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WKB Method for the Dirac Equation with the Central-Symmetrical Potential and Its Application to the Theory of Two Dimensional Supercritical Atoms

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Solutions of the Dirac equation in a strong external field are obtained in the WKB approximation. A field is considered strong if the electron binding energy exceeds $2mc^2$ and the discrete spectrum levels may be lowered into the lower continuum. The wave functions in the classically allowed and forbidden regions are found and the conditions for matching them on transition through the turning point are obtained. The WKB method is applied to the following problems: 1) generalization of the Bohr–Sommerfeld quantization conditions with allowance for relativistic effects and the spin in $2+1$ dimensions; 2) energy and width of the quasistationary level in the lower continuum.

1 Introduction

It is known [1, 2] that in three spatial dimensions the expression for the electron ground state energy in the Coulomb field of a point-charge $Z|e|$ becomes purely imaginary when $Z > 137$, and that its interpretation as electron energy no longer has a physical meaning. To determine the electron energy spectrum in the Coulomb field with such a charge we need to eliminate the singularity of the Coulomb potential of a point-charge at $r = 0$ by cutting off the Coulomb potential at small distances. This is equivalent to taking into account of the nucleus size. In three space dimensions the electron energy spectrum in the Coulomb field regulated at small distances was first considered by Pomeranchuk and Smorodinsky (see, for instance, [3]). With increasing Z in the region $Z > 137$, the electron energy levels in such a field were found to decrease, become negative, and may cross the boundary of the lower energy continuum, $E = -mc^2$. The value of $Z|e| = Z_{\rm cr}|e|$ at which the lowest electron energy level cross the boundary of the lower energy continuum is called the critical charge for the electron ground state [2, 4]. If Z continues to grow and enters the transcritical region with $Z > Z_{\rm cr}$, the lowest electron energy level "sinks" into the lower energy continuum, which result in a rearrangement of the vacuum of the QED. This rearrangement is constrained by Pauli exclusion principle. If the electron ground state at $Z < Z_{\rm cr}$ is vacant, two electron-positron pairs are created; if it is half-occupied, one pair is created; and if it is occupied, no pairs are created. The Coulomb potential is repulsive for the created positrons, so they go to infinity. Hence at $Z > Z_{\rm cr}$ a quasistationary state appears in the lower energy continuum and the new vacuum of QED, which corresponds to the filling of all the electron states with $E < -mc^2$, has the total electric charge $2e$ [2, 4]. Indeed, all the electron states with $E < -mc^2$ (the Dirac sea) were filled at $Z < Z_{\rm cr}$, so electrons created by the strong Coulomb field with $Z > Z_{\rm cr}$ cannot be described by means of a convenient wave function, and the notion of charged vacuum was introduced to describe these states [4, 5, 6, 7]. In terms of the new vacuum, the density of electric charge $\rho(r)$ is classical. It is a function characterising the spatial distribution of the real electric charge appearing in the new (charged) vacuum, while in terms of the old (uncharged) vacuum this function should be

interpreted as the probability of two electrons (with charge $2e$) being present at a given point in space.

We would like to see how the same system behaves in two dimensions. With this aim we shall apply the WKB method to the Dirac equation in a strong Coulomb field. Such approach works rather well for states with energy both $0 < E < mc^2$ and $E < -mc^2$. The obtained by this way quasiclassical formulae for the energy of quasistationary levels of the Dirac equation solutions in the lower continuum in $(2+1)$ dimensions allow to consider a wide range of problems in the theory of supercritical atoms.

2 The Dirac equation in an external Coulomb field in $2+1$ dimensions

Since [8] in $2+1$ dimensions the Dirac algebra may be represented in terms of the Pauli matrices as $\gamma^0 = \sigma^3$, $\gamma^k = i\sigma^k$, the Dirac equation for an electron minimally coupled to an external electromagnetic field has the form ($\hbar = c = m_e = 1$)

$$\left(i\frac{\partial}{\partial t} - H_D\right)\Psi = 0, \tag{1}$$

where

$$H_D = \vec{\alpha}\widehat{\vec{p}} + \beta - eA^0\widehat{I} = \sigma^1 p_2 - \sigma^2 p_1 + \sigma^3 - eA^0\widehat{I} \tag{2}$$

is the Dirac Hamiltonian, $p_\mu = i\partial_\mu + eA_\mu$ is the operator of generalized momentum of the electron, A_μ is the vector potential of the external electromagnetic field, $-e < 0$ ($e > 0$) is electric charge of the electron, and the conserved total angular momentum has only a single component, namely, $J_z = L_z + S_z$, where $L_z = -i\partial/\partial\varphi$ and $S_z = \sigma^3/2$.

Let us apply the Dirac equation (1), (2) to study two-dimensional hydrogen-like ion with nuclear charge $eZ \gg 1$. Consider the problem neglecting the nucleus size and assuming the vector potential to be Coulomb

$$A^0(r) = -\frac{Ze}{r}, \qquad A^x = A^y = 0 \tag{3}$$

for $0 \le r < \infty$.

We seek the solutions of the Dirac equation (1) in the field (3) in the polar coordinates in the form

$$\Psi(t, \vec{x}) = \frac{1}{\sqrt{2\pi}} \exp(-i\varepsilon t + il\varphi)\psi(r, \varphi), \tag{4}$$

where ε is the energy, l is an integer number and

$$\psi(r, \varphi) = \frac{1}{\sqrt{r}} \begin{pmatrix} F(r) \\ G(r)e^{i\varphi} \end{pmatrix}. \tag{5}$$

Note that the function (4) is an eigenfunction of the the Dirac Hamiltonian H_D and the total angular momentum J_z with eigenvalues ε and $l + 1/2$, respectively.

Substituting (4) and (5) into (1), and taking into account of the equations

$$p_x \pm p_y = -ie^{\pm i\varphi}\left(\frac{\partial}{\partial r} \pm \frac{i}{r}\frac{\partial}{\partial\varphi}\right),$$

we obtain

$$\frac{dF}{dr} - \frac{l+1/2}{r}F + (\varepsilon + 1 - V(r))\,G = 0, \tag{6}$$

$$\frac{dG}{dr} + \frac{l+1/2}{r}G - (\varepsilon - 1 - V(r))\,F = 0, \tag{7}$$

where $V(r) = -Z\alpha/r$, $\alpha = e^2 \approx 1/137$ is the fine structure constant.

The exact solutions and the energy eigenvalues with $\varepsilon < 1$ corresponding to stationary states of the Dirac equation may be found in full analogy with the case of three space dimensions [1]. Let us look for functions F and G in the form

$$F = \sqrt{1+\varepsilon}\cdot e^{-\rho/2}\rho^{\gamma}\,(Q_1 + Q_2)\,, \qquad G = \sqrt{1-\varepsilon}\cdot e^{-\rho/2}\rho^{\gamma}\,(Q_1 - Q_2)\,, \tag{8}$$

where

$$\rho = 2\lambda r, \qquad \lambda = \sqrt{1-\varepsilon^2}, \qquad \gamma = \sqrt{(l+1/2)^2 - (Z\alpha)^2}.$$

The value of γ is to be found by studying the behavior of the wave function at small r. The functions Q_1 and Q_2 which rendered the solutions of (6), (7) finite at $\rho = 0$ are given in terms of the confluent hypergeometric function $F(a, b; z)$ as:

$$Q_1 = AF(\gamma - \varepsilon Z\alpha/\lambda, 2\gamma + 1; \rho), \qquad Q_2 = BF(\gamma - \varepsilon Z\alpha/\lambda + 1, 2\gamma + 1; \rho).$$

The constants A and B are related by

$$B = \frac{\gamma - \varepsilon Z\alpha/\lambda}{l + 1/2 + Z\alpha/\lambda}A,$$

and the energy eigenvalues are defined by

$$\gamma - \varepsilon Z\alpha/\lambda = -n_r. \tag{9}$$

It is easy to show that the following values of the quantum number n_r are allowed: $n_r = 0, 1, 2, \ldots$, if $l \geqslant 0$, and $n_r = 1, 2, 3, \ldots$ if $l < 0$.

From the normalization condition for the wave function $\Psi(t, \vec{x})$ one can obtain the expression for the constant A:

$$A = \frac{1}{\Gamma(2\gamma+1)}\left\{\frac{\lambda\,[Z\alpha + \lambda(l+1/2)]\,\Gamma(2\gamma + n_r + 1)}{2Z\alpha\cdot n_r!}\right\}^{1/2}.$$

From (9) we find the electron energy spectrum in the Coulomb field (3):

$$\varepsilon = \left[1 + \frac{(Z\alpha)^2}{\left(n_r + \sqrt{(l+1/2)^2 - (Z\alpha)^2}\right)^2}\right]^{-1/2}.$$

It is seen that

$$\varepsilon_0 = \sqrt{1 - (2Z\alpha)^2}$$

for $l = n_r = 0$, and ε_0 becomes zero at $Z\alpha = 1/2$, whereas in three spatial dimensions ε_0 equals zero at $Z\alpha = 1$. Thus, in two space dimensions the expression for the electron ground state energy in the Coulomb field of a point-charge $Z|e|$ no longer has a physical meaning at a much lower value of $Z\alpha = 1/2$, and the corresponding solution of the Dirac equation oscillates near the point $r \to 0$.

To determine the electron energy spectrum in the Coulomb field with such a charge we need to eliminate the singularity of the Coulomb potential of a point-charge at $r = 0$ by cutting off the Coulomb potential at small distance r_N. This is equivalent to taking into account of the nucleus size.

3 WKB method for the Dirac equation in the strong external field

For finding the quasiclassical solutions of the system of equations (6), (7) it is convenient to write them in the matrix form:

$$\psi' = \frac{1}{\hbar} D\psi,\ \psi = \begin{pmatrix} F \\ G \end{pmatrix}, \qquad D = \begin{pmatrix} \hbar\aleph/r & -(\varepsilon + 1 - V(r)) \\ \varepsilon - 1 - V(r) & -\hbar\aleph/r \end{pmatrix}. \tag{10}$$

Here we have restored in an obvious view the reduced Planck constant $\hbar$, the prime denotes the derivative with respect to r, $\aleph = l + 1/2$, and the external electrostatic potential is $V(r) = -eA^0(r)$. The solution of the matrix equation (10) we shall look as the formal expansion in powers of $\hbar$:

$$\psi = \varphi \exp\left(\int y dr\right), \qquad y(r) = \frac{1}{\hbar} y_{-1}(r) + y_0(r) + \hbar y_1(r) + \cdots,$$
$$\varphi(r) = \sum_{n=0}^{\infty} \hbar^n \varphi^{(n)}(r), \tag{11}$$

where the upper (lower) component $\varphi_F^{(n)}$ $\left(\varphi_G^{(n)}\right)$ of the vector $\varphi^{(n)}$ corresponds to the radial wave function F (G). By substituting (11) into (10) and equating to zero the coefficient of each power of $\hbar$, we obtain the recurrence system

$$(D - y_{-1})\,\varphi^{(0)} = 0, \tag{12}$$

$$(D - y_{-1})\,\varphi^{(n+1)} = \left(\varphi^{(n)}\right)' + \sum_{k=0}^{n} y_{n-k}\varphi^{(k)}, \qquad n = 0, 1, \ldots \tag{13}$$

Using the first two equation of system of equations (12), (13) by the left and right vectors technique we find the terms y_{-1}, y_0 and $\varphi^{(0)}$. Solving the following equations of this system by the similar procedure one can find the terms $y_2, y_3, \ldots, \varphi^{(2)}, \varphi^{(3)}, \ldots$ in the expansions (11). But formulae for them are rather cumbrous, therefore in applications one usually restricts them to only first terms. Actually the reason of this is the fact that the expansions in powers of $\hbar$ (11) in the general case do not convergent and are asymptotic series, the finite number of terms of which gives the good approximation for the wave function, if a parameter of an expansion (the reduced Planck constant $\hbar$) is rather small. So we obtained (to within a normalization constant)

$$\psi = \frac{1}{\sqrt{qQ_\mp}} \exp\left[\int \left(\pm q + \frac{V'(r)}{2qQ_\mp}\right) dr\right] \begin{pmatrix} 1 + \varepsilon - V(r) \\ \mp Q_\mp \end{pmatrix}. \tag{14}$$

Employ the obtained formula to the problem about quasistationary state that is prolongation of the discrete level into the transcritical range $Z > Z_{\rm cr}$, when $\varepsilon < -1$.

To the Dirac system of equations (6), (7) there corresponds the effective potential

$$U(r, \varepsilon) = \varepsilon V - 1/2V^2 + \aleph^2/2r^2, \tag{15}$$

which corresponds to the attraction on small distances $r < r_-$ from nuclear (at $Z\alpha > |\aleph|$) and repulsion for $r > r_-$. So $U(r, \varepsilon)$ looks like a potential with a barrier. To eliminate the singularity of the Coulomb potential of a point-charge at $r = 0$ it is necessary to cut off the Coulomb potential $V(r)$ at some small distance r_N:

$$V(r) = \begin{cases} -Z\alpha/r, & r > r_N, \\ -(Z\alpha/r)\, f\,(r/r_N), & r \le r_N. \end{cases} \tag{16}$$

Here $f(x)$ is cutoff function, $0 \le x = r/r_N \le 1$. Most often the following models are used: $f(x) = 1$ and $f(x) = \left(3 - x^2\right)/2$.

4 The wave function of the Dirac electron in classically allowed and forbidden regions

The wave function of quasistationary state has the various look in the various regions.

I. The region $r_0 < r < r_-$ is classically allowed; there the wave functions (14) oscillate

$$G = C_1^{\pm}\left(\frac{\varepsilon - V + 1}{p}\right)^{1/2}\cos\Theta_1, \qquad F = C_1^{\pm}\,\mathrm{sgn}\left(\frac{\varepsilon - V - 1}{p}\right)^{1/2}\cos\Theta_2. \tag{17}$$

Here

$$p(r) = \sqrt{(\varepsilon - V)^2 - 1 - \frac{\aleph^2}{r^2}}$$

is quasiclassical moment for the radial motion of a particle, $C_1^{\pm}$ is normalization constant,

$$\Theta_1 = \int_{r_-}^{r}\left(p - \frac{\aleph w}{pr}\right)dr + \frac{\pi}{4}, \qquad \Theta_2 = \int_{r_-}^{r}\left(p - \frac{\aleph \widetilde{w}}{pr}\right)dr + \frac{\pi}{4},$$
$$w = \frac{1}{2}\left(\frac{V'}{1+\varepsilon - V} - \frac{1}{r}\right), \qquad \widetilde{w} = \frac{1}{2}\left(\frac{V'}{1-\varepsilon + V} - \frac{1}{r}\right).$$

Signs $\pm$ correspond to values $\aleph > 0$ and $\aleph < 0$. If a width γ of a level is small (it will be shown later) the wave function of quasistationary state can be normalized on a single particle localized in the region I, neglecting its penetrability into the classically forbidden regions $r < r_0$ and $r > r_-$ [10]. Here $\cos^2\Theta_i(r)$ can be replaced with average value 1/2:

$$\left|C_1^{\pm}\right| = \left[\int_{r_0}^{r_-}\frac{\varepsilon - V(r)}{p(r)}dr\right]^{-1/2} = \left(\frac{2}{T}\right)^{1/2},$$

where T is the frequency period of a relativistic particle inside a potential well.

II. The below-barrier region $r_- < r < r_+$ is classically forbidden. Here $p = iq$, and quantities q, y_{-1} and y_0 are real. As known [10] the wave function should exponentially damp inside of this region. So the solutions of the Dirac system of equations (6), (7) in the below-barrier region for $\aleph < 0$ are

$$\psi = \frac{C_2^-}{\sqrt{qQ_-}}\exp\left[-\int_{r_+}^{r}\left(q + \frac{V'(r)}{2qQ_-}\right)dr\right]\begin{pmatrix} -Q_- \\ \varepsilon - 1 - V(r)\end{pmatrix}, \tag{18}$$

III. In the region $r > r_+$ the divergent wave corresponds to the quasistationary state (taking off positron); for $\aleph < 0$:

$$\psi = \frac{C_3^-}{\sqrt{pP_-}}\exp\left[\int_{r_+}^{r}\left(ip + \frac{V'(r)}{2pP_-}\right)dr\right]\begin{pmatrix} iP_- \\ \varepsilon - 1 - V(r)\end{pmatrix}, \tag{19}$$

where $P_\pm = p \pm i\aleph/r$. The formulae (17)–(19) include the whole range of values of r (except for range $r < r_0$ for which the view of a wave function here is not written out), except for neighbourhoods of turning points r_- and r_+. For bypass of these points and sewing the solutions we shall use the usual method [10]. Closely to the r_- and r_+ the system (6) reduces to the Schrödinger equation with the effective potential linearly depending on $r - r_\pm$, the solution of which expressed through the Airy function; one can sew by the more elegant Zwaan method. So the relation between the constants in various regions is of the form

$$C_2^{\pm} = iC_3^{\pm} = \sigma C_1^{\pm}\left[\frac{|\aleph|}{\left(r_-^2 + \aleph^2\right)^{1/2} + r_-}\right]^{\sigma}\exp\left[-\int_{r_-}^{r_+}\left(q + \sigma\frac{V'(r)}{qQ_\pm}\right)dr\right], \tag{20}$$

where $\sigma = \mathrm{sgn}\,\aleph/2$.

Though the formulae (17)–(19) essentially differ from the formulae by nonrelativistic quasiclassics and more complicated from them, their application to concrete problems does not meet difficulties, as all quantities in functions F and G express in quadratures.

5 Position and width of quasistationary levels in the lower continuum

Let us find the energy of quasistationary states that are the prolongation of the discrete spectrum levels into supercritical region $Z > Z_{\rm cr}$, $\varepsilon < -1$. Neglecting the penetrability of a barrier in the region $r_- < r < r_+$ we obtain from (15) the quantization condition:

$$\int_{r_-}^{r_+} \left(p - \frac{\aleph w}{pr} \right) dr = \pi \left(n_r + \frac{\operatorname{sgn}(l+1/2)}{2} \right). \tag{21}$$

The equation (21) determines the real part of the level energy $\varepsilon_{nl} = \varepsilon - i\gamma/2$. It is easy to show that the condition (21) reproduces the exact expression of the energy spectrum in the case $0 < \varepsilon < 1$.

Calculating the integral in (21) for the potential (14) and taking into account that $|\varepsilon| \ll Z\alpha/r_N$, we arrive at the transcendental equation ε:

$$\frac{\varepsilon Z\alpha}{2k} \ln \frac{|\varepsilon|\, Z\alpha + kg}{|\varepsilon|\, Z\alpha - kg} - g \ln \frac{r_N e\mu}{2g^2} + \sigma \arccos \frac{g^2 - \varepsilon\aleph^2}{Z\alpha\mu} + I = \pi \left(n_r + \frac{\operatorname{sgn}(l+1/2)}{2} \right), \tag{22}$$

where

$$I = Z\alpha \int_{x_0}^{1} \left[\sqrt{f^2(x) - \frac{\rho^2}{x^2}} + \frac{\aleph}{2(Z\alpha)^2} \left(\frac{f'(x)}{f(x)} + \frac{1}{x} \right) \frac{1}{\sqrt{x^2 f^2(x) - \rho^2}} \right] dx, \quad e = 2.718\ldots$$

Let now us go to determination of the level width $\gamma = -2\,\mathrm{Im}\,\varepsilon_{nl}$ that coincides with the probability of the spontaneous creation of positrons. From the equations (6), (7) we obtain the expression for γ

$$\gamma = 2\,\mathrm{Im}\,[G^*(\infty)F(\infty)].$$

By the obtained formulae for G and F γ takes the form

$$\gamma = \gamma_0 \exp\left[-2\pi Z\alpha \left(\sqrt{1 + 1/k^2} - \sqrt{1 - \rho^2} \right) \right],$$
$$T = \frac{1}{\gamma_0} = -\frac{2}{k^2} \left[\varepsilon g + \frac{Z\alpha}{2k} \ln \left(\frac{|\varepsilon|\, Z\alpha + kg}{|\varepsilon|\, Z\alpha - kg} \right) \right].$$

6 Conclusions

In this paper we construct quasiclassical solutions of the (2+1)-dimensional Dirac equation with a strong Coulomb field. By the obtained formulae we obtain the spectrum of quasistationary levels (its position and width) in the lower energy continuum $\varepsilon < -1$ for a spherical superheavy nuclear with a charge $Z > Z_{\rm cr}$. Comparison of values of critical charge $Z_{\rm cr}$ obtained from exact solutions of the Dirac equation [9] with $Z_{\rm cr}$ obtained from the quasiclassical formula (20) shows good correlation. Note that in the ground state for the model I at $r_N = 0.03$ $Z \approx 108$ and 170 in $(2+1)$- and $(3+1)$-dimensional QED, respectively. Thus, the Dirac vacuum in two space dimensions in the presence of a strong Coulomb field is unstable against electron-positron production at significantly smaller values of the critical charge than in the case of three spatial dimensions. Another difference between these two cases results from the fact that electrons confined to a plane behave like a spinless fermion. So if the ground electron state at $Z < Z_{\rm cr}$ is vacant, one pair is created; if it is occupied, no pairs are created.

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