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QUASICLASSICAL THEORY OF TUNNEL IONIZATION OF AN ATOM BY PARALLEL ELECTRIC AND MAGNETIC FIELDS

The method of quasiclassical localized states is developed for the stationary Schrödinger equation with an arbitrary axially symmetrical electric potential of barrier type and potential of uniform magnetic field directed along the symmetry axis. Using this method in classically forbidden and allowed regions quasiclassical wave-functions for an arbitrary atom in the parallel uniform electric and magnetic fields are constructed. The general analytical expressions for leading term of the asymptotic (at small intensities of electrostatic and magnetic fields) behaviour of ionization rate of an atom in such electromagnetic field are found.
Keywords: tunneling ionization, Stark effect, quasiclassical approximation.

Introduction

The problem of an atom in an electromagnetic field plays the fundamental role in quantum mechanics and atomic physics and has many applications (see, for example, [1-3] and the references therein). Since the twenties [4] of the previous century, properties of an energy spectrum of hydrogen atom and other atoms in external fields of various configurations were intensively studied in the framework of the Schrödinger equation.

In order to construct a consistent theory of tunnel ionization of atoms, one should solve the problem of electron motion in the field created by nucleus and external electromagnetic field. In the case of parallel electric and magnetic fields, the Schrödinger equation does not permit complete separation of variables in any orthogonal system of coordinates. Therefore, the given problem has no exact analytical solution, and numerical methods are still demand significant computational efforts.

The quasiclassical theory of atomic particles decay elaborated in sixties (see for instance [3]) has allowed obtaining useful analytical formulae for ionization rate which are asymptotic in the limit of “weak” fields. Both neutral atom [1, 5, 6, 7] and negative ions like H^-, J^- etc. [5, 8] (the first of these problems is more complicated due to necessity of taking into account the Coulomb interaction between outgoing electron and atomic core) were considered.

Subsequently (see papers [9, 10] and references therein), the imaginary time method (ITM) was elaborated for study ionization of atoms by electric and magnetic fields where classical trajectories used but with imaginary time. Although this method is physically obvious, it is not able to take into account the Coulomb interaction between an atom and outgoing electron consequently. Second limitation of this method is accounting only *s*-states.

Among the relatively new quantum-mechanical methods for studying the processes of interaction of atomic particles with electric and magnetic fields, $1/n$ expansion method (n – principal quantum number), which is quite effective for highly excited (Rydberg) states of atoms and molecules, including the consideration of effects in strong external fields (see, for instance, [11]) occupies a special place.

Additionally, of practical interest is the case when the intensities of the external electric and magnetic fields are much smaller than the intensity of the characteristic atomic fields. If this condition is satisfied the breakup of the atomic particle occurs slowly compared to the characteristic atomic times and the leaking out of the electron takes place primarily in directions close to the direction of the electric field. Therefore, in order to determine the frequency of the passage of the electron through the barrier it is convenient to solve the Schrödinger equation near an axis directed along the electric field and passing through the atomic nucleus. This idea was used for solving the relativistic two-centre problem at large intercentre distances [12], for calculating the leading term (in intensity of electric field F) of the tunnel ionization rate of an atom in a constant uniform electric field in non-relativistic [5, 13] and relativistic [14-17] cases, and first two terms in non-relativistic case [18]. In our papers, such method called "*the method of quasiclassical localized states*" (MQLS) is shown to be free from the limitations of ITM.

In the present paper, our aim is to apply the MQLS to solving the problem of an arbitrary atom in the constant uniform electric and magnetic fields being parallel between themselves.

The paper is organized as follows. In section 2, the method of quasiclassical localized states is developed for the problem of atom in the barrier-type axially symmetrical electrostatic and constant uniform magnetic fields. In section 3, we analytically solve the Schrödinger equation for an atom in the parallel electric and magnetic fields in sub-barrier region. In section 4, we find the wavefunction in classically allowed range, calculate the leading term of tunnel ionization rate, and compare our results with ones of other authors in some limiting cases. In the last section of the paper, we discuss advantages of the elaborated method and further perspectives concerning its extension.

The MQLS in the problem of an atom in the axially symmetrical electrostatic and constant uniform magnetic fields

The Hamiltonian for an electron in the electromagnetic field is ($m_e = |e| = \hbar = 1$)

$$\hat{H} = \frac{1}{2}\left(\hat{\vec{p}} - \frac{1}{c}\vec{A}\right)^2 - \hat{\vec{\mu}}\vec{H} + V, \qquad (1)$$

where $\hat{\vec{p}} = -i\vec{\nabla}$, $\vec{A}$ and V are the vector and electrostatic potentials, respectively, $\hat{\vec{\mu}} = \mu_B \hat{\vec{s}}$ is the spin magnetic moment, $\mu_B = 1/2c$.

Consider the magnetic field directed along the negative z axis:

$$\vec{H} = (0,0,-H), \quad \vec{A} = \left(\frac{H}{2}y, -\frac{H}{2}x, 0\right). \qquad (2)$$

If the potential V is axially symmetrical, the Hamiltonian (1) can be rewritten in the form

$$\hat{H} = \frac{1}{2}\hat{\vec{p}}^2 + \frac{H}{2c}(m_l + 2m_s) + \frac{H^2\rho^2}{8c^2} + V, \qquad (3)$$

where $\rho = \sqrt{x^2 + y^2}$, $m_l = 0, \pm 1, \pm 2, \ldots \pm l$, l and m_l are respectively the orbital quantum number and its projection onto z axis, $m_s = \pm 1/2$ is the spin quantum number.

The spectrum of such quantum mechanical problem is a quasistationary. The energy of an electron is complex

$$E_c = E - i\Gamma/2, \qquad (4)$$

where E gives a position of a quasistationary level, $\Gamma = w/\hbar$ is its width, w is the rate of ionization.

Taking into account all the above mentioned, we obtain the following wave equation:

$$\Delta\Psi + 2\left[E - \tilde{V} - (H/2c)(m_l + 2m_s)\right]\Psi = 0, \qquad (5)$$

where $\tilde{V} = V + \left(H^2/8c^2\right)\rho^2$.

Since the potential $V(z,\rho)$ is axially symmetrical, the Hamiltonian (3) commutes with the operator of projection of total angular momentum of the electron onto a potential symmetry axis z, and equation (5) allows us to separate the azimuthal angle ϕ. For this purpose, we represent the solution of (5) in the form

$$\Psi = \psi(z,\rho)e^{im_l\phi}, \tag{6}$$

where $\psi(z,\rho)$ is a new unknown function.

Having substituted (6) into (5), we obtain the differential equation

$$\Delta\psi + \left[\frac{2}{\hbar^2}\left(E-\tilde{V}\right) - \frac{H}{\hbar c}(m_l+2m_s) - \frac{m^2}{\rho^2}\right]\psi = 0, \tag{7}$$

where the Planck constant $\hbar$ is renewed, and $m = |m_l|$.

We seek a solution of equation (7) in the form of the WKB expansion:

$$\psi = e^{S/\hbar}\sum_{n=0}^{\infty}\hbar^n\varphi^{(n)}. \tag{8}$$

Having substituted (8) into (7) and equated to zero the coefficients of each power of $\hbar$, we arrive at the hierarchy of equations

$$\left(\vec{\nabla}S\right)^2 = q^2, \qquad q^2 = 2\left(\tilde{V}-E\right); \tag{9}$$

$$2\vec{\nabla}S\vec{\nabla}\varphi^{(0)} + \left[\Delta S - \frac{H}{c}\left(m_l+2m_s\right)\right]\varphi^{(0)} = 0; \tag{10}$$

$$2\vec{\nabla}S\vec{\nabla}\varphi^{(n+1)} + \left[\Delta S - \frac{H}{c}\left(m_l+2m_s\right)\right]\varphi^{(n+1)} = = (m^2/\rho^2)\varphi^{(n)} - \Delta\varphi^{(n)}, \tag{11}$$

where $n = 0,1,2,\ldots$. Unfortunately, equations (9)-(11), similarly to the initial equation (5), do not permit exact separation of variables. In order to solve this problem, we use the idea of the localized states consisting in the following.

There are many cases when for solving quantum mechanical problem it is sufficient to find a wavefunction not in the whole configurational space but in the neighbourhood of manifold M of less dimension. States describes by such wavefunctions are called "localized states". In the sub-barrier region, unlike for the classically allowed range, the wavefunction is localized in the vicinity of the most probable tunnelling direction. It is natural to expand all the quantities in inseparable equations including their solutions, in the vicinity of the z axis. This idea was founded by Fock and Leontovich [19] and employed at solving diffraction problems [20] (the boundary-layer method), some quantum mechanical problems [21] (the parabolic equation method), and, finally, in the MQLS [14, 17]. Here we generalize the MQLS on equation (5).

Consider equation (9) and assume that

$$V(z,\rho) = V_0(z) + V_1\rho^2 + V_2(z)\rho^4 + \ldots,$$
$$V_k = \frac{1}{k!}\frac{\partial^k V(z,0)}{\partial\rho^{2k}}. \tag{12}$$

Solution of equation (9) can also be represented in the form of an expansion in powers of coordinate the ρ:

$$S(z,\rho) = s_0(z) + s_1(z)\rho^2 + s_2(z)\rho^4 + \ldots. \tag{13}$$

By inserting (13) into (9) and equating to zero the coefficients of each power of ρ, we obtain

$$(s_0')^2 = q_0^2, \quad q_0 = \sqrt{2(V_0-E)}; \tag{14}$$

$$s_0's_1' + 2s_1^2 = V_1 + \frac{H^2}{8c^2}; \tag{15}$$

$$s_0's_2' + 8s_1s_2 = V_2 - \frac{1}{2}\left(s_1'\right)^2; \tag{16}$$

$$s_0's_k' + 4ks_1s_k = V_k - \frac{1}{2}\sum_{j=1}^{k-1}s_j's_{k-j}' - 2\sum_{j=1}^{k-2}(j+1)(k-j)s_{j+1}s_{k-j}. \tag{17}$$

It is easy to show that in the sub-barrier region the solution of equation (14) is

$$s_0 = -\int q_0 dz + \text{const.} \tag{18}$$

Equation (15) is the nonlinear Riccati differential equation and are not solvable analytically in a general case. By making the substitution

$$s_1 = \frac{q_0(z)}{2}\left(\frac{1}{2}\frac{q_0'(z)}{q_0(z)} - \frac{\sigma'(z)}{\sigma(z)}\right), \qquad (19)$$

one can proceed from (15) to the linear second-order equation

$$\sigma'' + \left[\frac{1}{4}\left(\frac{q'_0}{q_0}\right)^2 - \frac{1}{2}\frac{q''_0}{q_0} - \frac{H^2}{4c^2q_0^2} - \frac{2V_1}{q_0^2}\right]\sigma = 0, \qquad (20)$$

which after substitution $q_0 \to \pm ip_0$ coincides with the equation obtained by Sumetskii within the parabolic equation method [21].

All the equations for s_2, s_3,... are linear, of first order and integrated in quadratures:

$$s_2 = \frac{q_0^2}{\sigma^4}\left\{\int \frac{\sigma^4}{q_0^3}\left[\frac{(s_1')^2}{2} - V_2\right]dz + \text{const}\right\}, \qquad (21)$$

$$s_k = \left(\frac{q_0}{\sigma^2}\right)^k \left\{\int \frac{\sigma^{2k}}{q_0^{k+1}}\left[\frac{1}{2}\sum_{j=1}^{k-1} s'_j s'_{k-j} + \right.\right.$$
$$\left. + 2\sum_{j=1}^{k-2}(j+1)(k-j)s_{j+1}s_{k-j} - V_k\right]dz +$$
$$\left. + \text{const}\right\}. \qquad (22)$$

The solutions of the equations (10), (11) are sought in the form

$$\varphi^{(n)} = \rho^m \sum_{k=0}^{\infty} \varphi_k^{(n)}(z)\rho^{2k}. \qquad (23)$$

By substituting (23) into the corresponding equations and equating to zero the coefficients of each power of ρ, we obtain the system of ordinary first-order linear differential equations solvable in quadratures.

The leading term of the wavefunction in the sub-barrier region is:

$$\Psi = \frac{C}{\sigma}\left(\frac{\rho\sqrt{q_0}}{\sigma}\right)^m \exp\left\{-\int_{z_1}^{z}\left[q_0(x) - \frac{H(m_l + 2m_s)}{2cq_0(x)}\right]dx + \right.$$
$$\left. + h_1(z)\rho^2 + im_l\phi\right\}. \qquad (24)$$

The MQLS in the problem of an atom in the parallel constant uniform electric and magnetic fields

If an arbitrary (not H-like) atom is placed in the constant uniform electric field, then an interaction potential at $r \gg 2Z/\gamma^2$ ($\gamma = \sqrt{-2E}$) is

$$V(z,\rho) \simeq -\frac{Z}{r} - Fz. \qquad (25)$$

The leading term $V_0(z) = -Z/z - Fz$ of expansion of (25) in powers of ρ^2 has a form of barrier (see Figure 1).

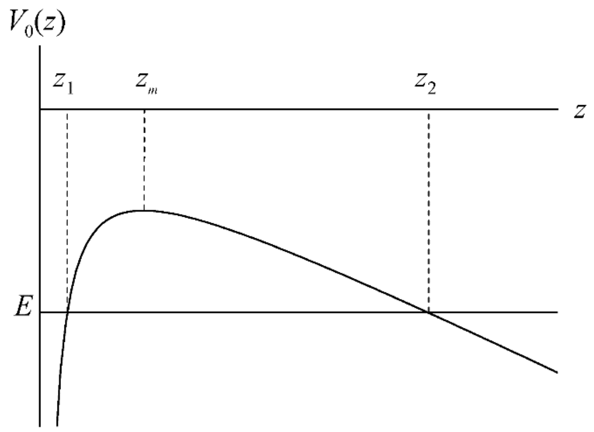

Fig. 1: The "potential" $V_0(z) = V(z,0)$; z_1, z_2 are roots of equation $q_0(z) = 0$, $z_m = \sqrt{Z/F}$ is the maximum point.

If $F \ll \gamma^3$ then the sub-barrier region is quite wide ($z_1 \ll z \ll z_2$). There is the range $z_1 \ll z \ll z_m$ where

$$\Psi \underset{z_1 \ll z \ll z_m}{\simeq} \Psi_0^{(as)}. \qquad (26)$$

Here $\Psi_0^{(as)}$ is the asymptotics (when $z \gg z_1$) of the unperturbed atomic wavefunction.

Using the MQLS elaborated one can find the quasiclassical localized wavefunction Ψ in the sub-barrier region $z_1 \ll z < z_2$ under the boundary condition (26). However, for this purpose we should solve the Riccati equation (15) writing

$$-2q_0 s_1' + 4s_1^2 = \frac{Z}{z^3} + \frac{H^2}{4c^2}. \tag{27}$$

We seek a solution of (27) in the form

$$s_1(z) = s_{10}(z) + s_{11}(z) + \ldots, \tag{28}$$

where $s_{1i+1}(z)/s_{1i}(z) \sim 1/z$. Then in zero approximation

$$-2q_0 s_{10}' + 4s_{10}^2 = \frac{H^2}{4c^2}. \tag{29}$$

The replacement $s_{10}(z) = H/4c + \chi_0(z)$ leads (29) to the Bernoulli equation for $\chi_0(z)$ which is solved analytically. Finally, the solution of (29) under the condition (26) is of the form

$$s_1(z) = -\frac{H}{4c}\coth\left[\frac{H}{2c}\int_{z_1}^{z}\frac{dx}{q_0(x)}\right]. \tag{30}$$

In the sub-barrier region, we obtain the wavefunction

$$\Psi_{II} = \frac{C_{II}\rho^m e^{im_l\phi}}{\sqrt{q_0(z)}\left\{\sinh\left[\frac{H}{2c}\int_{z_1}^{z}\frac{dx}{q_0(x)}\right]\right\}^{m+1}} \times$$
$$\times \exp\left\{-\int_{z_1}^{z}\left[q_0(x) - \frac{H(m_l+2m_s)}{2cq_0(x)}\right]dx + \right.$$
$$\left. + s_1(z)\rho^2\right\}, \tag{31}$$

where normalization constant

$$C_{II} = a\sqrt{\gamma}\left(\frac{H}{2c\gamma}\right)^{m+1}\left(\frac{Z}{2\gamma^2 e}\right)^{Z/\gamma} \times$$
$$\times \frac{(-1)^{\frac{m_l+m}{2}}}{2^m m!}\sqrt{\frac{2l+1}{4\pi}\frac{(l+m)!}{(l-m)!}}, \tag{32}$$

a is the asymptotic coefficient of asymptotic behaviour (at $r \gg 2Z/\gamma^2$) of unperturbed radial wavefunction:

$$R^{as}(r) = ar^{Z/\gamma-1}e^{-\gamma r}. \tag{33}$$

The wavefunction in the classically allowed region. The ionization probability

Continuing Ψ_{II} to classically allowed region $z > z_2$ we find

$$\Psi_{III} = \frac{C_{II}\exp\left\{-J_1 + \frac{H(m_l+2m_s)}{2c}J_2 + \frac{i\pi}{4}\right\}}{\sqrt{p_0(z)}\left\{\sinh\left[\frac{H}{2c}\left(J_2 + i\int_{z_2}^{z}\frac{dx}{p_0(x)}\right)\right]\right\}^{m+1}} \times$$
$$\times \rho^m \exp\left\{-i\int_{z}^{z_2}p_0(x)dx + s_1(z)\rho^2 + im_l\phi\right\}, \tag{34}$$

where

$$p_0(z) = iq_0(z) = \sqrt{\frac{2Z}{z} + 2Fz - \gamma^2}, \tag{35}$$

$$s_1(z) = \frac{H}{4c}\coth\left[\frac{H}{2c}\left(J_2 + i\int_{z_2}^{z}\frac{dx}{p_0(x)}\right)\right], \tag{36}$$

$$J_1 = \int_{z_1}^{z_2}q_0(z)dz, \quad J_2 = \int_{z_1}^{z_2}\frac{dz}{q_0(z)}. \tag{37}$$

Here J_1 is the so-called “barrier integral”.

As it is known [1], the ionization probability (rate) is equal to

$$w = \int_S \vec{j}d\vec{s}, \; \vec{j} = \frac{i}{2}\left(\Psi_{III}\vec{\nabla}\Psi_{III}^* - \Psi_{III}^*\vec{\nabla}\Psi_{III}\right). \tag{38}$$

Here S is a plane perpendicular to axis z and crossing it at $z > z_2$.

Substituting Ψ_{III} into the formula one can obtain the leading term of the ionization rate

$$w = \frac{\gamma a^2(2l+1)(l+m)!}{m!(l-m)!}\left(\frac{Z}{2\gamma^2 e}\right)^{2Z/\gamma} \times$$
$$\times \frac{\exp\left[-2J_1 + \frac{H(m_l+2m_s)}{c}J_2\right]}{\left(\frac{4c\gamma^2}{H}\sinh\frac{HJ_2}{c}\right)^{m+1}}. \tag{39}$$

After asymptotical (when $F \ll \gamma^3$) calculation of the integrals J_1 and J_2 we obtain the following result

$$w = \frac{a^2(2l+1)}{2^{m+1}m!\gamma^m}\frac{(l+m)!}{(l-m)!}\left[\frac{H\gamma/cF}{\sinh(H\gamma/cF)}\right]^{m+1} \times \\ \times\left(\frac{2\gamma^2}{F}\right)^{2Z/\gamma-m-1}\exp\left[-\frac{2\gamma^3}{3F}+\frac{H\gamma(m_l+2m_s)}{cF}\right]. \quad (40)$$

In the case of s-states ($l = m = 0$), after neglecting the electron spin ($m_s = 0$) formula (40) coincides with the result [22] obtained by ITM.

When $H \to 0$ the expression (40) is transformed into the well-known result of Smirnov and Chibisov [5] for ionization rate of an atom in electrostatic field.

In order to find the tunnel ionization rate of singly charged negative ions (i.e. H^-, J^-, etc.), in (40) it is necessary to put $Z = 0$. If the particle is in weakly bound states in the central field with small radius of action r_0 then beyond this radius the asymptotic behaviour of the unperturbed ($F = 0$) radial wavefunction is of the form [1]

$$R_{lm}^{(as)} = ar^{-1}e^{-\gamma r}, \quad (41)$$

where a is determined by means of normalization. When $\gamma r_0 \ll 1$ the behaviour of the wavefunction within the potential well $0 \leqslant r \leqslant r_0$ is inessential because the particle stands basically beyond the well. This gives $a \approx \sqrt{2\gamma}$ and the ionization rate

$$w = \frac{a^2(2l+1)}{m!\gamma^m}\frac{(l+m)!}{(l-m)!}\left[\frac{H}{2c\gamma\sinh(H\gamma/cF)}\right]^{m+1} \times \\ \times\exp\left[-\frac{2\gamma^3}{3F}+\frac{H\gamma(m_l+2m_s)}{cF}\right]. \quad (42)$$

In the case of s-states ($l = m = 0$), after neglecting the electron spin ($m_s = 0$) formula (42) coincides with the result [22] obtained by ITM or (when $H \to 0$) with the known result of Demkov and Drukarev [1, 8].

Conclusions

The method of quasiclassical localized states is elaborated to solve asymptotically the Schrödinger equation with barrier-type potentials which do not permit a complete separation of variables. It is based on physically clear ideas, applicable to arbitrary states (not only *s*-states as ITM) and takes into account the Coulomb interaction between the outgoing electron and atomic core during tunneling correctly. This method has allowed us to obtain for the first time the wavefunctions and general analytical expression for leading term of the asymptotic behaviour of ionization rate of an arbitrary atom (and negative ion) in the parallel electric and magnetic fields whose intensities F and H are much smaller than intensity of intra-atomic field.

Our next tasks are to generalize MQLS on other configurations of electric and magnetic fields (perpendicular, of arbitrary orientations, ununiform, non-stationary, laser fields of various polarizations, etc.) and to obtain higher orders of ionization probability expansion in powers of F and H in both the nonrelativistic and relativistic cases.

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КВАЗИКЛАССИЧЕСКАЯ ТЕОРИЯ ТУННЕЛЬНОЙ ИОНИЗАЦИИ АТОМА ПАРАЛЛЕЛЬНЫМИ ЭЛЕКТРИЧЕСКИМ И МАГНИТНЫМ ПОЛЯМИ

Метод квазиклассических локализованных состояний разработан для стационарного уравнения Шредингера с произвольным осесимметричным электрическим потенциалом барьерного типа и потенциалом однородного магнитного поля, направленного вдоль оси симметрии. С помощью этого метода построены квазиклассические волновые функции в классически запрещенной и разрешенной областях для произвольного атома в параллельных электрическом и магнитном полях. Найдены общие аналитические выражения для главного члена асимптотического (по напряженностях электростатического и магнитного полей) разложения вероятности ионизации атома в таком поле.
Ключевые слова: туннельная ионизация, эффект Штарка, квазиклассическое приближение.

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КВАЗІКЛАСИЧНА ТЕОРІЯ ТУНЕЛЬНОЇ ІОНІЗАЦІЇ АТОМА ПАРАЛЕЛЬНИМИ ЕЛЕКТРИЧНИМ ТА МАГНІТНИМ ПОЛЯМИ

Метод квазікласичних локалізованих станів розроблено для стаціонарного рівняння Шредінгера з довільним аксіально-симетричним електричним потенціалом бар'єрного типу та потенціалом однорідного магнітного поля, напрямленого вздовж осі симетрії. За допомогою цього методу побудовано квазікласичні хвильові функції в класично забороненій та дозволеній областях для довільного атома в паралельних електричному та магнітному полях. Отримано загальний аналітичний вираз для головного члена асимптотичного (за напруженостями електростатичного та магнітного полів) розкладу ймовірності іонізації атома в такому полі.
Ключові слова: тунельна іонізація, ефект Штарка, квазікласичне наближення.

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