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Relativistic Theory of Tunnel Ionization of an Atom in Parallel Electric and Magnetic Fields

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Abstract

The method of quasiclassical localized states is developed for the stationary Dirac 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 relativistic 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 (in intensities of electrostatic F and magnetic H fields) behaviour of ionization rate of an atom and negative ion in such electromagnetic field are found. Various limiting cases of the expression obtained are analyzed.

1 Introduction

The problem of an atom in electric and magnetic fields has fundamental meaning for a quantum mechanics and the atomic physics and has many applications (see, for example, [1, 2, 3] and the references therein). Since the twenties [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.

At the same time the interior logic of development of study of atomic systems with a high degree of ionization (the multiply charged ions) dictates, obviously, formulation of various qualitatively new problems, similar to those which were previously solved only for neutral or weakly ionized atoms. Essentially relativistic character of motion of electrons in the fields created by multiply charged ions (the characteristic velocity of the electron in H-like ions with nuclear charge Z is $\sim \alpha Z c$; α is the fine structure constant, c is the velocity of light) is the main feature of such ions that distinguishes them from neutral atoms. Thus, the consistent theory of tunnel ionization of such systems should be relativistic because relativistic effects are not small corrections, and fundamentally determine the orders of spectral characteristics.

In order to construct such a theory one should have the solution of the relativistic problem of motion of an electron in the field of nucleus and in the constant

uniform electric and magnetic fields. Since the Dirac 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 rather onerous.

The relativistic calculations of the linear Stark effect are carried out by means of perturbation theory [5, 6], and quadratic Stark effect was treated by means of RCGF (Relativistic Coulomb Green Function) method in the form of the expansion in powers of $Z\alpha$ [7]. However, the most of papers were basically devoted to position of quasistationary level, and there are only rare cases of calculation of width Γ in the relativistic case. In our previous paper [8] within quasiclassical approximation the hybrid version of spherically symmetrical model of the Stark effect, taking into account the Lorentz structure of interaction potential, was studied. Rather recently the probability of ionization of s-level, whose binding energy can be of order of the rest energy, in electric and magnetic fields has been calculated by means of generalization of the imaginary time method [9] and of so-called ADK-theory [10]. However, in the general case, widths of quasistationary states are not found until now.

Due to such situation in the theory and intensive experimental researches during last years, asymptotic methods of calculation of ionization probability, which are based on clear physical ideas about below-barrier electron transition, are gaining in importance. From this point of view it is worthwhile to use the WKB method (or quasiclassical approximation) which enables to find the approximative analytical solutions of the relativistic problem and to express required ionization probability in terms of quantum penetrability of the potential barrier which separates domains of discrete and continuous spectra. As is known, this method has rather high accuracy even for small quantum numbers. For the first time the three-dimensional version of WKB approximation for the Dirac equation with axially symmetrical potential was elaborated and used for the relativistic two-center problem in [11]. In the present work, we apply this method to the problem of tunnel ionization of an arbitrary multiply charged ions in parallel electric and magnetic fields.

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, 12, 13, 14] and negative ions like H^-, J^- etc. [12, 15] (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 [16, 17, 18] 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, [19]) 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 [11], 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 [20] and relativistic [21, 22, 23, 24] cases, and first two terms in non-relativistic case [25]. In [26], we solved such problem for parallel electric and magnetic field for the Schrödinger equation. In our last 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.

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 symmetric electrostatic and constant uniform magnetic fields. In section 3, we analytically solve the Dirac equation for an atom in the parallel constant uniform electric and magnetic fields in under-the-barrier range. 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 evolution.

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

For the bispinor Ψ the stationary Dirac equation is ($m_e = |e| = \hbar = 1$)

$$\begin{array}{ll} \sigma\,(c\mathbf{p} - \mathbf{A})\,\xi = (E - V + c^2)\eta, & \Psi = \left(\begin{array}{c} \xi \\ \eta \end{array} \right), \\ \sigma\,(c\mathbf{p} - \mathbf{A})\,\eta = (E - V - c^2)\xi, & \end{array} \qquad (1)$$

where $\mathbf{p} = -i\nabla$ is the momentum operator, c is the velocity of light, σ are the Pauli matrices, E is the electron energy including c^2, $\mathbf{A}$ and V are the vector and electrostatic potentials, respectively.

Consider the magnetic field directed along z axis:

$$\mathbf{H} = (0, 0, H), \quad \mathbf{A} = (-Hy/2, Hx/2, 0). \qquad (2)$$

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

$$E_c = E - i\Gamma/2, \tag{3}$$

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

By inserting the first equation of (1) into the second one and using the substitution

$$\xi = (W^+)^{1/2}\Phi, \qquad W^\pm = E - V \pm c^2, \tag{4}$$

we arrive at the matrix equation

$$\Delta\Phi + \hat{k}^2\Phi = 0, \; \hat{k}^2 = \frac{1}{\hbar^2 c^2}\left[(E-V)^2 - c^4 - \frac{H^2\rho^2}{4}\right] - \frac{\Delta V}{2W^+} -$$

$$- \frac{3}{4}\left(\frac{\nabla V}{W^+}\right)^2 + \frac{i}{W^+}\sigma\left[\nabla V, \nabla\right] - \frac{iH}{\hbar c}\frac{\partial}{\partial\phi} - \frac{H}{\hbar c}\Sigma, \tag{5}$$

where

$$\Sigma = \begin{pmatrix} -\dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial\rho} - 1 & e^{-i\phi}\dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial z} \\ e^{i\phi}\dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial z} & \dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial\rho} + 1 \end{pmatrix}.$$

Here we have restored the reduced Planck constant $\hbar$. Since the potential V is axially symmetrical, the Hamiltonian 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 φ. For this purpose we represent the solution of (5) in the form

$$\Phi = \begin{pmatrix} \psi_1(z,\rho)\exp\left[i\left(m - 1/2\right)\phi\right] \\ \psi_2(z,\rho)\exp\left[i\left(m + 1/2\right)\phi\right] \end{pmatrix}, \tag{6}$$

where $\psi_{1,2}$ are new unknown functions, m is the projection of the total angular momentum of the electron onto a potential symmetry axis z.

By defining the spinor

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

and by substituting (6) into (5), we obtain the matrix differential equation for ψ

$$(\Delta + \hat{\partial})\psi = (\hbar^{-2}q^2 + \hbar^{-1}\gamma_1 + \gamma_2)\psi, \tag{7}$$

where

$$q = \frac{1}{c}\sqrt{c^4 - (E-V)^2 + \frac{H^2\rho^2}{4}}, \quad \hat{\partial} = \frac{1}{W^+}\left(\frac{\partial V}{\partial\rho}\frac{\partial}{\partial z} - \frac{\partial V}{\partial z}\frac{\partial}{\partial\rho}\right)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

$$\gamma_1 = \begin{pmatrix} -m - 1/2 - \dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial\rho} & \dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial z} \\ \dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial z} & -m + 1/2 + \dfrac{\rho}{2W^+}\dfrac{\partial V}{\partial\rho} \end{pmatrix},$$

$$\gamma_2 = \begin{pmatrix} a_{m-1/2} & b_{m+1/2} \\ b_{m-1/2} & a_{-m-1/2} \end{pmatrix},$$

$$a_\mu(z,\rho) = \frac{\mu^2}{\rho^2} + \frac{1}{W^+} \left[\frac{\mu}{\rho} \frac{\partial V}{\partial \rho} + \frac{\Delta V}{2} + \frac{3}{4} \frac{(\nabla V)^2}{W^+} \right], \quad b_\mu(z,\rho) = -\frac{\mu}{\rho W^+} \frac{\partial V}{\partial z}.$$

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

$$\psi = \varphi \exp(\hbar^{-1} S), \quad \varphi = \sum_{n=0}^{\infty} \hbar^n \varphi^{(n)}. \tag{8}$$

Here $\varphi^{(n)}$ is a bispinor (the upper component corresponds to the function ψ_1, the lower to ψ_2). Having substituted ψ, determined by (8), into (7) and equated to zero the coefficients of each power of $\hbar$, we arrive at the hierarchy of equations

$$(\nabla S)^2 - q^2 = 0, \tag{9}$$

$$2\nabla S \cdot \nabla \varphi^{(0)} + \left(\Delta S + \hat{\partial} S - \gamma_1 \right) \varphi^{(0)} = 0, \tag{10}$$

$$2\nabla \cdot S \nabla \varphi^{(n+1)} + \left(\Delta S + \hat{\partial} S - \gamma_1 \right) \varphi^{(n+1)} = -\Delta \varphi^{(n)} - \hat{\partial} \varphi^{(n)} + \gamma_2 \varphi^{(n)}, \tag{11}$$

where $n = 0, 1, 2, \ldots$ Unfortunately, equations (9)–(11), similarly to the initial equation (1), 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 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 [27] and employed at solving diffraction problems [28] (the boundary-layer method), some quantum mechanical problems [29] (the parabolic equation method), and, finally, in the MQLS [24, 26]. Here we generalize the MQLS on the equation (1).

Consider equation (9) and assume that

$$q^2(z,\rho) = q_0^2(z) + \sum_{k=1}^{\infty} Q_k(z)\rho^{2k}, \quad q_0^2(z) = q^2(z,0), \quad Q_k = \frac{1}{(2k)!} \frac{\partial^{2k} q^2(z,0)}{\partial \rho^{2k}}. \tag{12}$$

According to the above speculations, the solution of equation (9) can also be represented in the form of an expansion in powers of the coordinate ρ:

$$S(z,\rho) = \sum_{n=0}^{\infty} s_n(z)\rho^{2n}. \tag{13}$$

By inserting (13) into (9) and equating to zero the coefficients of each power of ρ, we obtain the recurrent system of first-order differential equations

$$(s_0')^2 - q_0^2 = 0, \tag{14}$$

$$2s_0's_1' + 4s_1^2 = Q_1 + \frac{H^2}{4c^2}, \tag{15}$$

$$2s_0's_2' + 16s_1s_2 = Q_2 - (s_1')^2, \ldots, \tag{16}$$

$$2s_0's_n' + 16s_1s_n = Q_n - \sum_{j=1}^{n-1} s_j's_{n-j}' - 4\sum_{j=1}^{n-2}(j+1)(n-j)s_{j+1}s_{n-j}, \tag{17}$$

from which the values s_n $(n = 0, 1, 2, \ldots)$ are successively determined. Here the prime means the derivative with respect to z. Note that if in the expansion (13) the coefficients of negative and odd powers of ρ are taken into account, after substitution of (13) into (9) they will be equal to zero. The similar situation will arise later for the functions $\varphi^{(n)}$.

Consider the first two equations of the given system. It is easy to show that the solution of equation (14) is

$$s_0 = \pm \int q_0 dz + C_0, \quad C_0 = const. \tag{18}$$

In the below-barrier range, the wave function should decrease exponentially with increasing z, and in (18), the negative sign should be chosen.

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

$$\sigma'' + \left[\frac{1}{4}\left(\frac{q_0'}{q_0}\right)^2 - \frac{1}{2}\frac{q_0''}{q_0} - \frac{Q_1}{q_0^2}\right]\sigma = 0. \tag{20}$$

In the nonrelativistic limit $c \to \infty$, equation (20) is transformed into the similar equation, obtained by Sumetsky [29] by solving the Schrödinger equation with an axially symmetrical potential by the parabolic equation method.

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

$$\varphi^{(n)}(z, \rho) = \begin{pmatrix} \rho^{|m-1/2|} \sum\limits_{k=0}^{\infty} \varphi_{1k}^{(n)}(z)\rho^{2k} \\ \rho^{|m+1/2|} \sum\limits_{k=0}^{\infty} \varphi_{2k}^{(n)}(z)\rho^{2k} \end{pmatrix}. \tag{21}$$

By substituting (21) into the corresponding equations and equating to zero the coefficients of each power of ρ in the each of the two components, we obtain the system of ordinary first-order differential equations being solvable. Since in the

exponent we restricted ourselves to the first two terms s_0 and s_1 in the expansion of s in ρ^2, in order to avoid exceeding the accuracy of the approximation chosen by us in the pre-exponent, it is sufficient to take into account only the leading term in $\varphi^{(0)}$, and to neglect $\varphi^{(1)}$.

Thus, for $m > 0$ we obtain:

$$\varphi_{10}^{(0)} = \frac{C_1^{(+)}}{\sqrt{q_0}} \left[\frac{\sqrt{q_0}}{\sigma} \exp\left(\frac{H}{2c} \int \frac{dz}{q_0} \right) \right]^{|m|+1/2},$$

$$\varphi_{20}^{(0)} = \frac{C_1^{(+)}}{\sqrt{q_0}} \left[\frac{\sqrt{q_0}}{\sigma} \exp\left(\frac{H}{2c} \int \frac{dz}{q_0} \right) \right]^{|m|+3/2} \left[\int \frac{\sigma A_1(z)}{q_0 \sqrt{q_0}} dz + C_2^{(+)} \right], \qquad (22)$$

where

$$A_1(z) = \frac{1}{W_0^+} \left[\left(s_1 - \frac{H}{4c} \right) V_0' - q_0 V_1 \right], \qquad C_{1,2}^{(+)} = \text{const},$$

$$V_0(z) = V(z, 0), \quad V_1(z) = \frac{1}{2} \frac{\partial^2 V(z, 0)}{\partial \rho^2}, \quad W_0^\pm = W^\pm(z, 0).$$

In the case $m < 0$, the functions $\varphi_{10}^{(0)}(z)$ and $\varphi_{20}^{(0)}(z)$ can be obtained from (22) by simultaneous replacements: $\varphi_{10}^{(0)} \to \varphi_{20}^{(0)}$, $\varphi_{20}^{(0)} \to -\varphi_{10}^{(0)}$, $C_{1,2}^{(+)} \to C_{1,2}^{(-)}$.

Note all equations for next corrections (s_2, s_3, ... in the exponent as well as $\varphi_{1i}^{(j)}$ and $\varphi_{2i}^{(j)}$ ($i, j = 1, 2, \dots$) in pre-exponent) are linear, of first order and integrated in quadratures. Moreover, if it is necessary to find the first l terms of the expansion (13), then in each function $\varphi^{(n)}$ of (22) one has to take into account the first $l - n - 1$ ($n = 0, 1, \dots, l - 2$) terms of the expansion in ρ.

The lower component η of Ψ is obtained from the upper one ξ by the operation

$$\xi \xrightarrow[W^+ \to W^-]{} \eta. \qquad (23)$$

In the next section, we will consider a specific potential consisting of a Coulomb term and the potential of a constant homogeneous electric field.

Thus we have obtained the quasiclassically localized solutions Ψ of the Dirac equation (1) with arbitrary axial-symmetric potential of a barrier type within the constants C_0, $C_k^\pm$ ($k = 2, 3$). In order to determine them, one should take a certain potential and normalize the wave function. In the next section, we shall consider the potential V consisting of the Coulomb interaction and of the constant uniform electric field being parallel to the magnetic one.

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

If an arbitrary (including multi-electron) atom is placed in the constant uniform electric field, then an interaction potential at $r \gg 2Z/\lambda^2$ is

$$V(z, \rho) \sim -\frac{Z}{r} - Fz, \qquad (24)$$

where Z is the nuclear charge, $F = \text{const}$ is the electric field intensity, $\lambda = c\sqrt{1 - \varepsilon^2}$, $\varepsilon = E/c^2$.

Similarly to the WKB method for the Dirac equation with spherically symmetrical potential [8], we represent the quantity $q_0(z)$ as $q_0 = \sqrt{2\left(U_{\text{eff}} - E_{\text{eff}}\right)}$, where according to the expressions (7), (12) $E_{\text{eff}} = -\lambda^2/2$ is the effective energy and effective potential is equal to

$$U_{\text{eff}}(z, \varepsilon) = \varepsilon V_0 - V_0^2/2c^2, \quad V_0 = -Z/z - Fz. \tag{25}$$

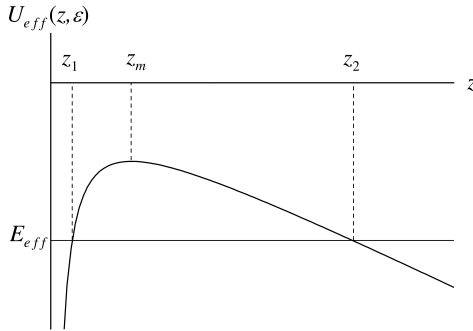The form of the effective potential $U_{\text{eff}}(z, \varepsilon)$ is shown in Fig. 1.

Figure 1: The dependence of the effective potential $U_{\text{eff}}(z, \varepsilon)$ on coordinate z; z_1, z_2 are roots of equation $q_0(z) = 0$, $z_m = \sqrt{Z/F}$ is the maximum point.

If $F \ll \lambda^4/4Z$ 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

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

$$\Psi_0(\mathbf{r}) = \begin{pmatrix} f(r)\,\Omega_{jlm}(\mathbf{n}) \\ ig(r)\,\Omega_{jl'm}(\mathbf{n}) \end{pmatrix}, \quad l = j \pm 1/2, \quad l' = 2j - l, \quad \mathbf{n} = \mathbf{r}/r, \tag{27}$$

$$\left. \begin{matrix} f(r) \\ g(r) \end{matrix} \right\} \simeq \pm\sqrt{1 \pm \varepsilon}\, A r^{\varepsilon Z/\lambda - 1} e^{-\lambda r}. \tag{28}$$

Here j and l are the total and orbital moments, respectively, A is the asymptotic coefficient.

We can find the quasiclassical localized wave function Ψ in the range $z_1 \ll z < z_2$ under the boundary condition (26) by means of the elaborated MQLS. However, for this purpose we should solve the Riccati equation (15) writing

$$2q_0 s_1' + 4s_1^2 = \frac{Z}{c^2 z^3}\left[E - V_0(z)\right] + \frac{H^2}{4c^2}. \tag{29}$$

We seek a solution of (29) in the form

$$s_1(z) = s_{10}(z) + s_{11}(z) + \cdots, \tag{30}$$

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

$$2q_0 s'_{10} + 4s^2_{10} = \frac{H^2}{4c^2}. \tag{31}$$

The replacement $s_{10}(z) = H/4c + \chi_0(z)$ leads (31) to the Bernoulli equation for $\chi_0(z)$ which is solved analytically and under the condition (26) we obtain

$$s_1(z) = -\frac{H}{4c} \coth\left(\frac{H}{2c} \int_{z_1}^{z} \frac{dx}{q_0(x)} \right). \tag{32}$$

Finally, in the under-the-barrier range we obtain the wave function

$$\Psi^{(\pm)} = \frac{C^{(\pm)}}{\sigma} \left(\frac{\sqrt{q_0}\rho}{\sigma} \right)^{|m|-1/2} \begin{pmatrix} \sqrt{c^2 + E_0 - V_0}\,\delta_{m,|m|} \\ \sqrt{c^2 + E_0 - V_0}\,\delta_{-m,|m|} \\ i\sqrt{c^2 - E_0 + V_0}\,\delta_{m,|m|} \\ -i\sqrt{c^2 - E_0 + V_0}\,\delta_{-m,|m|} \end{pmatrix} \times$$

$$\times \exp\left\{ -\int_{z_1}^{z} \left[q_0(x) + \frac{H(|m|+1/2)}{2cq_0(x)} \right] dx + s_1(z)\rho^2 + i(m \mp 1/2)\phi \right\}, \tag{33}$$

where the upper (lower) sign corresponds to $m > 0$ ($m < 0$), δ_{ij} is the Kronecker symbol,

$$q_0 = \frac{1}{c}\sqrt{c^4 - (E - V_0)^2}, \qquad \sigma = \frac{c\lambda}{H}\sqrt{q_0}\left[1 - \frac{H}{c}\exp\left(\int_{z_1}^{z} \frac{dz}{q_0} \right) \right],$$

$$C^{(\pm)} = C_1^{(\pm)}\sqrt{\lambda}\left(\frac{Z}{2\lambda^2 e} \right)^{\varepsilon Z/\lambda} e^{-Z\alpha\arccos\varepsilon}, \quad k = (-1)^{j-l+1/2}(j+1/2),$$

$$C_1^{(+)} = \frac{A\sqrt{\lambda}}{c}\frac{(-1)^{|m|+1/2}\mathrm{sgn}k}{2^{|m|-1/2}(|m|-1/2)!}\sqrt{\frac{(j+|m|)!}{4\pi(j-|m|)!}}, \; C_1^{(-)} = C_1^{(+)}(-1)^{|m|+1/2}\mathrm{sgn}k.$$

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

Let us continue $\Psi^{(\pm)}$ to classically allowed region $z > z_2$. Using for this the so-called Zwaan method [1] we obtain

$$\Psi^{(\pm)} = \frac{B^{(\pm)}}{\sigma} \left(\frac{\sqrt{p_0}\rho}{\tilde{\sigma}} \right)^{|m|-1/2} \begin{pmatrix} \sqrt{E - V_0 + c^2}\delta_{m,|m|} \\ \sqrt{E - V_0 + c^2}\delta_{-m,|m|} \\ \sqrt{E - V_0 - c^2}\delta_{m,|m|} \\ -\sqrt{E - V_0 - c^2}\delta_{-m,|m|} \end{pmatrix} \times$$

$$\times \exp\left\{ i\int_{z_2}^{z} \left[p_0(x) - \frac{H(|m|+1/2)}{2cp_0(x)} \right] dx + s_1(z)\rho^2 + i(m \mp 1/2)\phi \right\}, \tag{34}$$

where

$$B^{(\pm)} = C^{(\pm)} \exp\left[-J_1 - \frac{H(|m|+1/2)}{c}J_2 + \frac{i\pi}{4}\right],$$

$$\tilde{\sigma} = \frac{c\lambda}{H}\sqrt{q_0}\left[1 - \exp\left(-\frac{H}{c}J_2 - \frac{iH}{c}\int\limits_{z_2}^{z}\frac{dz}{p_0}\right)\right], \tilde{s_1} = \frac{ip_0}{2}\left(\frac{\tilde{\sigma}'}{\tilde{\sigma}} - \frac{1}{2}\frac{p_0'}{p_0}\right).$$

$$p_0(z) = iq_0(z) = c^{-1}\sqrt{(E-V_0)^2 - c^4}, \quad J_1 = \int\limits_{z_1}^{z_2} q_0(z)dz, \quad J_2 = \int\limits_{z_1}^{z_2}\frac{dz}{q_0(z)}.$$

The ionization rate is equal to the total probability flux through the plane S which is perpendicular to z-axis and located in the domain $z > z_2$:

$$w = c\int\limits_{S}\Psi^{+}\alpha\Psi d\mathbf{S} = c\int\limits_{0}^{2\pi}d\phi\int\limits_{0}^{\infty}(\Psi^{+}\alpha_z\Psi)\rho d\rho, \tag{35}$$

where $\alpha = (\alpha_x, \alpha_y, \alpha_z)$ is the Dirac α matrices vector.

Substituting (34) into the formula (35) one can obtain the leading term of the ionization rate

$$w = \frac{2\lambda|A|^2}{(|m|-1/2)!}\frac{(j+|m|)!}{(j-|m|)!}\left(\frac{Z}{2\lambda^2 e}\right)^{\frac{2\varepsilon Z}{\lambda}}\frac{e^{-2J_1-2Z\alpha\arccos\varepsilon}}{\left[\frac{2c\lambda^2}{H}\left(1 - \exp\left[-\frac{2H}{c}J_2\right]\right)\right]^{|m|+1/2}}. \tag{36}$$

After asymptotical (at $F \ll \lambda^4/16Z$) calculation of the barrier integrals J_1 and J_2 we obtain the following result

$$w = \frac{2\lambda|A|^2}{(|m|-1/2)!}\frac{(j+|m|)!}{(j-|m|)!}\frac{e^{2Z\alpha\arccos\varepsilon}}{\left[\frac{c\lambda^2}{H}\left(1 - e^{-2\frac{H}{F}\arccos\varepsilon}\right)\right]^{|m|+1/2}} \times$$

$$\times \left(\frac{2\lambda^2}{F}\right)^{\frac{2\varepsilon Z}{\lambda}-|m|-1/2}\exp\left\{-\frac{c^3\Phi(\varepsilon)}{F}\right\}, \tag{37}$$

where

$$\Phi(\varepsilon) = \arccos\varepsilon - \varepsilon\sqrt{1-\varepsilon^2}. \tag{38}$$

For s-states ($j = |m| = 1/2$), formula (36) within the factor 2 coincides with the result of [9] obtained in the framework of the relativistic version of ITM.

When $H \to 0$ the expression (36) is transformed into our previous result [24] 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 (36) 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 ($F = 0$, $H = 0$) radial wavefunctions are of the form

$$\left.\begin{array}{c}f(r)\\g(r)\end{array}\right\} = \pm\sqrt{1\pm\varepsilon}A_0\frac{e^{-\lambda r}}{r}, \tag{39}$$

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 $|A_0|^2 \approx \lambda$ and the ionization rate

$$w = \frac{2\lambda^2}{(|m| - 1/2)!} \frac{(j + |m|)!}{(j - |m|)!} \left[\frac{2c\lambda^4}{FH} \left(1 - e^{-2\frac{H}{F} \arccos \varepsilon} \right) \right]^{-|m| - 1/2} \exp \left\{ -\frac{c^3 \Phi(\varepsilon)}{F} \right\}.$$
(40)

Conclusion

The method of quasiclassical localized states is elaborated to solve asymptotically the Dirac 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 relativistic and spin-orbital effects as well as 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 task is 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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