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# Method of Quasiclassical Localized States in the Theory of Tunnel Ionization of an Atom by Parallel Electric and Magnetic Fields

**O.K. Reity, V.K. Reity, V.Yu. Lazur**

*Department of Theoretical Physics, Uzhhorod National University, 54 Voloshyna Street, Uzhhorod 88000, Ukraine*

**Abstract**

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 quasiclassical wavefunctions for an arbitrary atom in the parallel uniform electric and magnetic fields are constructed in classically forbidden and allowed regions. The general analytical expressions for leading term of the asymptotic (at small intensities of electrostatic $F$ and magnetic $H$ fields) behaviour of ionization rate of an atom in such electromagnetic field are found. Various limiting cases of the expression obtained is analysed.

## 1 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, 2, 3] and the references therein). Since the twenties (see, for instance, review in [4]), properties of an energy spectrum of hydrogen atom and other atoms in external fields were rather 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 constant uniform electric and magnetic fields. Since the Schrödinger equation with such superpositional potential does not permit complete separation of variables in any orthogonal system of coordinates, 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 electrical 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 (or Dirac) equation near an axis directed along the electric field and passing through the atomic nucleus. This idea was used for solving the relativistic two-center problem at large intercenter 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, 15, 16, 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 limitations of ITM.

In the present paper, our aim is to apply the method of quasiclassical localized states to solving the problem of an atom in the parallel constant uniform electric and magnetic field.

# 2 The MQLS in the problem of an atom in the axially symmetric electrostatic and constant uniform magnetic fields

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

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

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 $z$ axis:

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

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

$$\hat{\mathcal{H}} = \frac{1}{2}\hat{\vec{p}}^2 - \frac{H}{2c}(m_l + 2m_s) + \frac{H^2\rho^2}{4c^2} + V, \tag{3}$$

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 quasistationary. The energy of an electron is complex

$$E_c = E - i\Gamma/2, \tag{4}$$

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

Considering all the above mentioned, we obtain the following wave equation:

$$\Delta\Psi + 2\left(\tilde{E} - V - \frac{H^2\rho^2}{4c^2}\right)\Psi = 0, \tag{5}$$

$$\tilde{E} = E + \frac{H}{2c}(m_l + 2m_s).$$

Since the potential $V$ is axially symmetrical ($V = V(z, \rho)$), 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) permits separation of a variable $\phi$. 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.

By substituting (6) into (5) we obtain the differential equation

$$\Delta\psi + \left[\frac{2}{\hbar^2}\left(\tilde{E} - V\right) - \frac{m^2}{\rho^2} - \frac{H^2\rho^2}{4c^2}\right]\psi = 0, \tag{7}$$

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

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

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

$$2\vec{\nabla}S\vec{\nabla}\varphi^{(0)} + \Delta S\,\varphi^{(0)} = 0; \tag{10}$$

$$2\vec{\nabla}S\vec{\nabla}\varphi^{(n+1)} + \Delta S\,\varphi^{(n+1)} = (m^2/\rho^2)\varphi^{(n)} - \Delta\varphi^{(n)}, \tag{11}$$

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 used 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 wave function not in the whole configurational space but in the neighbourhood of manyfold $M$ of less dimension. States describes by such wave functions are called "localized states". In the under-the-barrier range, unlike for the classically allowed range, the wave function 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 the equation (5).

Consider equation (9) and assume that

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

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

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

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

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

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

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

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

It is easy to show that the solution of equation (14) is

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

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

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

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

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

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

The all equations for $s_2,\ s_3,\ \ldots$ are linear, of first order and integrated in quadratures:

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

$$s_k = \left(\frac{q_0}{\sigma^2}\right)^k\left\{\int \frac{\sigma^{2k}}{q_0^{k+1}}\left[\frac{1}{2}\sum_{j=1}^{k-1} s_j' s_{k-j}' + 2\sum_{j=1}^{k-2}(j+1)(k-j)s_{j+1}s_{k-j} - V_k\right]dz\right.$$
$$\left. + \mathrm{const}\right\}. \tag{22}$$

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

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

By substituting (23) into the corresponding equations and equating to zero the coefficients of each power of $\rho$, we obtain the system of ordinary first-order differential equations which are solvable ($k = 1, 2, 3, \ldots$):

$$\varphi_0^{(0)} = \frac{1}{\sqrt{q_0}}\left(\frac{\sqrt{q_0}}{\sigma}\right)^{m+1}, \tag{24}$$

$$\varphi_k^{(0)} = \frac{1}{\sqrt{q_0}}\left(\frac{\sqrt{q_0}}{\sigma}\right)^{m+2k+1}\left\{\int \frac{1}{\sqrt{q_0}}\left(\frac{\sigma}{\sqrt{q_0}}\right)^{m+2k+1}\sum_{j=1}^{k}\left(s_k'\varphi_{k-j}^{(0)}{}' + \right.\right.$$
$$\left.\left. + \left[2(j+1)(m+2k-j+1)s_{k+1} + s_k''/2\right]\varphi_{k-j}^{(0)}\right)dz + \mathrm{const}\right\}, \tag{25}$$

$$\varphi_0^{(n)} = \frac{1}{\sqrt{q_0}}\left(\frac{\sqrt{q_0}}{\sigma}\right)^{m+1}\left\{\int \frac{1}{\sqrt{q_0}}\left(\frac{\sigma}{\sqrt{q_0}}\right)^{m+1}\left[2(m+1)\varphi_1^{(n-1)}\right.\right.$$
$$\left.\left. + \varphi_0^{(n-1)}{}''/2\right]dz + \mathrm{const}\right\}, \tag{26}$$

$$\varphi_k^{(n)} = \frac{1}{\sqrt{q_0}}\left(\frac{\sqrt{q_0}}{\sigma}\right)^{m+2k+1}\left\{\int \frac{1}{\sqrt{q_0}}\left(\frac{\sigma}{\sqrt{q_0}}\right)^{m+2k+1}\left[\sum_{j=1}^{k}\left(s_k'\varphi_{k-j}^{(n)}{}' + \right.\right.\right.$$
$$\left. + \left[2(j+1)(m+2k-j+1)s_{k+1} + s_k''/2\right]\varphi_{k-j}^{(n-1)}\right) +$$
$$\left.\left. + 2(k+1)(m+k+1)\varphi_{k+1}^{(n-1)} + \varphi_k^{(n-1)}{}''/2\right]dz + \mathrm{const}\right\}. \tag{27}$$

The leading term of the wave function in the under-the-barrier range is:

$$\Psi = \frac{C}{\sigma}\left(\frac{\rho\sqrt{q_0}}{\sigma}\right)^m \exp\left\{-\left[\int\limits_{z_1}^{z} q_0(z')dz' + h_1(z)\rho^2\right] + im_l\phi\right\}. \tag{28}$$

# 3 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 $r \gg 2Z/\gamma^2$ ($\gamma = \sqrt{-2\tilde{E}}$) is

$$V(z,\rho) \sim -\frac{Z}{r} - Fz. \tag{29}$$

If $F \ll \gamma^3$, $H/c \ll \gamma^2$ the energy spectrum $E$ of an atom can be found by means of the first-order perturbation theory:

$$E = E_0 - \frac{H}{2c}(m_l + 2m_s), \tag{30}$$

where $E_0$ is the energy of unperturbed atom. Then $\tilde{E} = E_0$.

The leading term $V_0(z) = -Z/z - Fz$ of expansion of (29) in powers of $\rho^2$ has a form of barrier (see fig. 1).

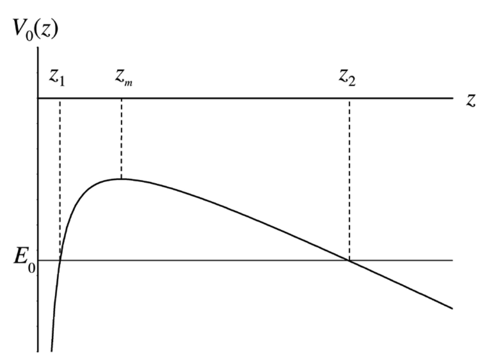


Figure 1: The "potential" $V_0(z) = V(z,0)$; $z_1$, $z_2$ are roots of equation $q_0(z) = 0$, $z_m = \sqrt{Z/F}$ is the maximum point.

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

$$\Psi \underset{z_1 \ll z \ll z_m}{\simeq} \Psi_0^{(as)}. \tag{31}$$

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

By means of the elaborated MQLS one can find the quasiclassical localized wave function $\Psi$ in the under-the-barrier range $z_1 \ll z < z_2$ under the boundary condition (31). However, for this purpose we should solve the Riccati equation (15) writing

$$2q_0 s_1' + 4s_1^2 = \frac{Z}{z^3} + \frac{H^2}{4c^2}. \tag{32}$$

We seek a solution of (32) in the form

$$s_1(z) = s_{10}(z) + s_{11}(z) + \ldots, \tag{33}$$

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

$$2q_0 s_{10}' + 4s_{10}^2 = \frac{H^2}{4c^2}. \tag{34}$$

The replacement $s_{10}(z) = H/4c + \chi_0(z)$ leads (34) to the Bernoulli equation for $\chi_0(z)$ which is solved analytically and under the condition (31) we obtain

$$s_1(z) \approx \frac{H}{4c} \coth \frac{H[\gamma - q_0(z)]}{2cF}. \tag{35}$$

In the under-the-barrier range we obtain the wave function

$$\Psi_{II} = \frac{C_{II} \rho^m e^{i m_l \phi}}{\sqrt{q_0(z)} \left\{ \sinh \frac{H[\gamma - q_0(z)]}{2cF} \right\}^{m+1}} \exp\left\{ -\int_{z_1}^{z} q_0(z') dz' - s_1(z) \rho^2 \right\}, \tag{36}$$

where normalization constant

$$C_{II} = a\sqrt{\gamma} \left( \frac{H}{2c\gamma} \right)^{m+1} \left( \frac{Z}{2\gamma^2 e} \right)^{Z/\gamma} \frac{(-1)^{\frac{m_l+m}{2}}}{2^m m!} \sqrt{\frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!}}, \tag{37}$$

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

$$R^{as}(r) = a r^{Z/\gamma - 1} e^{-\gamma r}. \tag{38}$$

# 4 The wave function in the classically allowed region. The ionization probability

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

$$\Psi_{III} = \frac{C_{II} e^{-J} \rho^m e^{i m_l \phi + i\pi/4}}{\sqrt{p_0(z)} \left\{ \sinh \frac{H[\gamma + i p_0(z)]}{2cF} \right\}^{m+1}} \exp\left\{ -i \int_{z}^{z_2} p_0(z') dz' - \bar{s}_1(z) \rho^2 \right\}, \tag{39}$$

where

$$p_0(z) = iq_0(z) = \sqrt{\frac{2Z}{z} + 2Fz - \gamma^2}, \quad \bar{s}_1(z) = \frac{H}{4c} \coth \frac{H[\gamma + ip_0(z)]}{2cF}, \tag{40}$$

$$J = -\int_{z_1}^{z_2} q_0(z) dz \tag{41}$$

is the so-called "barrier integral".

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

$$w = \int_S \vec{j} d\vec{s}, \quad \vec{j} = \frac{i}{2} \left( \Psi_{III} \vec{\nabla} \Psi^*_{III} - \Psi^*_{III} \vec{\nabla} \Psi_{III} \right). \tag{42}$$

Here $S$ is the plane perpendicular to axis z and located at $z > z_2$.

Substituting $\Psi_{III}$ into the formula one can obtain the leading term of the ionization rate

$$w = \frac{\gamma a^2 (2l+1)(l+m)!}{m!(l-m)!} \left( \frac{Z}{2\gamma^2 e} \right)^{2Z/\gamma} \left( \frac{H}{4c\gamma^2 \sinh \frac{H\gamma}{cF}} \right)^{m+1} e^{-2J}. \tag{43}$$

After asymptotical (at $F \ll \gamma^4/16Z$) calculation of the barrier integral $J$ we obtain the following result

$$w = \frac{a^2(2l+1)}{2^{m+1} m! \gamma^m} \frac{(l+m)!}{(l-m)!} \left[ \frac{H\gamma/cF}{\sinh(H\gamma/cF)} \right]^{m+1} \left( \frac{2\gamma^2}{F} \right)^{2Z/\gamma - m - 1} e^{-2\gamma^3/3F}. \tag{44}$$

For $s$-states ($l = m = 0$) formula (44) coincides with the result [22] obtained by ITM.

When $H \to 0$ the expression (44) is transformed into well-known result of Smirnov and Chibisov [5] for ionization rate of an atom in electrostatic field.

For finding the tunnel ionization rate of singly charged negative ions (i.e. $H^-$, $J^-$ etc.), in (44) 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]

$$R^{(as)}_{lm} = a r^{-1} e^{-\gamma r}, \tag{45}$$

where $a$ is determined by means of normalization. When $r_0 \ll 1$ 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

$$w = \frac{a^2(2l+1)}{m! \gamma^m} \frac{(l+m)!}{(l-m)!} \left[ \frac{H}{2c\gamma \sinh(H\gamma/cF)} \right]^{m+1} e^{-2\gamma^3/3F}. \tag{46}$$

. For $s$-states the formula (46) coincides with the result [22] obtained by ITM or with the known result of Demkov and Drukarev [1, 8] when $H \to 0$.

## Conclusion

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 expressions for leading term of the asymptotic behaviour of ionization rate of an arbitrary atom (and negative ion) in the parallel constant uniform 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 fields, fields of arbitrary orientations, ununiform fields, non-stationary fields, strong laser field of various polarizations) and to obtain higher orders of ionization probability expansion in powers of $F$ and $H$ in both the non-relativistic and relativistic cases.

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