT:[b)]

$$\delta W=-i\eta\ \ln\ \kappa r_1-\int_{t_1}^{0}\delta V(\mathbf{r}(t))dt, \tag{6}$$

where $\mathbf{r}(t)$ is the subbarrier trajectory, $r_1=r(t_1)$, and $\eta=Z/\kappa$ is the Sommerfeld parameter. From Eqs. (3)–(6) we obtain after simple but tedious calculations

$$w(\mathscr{E},\mathscr{H})=|A_{\kappa s}|^2\left[\frac{2}{\epsilon}C(\gamma,\theta)\right]^{2\eta}w_{short}(\mathscr{E},\mathscr{H}), \tag{7}$$

where $w_{short}(\mathscr{E},\mathscr{H})$ is defined in Eq. (5),

$$C(\gamma,\theta)=\ \exp\left\{\ln\frac{\tau_0}{2\gamma}+\int_0^{\tau_0}d\tau\left[\frac{\gamma}{\xi(\tau)}-\frac{1}{\tau_0-\tau}\right]\right\}, \tag{8}$$

$$\xi(\tau)=\left\{\frac{1}{4}(\tau_0^2-\tau^2)^2\ \cos^2\theta+\tau_0^2\left[\left(\frac{\cosh\ \tau_0-\ \cosh\ \tau}{\sinh\ \tau_0}\right)^2-\left(\frac{\sinh\ \tau}{\sinh\ \tau_0}-\frac{\tau}{\tau_0}\right)^2\right]\sin^2\theta\right\}^{1/2} \tag{8a}$$

and $A_{\kappa s}$ is the asymptotic coefficient of the s-state wave function (in a free atom) at large distances:

$$\psi_0(r)\approx A_{\kappa s}\sqrt{\frac{\kappa^3}{2\pi}}\,e^{-\kappa r}(\kappa r)^{\eta-1},\quad r\gg\kappa^{-1} \tag{9}$$

(in the case of three-dimensional δ-function potential $A=1$, and for the ns levels of the hydrogen atom $|A_{ns}|=2^{n-1/2}/n!$). The Coulomb interaction gives the factor in the square brackets in Eq. (7) but does not change the function $g(\gamma,\theta)$ appearing in the exponential.

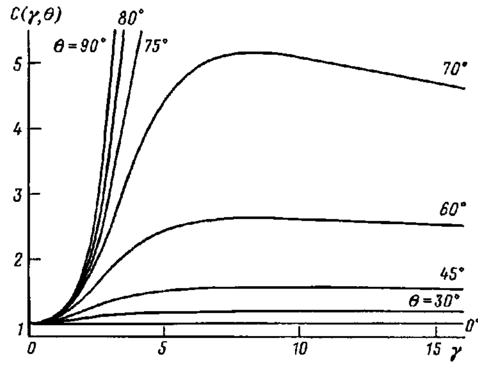

FIG. 2. Coulomb factor $C(\gamma,\ \theta)$ in the ionization probability of the atoms. See Eq. (7).

Since $C=1+\frac{1}{9}\sin^2\theta\gamma^2+\dots$ for $\gamma\ll 1$ (''weak'' magnetic field), expression (7) reduces in this case to the well-known[1–3,10] Coulomb factor $(2\kappa^3/\mathscr{E})^{2\eta}\gg 1$. In the other limiting case ($\gamma\to\infty$) the function $C(\gamma,\theta)$ becomes a constant, equal to $1/\cos\theta$, if $\theta\neq\pi/2$ (see Fig. 2).

A numerical calculation using Eqs. (5) and (8) gives the curves presented in Figs. 1 and 2. A magnetic field decreases the ionization probability, stabilizing the level. This is due to the fact that when the field $\mathscr{H}$ is switched on, the subbarrier trajectory of the electron becomes ''twisted'' and the barrier width b increases. At the same time, the Coulomb interaction greatly increases the ionization probability of a neutral atom as compared with a negative ion (with the same binding energy $\kappa^2/2$ and comparable values of $|A_{\kappa l}|^2$).

We underscore the fact that the expressions (5) and (7) are asymptotically exact for sufficiently weak fields ($\epsilon,\ h\ll 1$), when the ionization probability w is exponentially small. It should be noted that in the case $\theta=\pi/2$ and $\gamma>1$ (crossed electric and magnetic fields, Lorentzian ionization) the probability w, though small, by no means vanishes (in contrast to the assertion made in Ref. 6).

3. By calculating the level width $\Gamma=\hbar w(\mathscr{E},\mathscr{H})$ one can investigate the asymptotic behavior of the higher orders of the perturbation theory. Expanding the energy in the perturbation series

$$E=\sum_{k=0}^{\infty} E_{2k}(\gamma)\mathscr{E}^{2k},\qquad \gamma=h/\epsilon \tag{10}$$

and using the dispersion relations,[13] we obtain from Eqs. (7) and (5) in the limit $k\to\infty$

$$E_{2k}\approx(2k)!a^{2k}k^{\beta}\left(c_0+\frac{c_1}{k}+\dots\right),\qquad a=\frac{3}{2\kappa^3 g(\gamma,\theta)} \tag{11}$$

(here we are studying the ground state, for which the odd orders of the perturbation theory vanish identically).

A numerical analysis of Eq. (4) showed that, together with the real solution $\tau_0(\gamma,\theta)$ found above, the equation also has a complex solution $\tau_c(\gamma,\theta)$, for which $\tau_c = i\pi[1 - i\gamma^{-1}\sin\theta + O(\gamma^{-3})]$ in the limit $\gamma\to\infty$. It corresponds to the function $g_c(\gamma,\theta)$ represented by the dashed curve in Fig. 1. It is obvious from Fig. 1 that there exists a $\gamma_*(\theta)$ such that $|g_c(\gamma,\theta)| < g(\gamma,\theta)$ for $\gamma > \gamma_*(\theta)$. In this case the asymptotic form of the perturbation-theory coefficient is determined not by the saddle point τ_0 but rather by the second solution τ_c (and its complex conjugate):

$$E_{2k} \approx (-1)^k (2k)! \,\mathrm{Re}(c_c a_c^{2k}) k^{\beta_c}, \quad k\to\infty, \tag{11a}$$

where $a_c = 3/2g_c$ and c_c are complex parameters. For $\kappa = 1$ and $\theta = 0$ (ground state of the hydrogen atom, parallel fields) we have

$$g(\gamma,0) \equiv 1, \quad g_c(\gamma,0) = i\frac{3\pi}{2\gamma}\left(1 + \frac{\pi^2}{3\gamma^2}\right),$$

whence

$$\gamma_*(\theta=0) = \pi[(\sqrt{2}+1)^{1/3} - (\sqrt{2}-1)^{1/3}]^{-1} = 5.270\ldots. \tag{12}$$

If $\gamma < \gamma_*$, then the perturbation-theory series is a sign-constant series, since the parameter $a > 0$. If $\gamma > \gamma_*$, however, then the signs of E_{2k} should alternate in accordance with Eq. (11a). We checked this by calculating directly the higher orders of the perturbation theory all the way to $2k = 80$ (for $2k \leqslant 10$ our results agree with Ref. 14). It was shown that the structure of the perturbation series does indeed change between $\gamma = 5$ and 5.5 (including alternation of the signs of E_{2k}). Moreover, for $\gamma < \gamma_*$ the coefficients E_{2k} are still all of the same order of magnitude (since the asymptotic parameter $a = 3/2$ does not depend on γ), and for $\gamma > \gamma_*$ additional (and very rapid) growth of the coefficients starts in accordance with the decrease in $|g_c(\gamma)|$.

In summary, complex subbarrier trajectories can be important for determining the higher orders of the perturbation theory. The expression (7) for the level width $\Gamma = \hbar\omega$ does not change, however, since such trajectories do not satisfy the boundary conditions corresponding to the emergence of the particle from under the barrier and escape of the particle to ∞.

The pre-exponential factor[c)] in Eqs. (5) and (7) was also calculated. This makes it possible to compare the computational results with the experimental data. For lack of space, we defer a discussion of these questions to a more detailed publication.

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[a)]We note that the parameter γ is analogous to the well-known Keldysh parameter in the theory of multiphoton ionization of atoms.[9]

[b)]A check on this procedure is that the arbitrary matching point r_1 should drop out of the final answer, as happens in Eqs. (7) and (8).

[c)]The pre-exponential factor was found to be a sharp function of γ for $\gamma \gg 1$, i.e., in the region of strong magnetic fields, and it must be taken into account when making comparisons with experiments.

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