# **New Exact Solution of Dirac-Coulomb Equation with Exact Boundary Condition**

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**Abstract** It usually writes the boundary condition of the wave equation in the Coulomb field as a rough form without considering the size of the atomic nucleus. The rough expression brings on that the solutions of the Klein-Gordon equation and the Dirac equation with the Coulomb potential are divergent at the origin of the coordinates, also the virtual energies, when the nuclear charges number  $Z > 137$ , meaning the original solutions do not satisfy the conditions for determining solution. Any divergences of the wave functions also imply that the probability density of the meson or the electron would rapidly increase when they are closing to the atomic nucleus. What it predicts is not a truth that the atom in ground state would rapidly collapse to the neutron-like. We consider that the atomic nucleus has definite radius and write the exact boundary condition for the hydrogen and hydrogen-like atom, then newly solve the radial Dirac-Coulomb equation and obtain a new exact solution without any mathematical and physical difficulties. Unexpectedly, the *K* value constructed by Dirac is naturally written in the barrier width or the equivalent radius of the atomic nucleus in solving the Dirac equation with the exact boundary condition, and it is independent of the quantum energy. Without any divergent wave function and the virtual energies, we obtain a new formula of the energy levels that is different from the Dirac formula of the energy levels in the Coulomb field.

### **1 Introduction**

The Dirac equation for the hydrogen atom has been treated in modern mathematical physics textbooks [\[1\]](#page-8-0). It is well known that the Dirac equation succeed in many respects. The Dirac equation is compatible with the theory of relativity, and it describes the spin of the electron and its magnetic moment in a completely natural way and so on. Especially, the distinguished Dirac formula of energy levels in Coulomb field can explain the fine-structure of the hydrogen atom. This is one of the important indicates of the achievements of the Dirac

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theory. However, the Dirac operator is not apple-pie. According to Ref. [\[1\]](#page-8-0), the main difficulty with a quantum mechanical on-particle interpretation is the occurrence of states with negative (kinetic) energy. Interaction may cause transitions to negative energy states, so that there is no hope for a stability of matter within that framework. On the other hand, we have to be aware of the fact that a quantum mechanical interpretation leads to inconsistencies if pushed too far. The localization problem and the Klein paradox are still no clear solution, even in quantum electrodynamics. Investigating the Dirac equation, one should be not too far from Dirac's point of view: "... a book on the new physics, if not purely descriptive of experimental work, must be essentially mathematical". Here we start with the above reference and take new attention to one of the mathematical difficulties concealed in the Dirac equation with a Coulomb potential, which have not been obtained any logical mathematical explain, and we show finally that these paradoxes do not exists actually, such as the virtual energies and the divergence of all wave function on the ground state as  $r \to 0$  in pure Coulomb field. We show that all of this kind of difficulties is due to the original incorrect mathematical methods for solving the radial Dirac equation.

It is also well known that, according to the boundary condition to solve Schrödinger equation  $\lceil 2 \rceil$  for the hydrogen atom one can naturally obtain the Bohr formula  $\lceil 3 \rceil$  of energy levels, this is the prominent sign that the quantum mechanics is different from the classical mechanics. Considering the relativistic effect, Dirac introduced his relativistic wave equation for the single electron  $\begin{bmatrix} 4 \end{bmatrix}$  in 1928. Darwin  $\begin{bmatrix} 5 \end{bmatrix}$  and Gordon  $\begin{bmatrix} 6 \end{bmatrix}$  $\begin{bmatrix} 6 \end{bmatrix}$  $\begin{bmatrix} 6 \end{bmatrix}$  first obtain the exact solution of the Dirac equation with a Coulomb potential. Biedenharm [\[7\]](#page-8-0), Wong and Yeh [[8,](#page-8-0) [9\]](#page-8-0), Su [[10](#page-8-0)] etc. also constructed the different second Dirac equation and obtain the different form of solutions. Nenciu [\[11\]](#page-8-0), Kalus and Wüst [\[12\]](#page-8-0) investigated the different construction methods of self-adjoint extension of the Dirac operators with coulomb potential, and it is also showed that the distinguished self-adjoint extensions given by the two methods are identical. In history, it was ineffectual to use the Klein-Gordon equation  $[13, 14]$  $[13, 14]$  $[13, 14]$  $[13, 14]$  $[13, 14]$ , to describe the hydrogen atom because its eigenvalues of the quantum energy is incompletely agrees accurately with the experimentally observed hydrogen spectra. We investigated the mathematical foundation of constructing all wave equations for the quantum system by the numbers and found some mathematical problems that have been ignored in the Dirac equation. We know that all wave equations for the quantum system have not been strictly demonstrated in quantum mechanics, but the Schrödinger equation has not any mathematical difficulty, it is regarded as a fundamental assumption and is generally accepted. However the original solution of the Dirac equation in Coulomb field is divergent at the origin of coordinate and the energies for all atoms with nuclear charges number  $Z > 137$  are the virtual numbers, all of these problems are actually serious mistakes from the incorrect mathematical methods. If a solution of some wave equation contains some mathematical or physical difficulties even mistakes, it should imply some new laws that have not been found [\[15\]](#page-8-0). The mathematical difficulties concealed in the Dirac equation with the Coulomb potential should imply some new conclusions that have not been found also.

For briefness to discuss the essential of the problems, we only focus on the original exact solution of the Dirac equation for the hydrogen atom in present paper. It is should be accentuated that the boundary condition exerts decisive action in solving the wave equation [\[16–](#page-8-0)[23\]](#page-9-0). However such important condition is not always attended in the history of the relativistic quantum mechanics  $[24–30]$ . That the whole Dirac wave functions of the hydrogen and hydrogen-like atom are divergent at the origin of the coordinate implies that the atom on the ground state would collapse to the neutron-like. By all appearances, the deduction falls short of the true. In fact, the original mathematical methods for solving the radial Dirac equation are incorrect, although one can obtain the fine-structure formula of <span id="page-2-0"></span>the energy-levels. This is why we have those mathematical difficulties. For finding the correct eigensolution of the some differential equations that cannot be optimized such as the radial Dirac equation with the Coulomb potential, there is some theorems which need to be proved [[31](#page-9-0), [32\]](#page-9-0). Any wave function must accord with the conditions for determining solution and the physical signification. The virtual energies and the divergence of the original solution for the Dirac equation are due to the rough boundary condition. Writing the exact boundary condition and solving the Dirac equation outside the nucleus again, one can obtain a new exact wave function which has no any mathematical paradox, including the divergence of the wave function and the virtual energies. Howvere, the new strict mathematical deduction indicates that the *K* value constructed by Dirac is naturally written in the radius of the hydrogen atom, one can find that the new formula of the energy levels is no longer the Dirac formula, it is the correct result from a correct mathematical method for solving the redial Dirac equation.

#### **2 Rough Boundary Condition and Divergence of Dirac Function**

Using the Schrödinger equation to describe the quantum system of the hydrogen atom, it usually does not consider the size of the atomic nucleus. The boundary condition of the atom with nuclear charges number *Z* is written as the rough form

$$
R(r \to 0) \neq \pm \infty, \qquad R(r \to \infty) = 0, \quad -\infty < R(0 < r < \infty) < \infty \tag{1}
$$

where *R* is the radial wave function. Solving the Schrödinger equation by using this rough boundary condition, the Bohr formula of the energy levels is naturally obtained, it is one of the most consummate parts in quantum mechanics. In Dirac theory, because of absence for considering size of the atomic nucleus, one still uses the above rough boundary condition to solve the radial Dirac equation and obtains the distinguished Dirac formula of the energy levels in the Coulomb field [[33\]](#page-9-0)

$$
E = \frac{mc^2}{\sqrt{1 + \alpha^2/(n_r + \sqrt{K^2 - Z^2\alpha^2})^2}}
$$
(2)

where  $K = \pm 1, \pm 2, \pm 3, \ldots$ , constructed by Dirac,  $n_r = 0, 1, 2, \ldots$ , and  $\alpha$  is the fine structure constant. It sticks out a mile, for the ground state or S-state,  $n = 0$ ,  $K = \pm 1$ , when *Z >* 137, the energies of the system must be virtual numbers. This is a pure mathematical problem. We don't think that those explain which departure mathematics too far are correct.

On the other hand, the corresponding Dirac wave function takes the form with two components

$$
R(r) = \begin{pmatrix} e^{-ar} \sum_{v=0}^{n} b_v(ar) \sqrt{\frac{K^2 - Z^2\alpha^2 + v - 1}{K^2 - Z^2\alpha^2}} \\ e^{-ar} \sum_{v=0}^{n} d_v(ar) \sqrt{\frac{K^2 - Z^2\alpha^2}{K^2 - Z^2\alpha^2}} \end{pmatrix}
$$
(3)

where  $a = \sqrt{m^2c^4 - E^2}/\hbar c$  and the coefficients of the polynomial satisfy the system of the recursive relations

$$
\frac{1}{\lambda}b_{\nu-1} + d_{\nu-1} - Z\alpha b_{\nu} - (K + \sqrt{K^2 - Z^2\alpha^2} + \nu)d_{\nu} = 0,
$$
  
\n
$$
b_{\nu-1} + \lambda d_{\nu-1} + (K - \sqrt{K^2 - Z^2\alpha^2} - \nu)b_{\nu} + Z\alpha d_{\nu} = 0
$$
\n(4)

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<span id="page-3-0"></span>where  $\lambda = \sqrt{\frac{mc^2 - E}{mc^2 + E}}$ . However the wave function for the S-state is divergent, as  $K = 1$ , whatever  $n_r$  takes any value, the expression  $(3)$  becomes

$$
R(r \to 0) = \lim_{r \to 0} \left( \frac{(ar)^{\sqrt{K^2 - Z^2 \alpha^2} - 1} + \sum_{\nu=1}^{n_r} b_{\nu}(ar)^{\sqrt{K^2 - Z^2 \alpha^2} + \nu - 1}}{(ar)^{\sqrt{K^2 - Z^2 \alpha^2} - 1} + \sum_{\nu=1}^{n_r} d_{\nu}(ar)^{\sqrt{K^2 - Z^2 \alpha^2} + \nu - 1}} \right) e^{-ar} = \left( \infty \right)
$$
(5)

this is a typical mathematical difficulty, which the solution balance out the condition for determining solution of the wave equation.

Any mathematical difficulty in physical theory must lead to some deductions that contravene the order of nature. When looking from a physical point of view, the divergence of the Dirac wave function for S-state implies that the probability density of the electron around the nucleus rapidly increases as it close to the atomic nucleus. The probability density from the wave function with two components is defined as

$$
\rho(r,t) = R^+(r,t)R(r,t). \tag{6}
$$

According to  $(3)$  $(3)$ , we have

$$
R^{+} = e^{-ar} \left( \sum_{\nu=0}^{n} b_{\nu}(ar)^{\nu+\sqrt{K^{2}-Z^{2}\alpha^{2}}-1} \sum_{\nu=0}^{n} d_{\nu}(ar)^{\nu+\sqrt{K^{2}-Z^{2}\alpha^{2}}-1} \right).
$$
 (7)

In this case the radial probability density of the electron for the relativistic hydrogen is as follows

$$
\rho = \left[ e^{-ar} \sum_{\nu=0}^{n} b_{\nu}(ar)^{\nu+\sqrt{K^2 - Z^2 \alpha^2 - 1}} \right]^2 + \left[ e^{-ar} \sum_{\nu=0}^{n} d_{\nu}(ar)^{\nu+\sqrt{K^2 - Z^2 \alpha^2 - 1}} \right]^2.
$$
 (8)

For S-state which implies  $K = 1$ , as  $r \to 0$ , the above formula becomes

$$
\lim_{r \to 0} \rho = \infty \tag{9}
$$

what this result predicts should be that the hydrogen and hydrogen-like atom in the ground state must rapidly collapse to the neutron-like. However the fact is not thusness. That is to say, the original solution of the Dirac equation for the hydrogen and hydrogen-like atom neither agrees with the mathematical principle nor agrees with the physical signification. Unexpectedly, such divergence was defined as so-called "mild divergence" [[34](#page-9-0)–[36](#page-9-0)] so that hardly might one open out its actual meaning, and the correct deduction have been buried. We know that the Klein-Gordon for the meson without spin has the same divergence, but the Klein-Gordon divergence in the Coulomb field can be eliminated by the suitable mathematical method. Only one demonstrate some new theorems for finding the eigensolutions set of some differential equations with the variable coefficient can find the correct eigenvalues set of the corresponding wave equations [\[31,](#page-9-0) [32\]](#page-9-0).

Using a cut-off procedure for the potential that is similar to the case of considering an extended nucleus to blench the divergence should be independent of the exact solution for the Dirac equation with the Coulomb potential, and it oppresses the exact solution of the wave equation. For the exact solution, why coming forth the mathematical difficulty such <span id="page-4-0"></span>as the expression  $(5)$  $(5)$  and  $(9)$  $(9)$  $(9)$  and the virtual energies is that the size of the nucleus of the hydrogen atom is not considered in the rough boundary condition ([1\)](#page-2-0), and the nuclear are regarded as the point in geometrical meaning. The point in geometrical meaning falls short of the actual case of the atomic nucleus. In fact, the necessary of the normalizable wave function of the hydrogen atom has been discussed home and widely in some modern physics textbook [\[37\]](#page-9-0). Now one should consider the actual size of the atomic nucleus to rewrite the boundary condition then find the eigensolution of the Dirac equation for the hydrogen and hydrogen-like atom.

#### **3 Exact Boundary Condition and New Solution of Dirac Equation**

Boundary conditions for any wave equations are written out basing on the structure of the physical model and distributing character of the physical quantity. Consider two basic facts, one is that the atomic nucleus has definite size, we suppose its equivalent radius or barrier width is *δ*. Another is that the electron does not enter the inside of the atomic nucleus, and does not collide to and rub with the atomic nucleus. In this way, any wave equation that describes the atom has the same exact boundary condition

$$
R(r \le \delta) \neq \pm \infty, \qquad R(r \to \infty) = 0, \quad -\infty < R(\delta < r < \infty) < \infty \tag{10}
$$

one would recover the Bohr formula of the energy levels if uses this exact condition to solve the Schrödinger equation for the hydrogen atom. It is well known that the Schrödinger equation is very consummate in mathematics. However the new formula of the energy levels coming from the Dirac equation with the exact boundary condition is not as exact as the Dirac formula with the rough boundary condition and the divergence for the wave function. Of course, one would obtain the satisfying formula that is as exact as the distinguished Dirac formula when considering the spin-orbit coupling in the Dirac equation. It should be not one and only choice that for explaining the fine structure of the hydrogen atom one still uses the rough boundary condition for the Dirac equation and still blench those mathematical and physical difficulty such as the divergence and the virtual energies. One note that the boundary conditions are related to the self-adjointness of the operator, also one of methods to obviate the divergence of the Dirac function was given by Deck, Amar and Fralick [\[38\]](#page-9-0).

Now use the exact boundary condition (10) to solve the radial Dirac equation of the hydrogen atom. It usually introduces a mathematical transformation

$$
R = \begin{pmatrix} F(r)/r \\ G(r)/r \end{pmatrix} \tag{11}
$$

and translate the radial Dirac equation for the hydrogen atom [\[39,](#page-9-0) [40](#page-9-0)]

$$
\left[c\hat{p}_r\begin{pmatrix}0&i\\-i&0\end{pmatrix}-\frac{\hbar cK}{r}\begin{pmatrix}0&1\\1&0\end{pmatrix}+mc^2\begin{pmatrix}1&0\\0&-1\end{pmatrix}\right]R=\left(E+\frac{e^2}{4\pi\varepsilon_0r}\right)R\tag{12}
$$

into the following form

$$
\left(\frac{E - mc^2}{\hbar c} + \frac{\alpha}{r}\right)F + \left(\frac{K}{r} + \frac{d}{dr}\right)G = 0,
$$
\n
$$
\left(\frac{E + mc^2}{\hbar c} + \frac{\alpha}{r}\right)G + \left(\frac{K}{r} - \frac{d}{dr}\right)F = 0
$$
\n(13)

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where  $K = \pm 1, \pm 2, \ldots$ . Considering the exact boundary condition ([10](#page-4-0)), introduce the transform

$$
\xi = r - \delta \quad (\xi \ge 0) \tag{14}
$$

the boundary  $(10)$  $(10)$  can be overwritten as follows

$$
R(\xi \to 0) \neq \pm \infty, \qquad R(\xi \to \infty) = 0, \quad -\infty < R(0 < \xi < \infty) < \infty \tag{15}
$$

then  $r = \xi + \delta$ , substituting it into [\(13\)](#page-4-0), one obtains

$$
\left(\frac{E - mc^2}{\hbar c} + \frac{\alpha}{\xi + \delta}\right)F + \left(\frac{K}{\xi + \delta} + \frac{d}{d\xi}\right)G = 0,
$$
\n
$$
\left(\frac{E + mc^2}{\hbar c} + \frac{\alpha}{\xi + \delta}\right)G + \left(\frac{K}{\xi + \delta} - \frac{d}{d\xi}\right)F = 0.
$$
\n(16)

Because  $F \to 0$ ,  $G \to 0$  as  $\xi \to \infty$ , the system of differential equations (16) has the formal solutions with weight function of asymptotic solutions

$$
F = e^{-a\xi} f(\xi), \qquad G = e^{-a\xi} g(\xi). \tag{17}
$$

Substituting  $(17)$  into  $(16)$ , one then obtains

$$
\left[\frac{E - mc^2}{\hbar c}(\xi + \delta) + \alpha\right]f + (\xi + \delta)\frac{dg}{d\xi} + [K - a(\xi + \delta)]g = 0,
$$
\n
$$
\left[\frac{E + mc^2}{\hbar c}(\xi + \delta) + \alpha\right]g - (\xi + \delta)\frac{df}{d\xi} + [K + (a\xi + \delta)]f = 0
$$
\n(18)

the eigensolutions of  $(18)$  correspond to quantum energy are two interrupted series which the number of terms is determined by the eigenvalues.

In order to find the general series solutions for  $(18)$ , it is assumed that the formal solutions are

$$
f(\xi) = \sum_{\nu=0}^{\infty} b_{\nu} \xi^{\sigma+\nu}, \qquad g(\xi) = \sum_{\nu=0}^{\infty} d_{\nu} \xi^{\sigma+\nu}.
$$
 (19)

Substituting into  $(18)$ , one obtains the linear system of recursive relations

$$
\sum_{\nu=0}^{\infty} \left[ \frac{E-mc^2}{\hbar c} b_{\nu-1} + \frac{E-mc^2}{\hbar c} \delta b_{\nu} + \alpha b_{\nu} + K d_{\nu} + K d_{\nu} + (\sigma + \nu) d_{\nu} + \delta (\sigma + \nu + 1) d_{\nu+1} - a d_{\nu-1} - \delta a d_{\nu} \right] \xi^{\sigma+\nu} = 0,
$$
\n
$$
\sum_{\nu=0}^{\infty} \left[ \frac{E+mc^2}{\hbar c} d_{\nu-1} + \frac{E+mc^2}{\hbar c} \delta d_{\nu} + \alpha d_{\nu} + K b_{\nu} - (\sigma + \nu) b_{\nu} - \delta (\sigma + \nu + 1) b_{\nu+1} + a b_{\nu-1} + \delta a b_{\nu} \right] \xi^{\sigma+\nu} = 0.
$$
\n(20)

hence the coefficient of the power series satisfy the following system of recursive relations

$$
\frac{E - mc^2}{\hbar c} b_{\nu-1} + \left(\frac{E - mc^2}{\hbar c} \delta + \alpha\right) b_{\nu} - ad_{\nu-1} \n+ \delta(\sigma + \nu + 1) d_{\nu+1} + (K + \sigma + \nu - \delta a) d_{\nu} = 0,
$$
\n
$$
\frac{E + mc^2}{\hbar c} d_{\nu-1} + \left(\frac{E + mc^2}{\hbar c} \delta + \alpha\right) d_{\nu} + ab_{\nu-1} \n- \delta(\sigma + \nu + 1) b_{\nu+1} + (K - \sigma - \nu + \delta a) b_{\nu} = 0.
$$
\n(21)

<span id="page-5-0"></span>

<span id="page-6-0"></span>Corresponding to  $v = -1$  the indicial equations are given that  $\delta \sigma b_0 = 0$  and  $\delta \sigma d_0 = 0$ . Because  $\delta \neq 0$ ,  $b_0 \neq 0$  and  $d_0 \neq 0$ , one obtains

$$
\sigma = 0 \tag{22}
$$

so that the wave functions satisfy the boundary condition at  $r \to \delta$  namely  $\xi \to 0$ , the above equations reduce to

$$
\frac{E - mc^2}{\hbar c} b_{\nu-1} + \left( \frac{E - mc^2}{\hbar c} \delta + \alpha \right) b_{\nu} - ad_{\nu-1} + \delta(\nu + 1) d_{\nu+1} + (K + \nu - \delta a) d_{\nu} = 0,
$$
\n
$$
\frac{E + mc^2}{\hbar c} d_{\nu-1} + \left( \frac{E + mc^2}{\hbar c} \delta + \alpha \right) d_{\nu} + ab_{\nu-1} - \delta(\nu + 1) b_{\nu+1} + (K - \nu + \delta a) b_{\nu} = 0.
$$
\n(23)

Respectively evaluate for  $v = 0, 1, 2, \ldots, n_r$ ,  $b_{n_r+1} = d_{n_r+1} = 0$ , make use of that  $b_{-2} =$  $d_{-2} = 0$  and  $b_{-1} = d_{-1} = 0$ , (23) give

$$
\left(\frac{E - mc^2}{\hbar c}\delta + \alpha\right)b_0 + (K - \delta a)d_0 + \delta d_1 = 0,(K + \delta a)b_0 + \left(\frac{E + mc^2}{\hbar c}\delta + \alpha\right)d_0 - \delta b_1 = 0,\frac{E - mc^2}{\hbar c}b_0 + \left(\frac{E - mc^2}{\hbar c}\delta + \alpha\right)b_1 - ad_0 + (K + 1 - \delta a)d_1 + 2\delta d_2 = 0,ab_0 + (K - 1 + \delta a)b_1 + \frac{E + mc^2}{\hbar c}d_0 + \left(\frac{E + mc^2}{\hbar c}\delta + \alpha\right)d_1 - 2\delta b_2 = 0,\vdots
$$
\n(24)

$$
\frac{E - mc^2}{\hbar c} b_{n_r - 1} + \left( \frac{E - mc^2}{\hbar c} \delta + \alpha \right) b_{n_r} - ad_{n_r - 1} + (K + n_r - \delta a) d_{n_r} = 0,
$$
  
\n
$$
ab_{n_r - 1} + (K - n_r + \delta a) b_{n_r} + \frac{E + mc^2}{\hbar c} d_{n_r - 1} + \left( \frac{E + mc^2}{\hbar c} \delta + \alpha \right) d_{n_r} = 0,
$$
  
\n
$$
\frac{E - mc^2}{\hbar c} b_{n_r} - ad_{n_r} = 0,
$$
  
\n
$$
ab_{n_r} + \frac{E + mc^2}{\hbar c} d_{n_r} = 0.
$$

The last two formulas are linearly dependent. Use  $(E + mc^2)/\hbar c$  to multiply the third for-The last two formulas are linearly dependent. Use  $(E + mc<sup>2</sup>)/nc$  to multiply the finite formula from bottom, and the  $\sqrt{m<sup>2</sup>c<sup>4</sup> - E<sup>2</sup>}/\hbar c$  to multiply the fourth formula from bottom, and then add the two new formulas, it is given as follows

$$
[\alpha(E + mc^2) + (K - n_r)\sqrt{m^2c^4 - E^2}]b_{n_r}
$$
  
+  $t[(K + n_r)(E + mc^2) + \alpha\sqrt{m^2c^4 - E^2}]d_{n_r} = 0.$  (25)

Substituting for the second formula from the bottom, one will obtain a new formula of the energy levels for the hydrogen atom

$$
E = \frac{mc^2}{\sqrt{1 + (\frac{\alpha}{n_r})^2}} \quad (n_r = 1, 2, 3, \ldots).
$$
 (26)

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One can strictly demonstrate that  $n_r \geq 1$ . It is different from the Dirac formula of the energy levels for the hydrogen atom. This result is the inevitable deduction of the Dirac equation with the exact boundary condition for the hydrogen atom. With the exact boundary condition  $(10)$  $(10)$  $(10)$  and the new formula of the energy levels  $(26)$ , all of the corresponding wave functions satisfy the boundary conditions and there is not any virtual energies.

According to ([11](#page-4-0), [14,](#page-5-0) [16](#page-5-0), [19,](#page-5-0) [23\)](#page-6-0), the whole wave function with the exact boundary condition is as follows

$$
R = \begin{pmatrix} \frac{e^{-a\xi}}{\xi + \delta} \sum_{\nu=1}^{n_r} b_{\nu} \xi^{\nu} \\ \frac{e^{-a\xi}}{\xi + \delta} \sum_{\nu=1}^{n_r} d_{\nu} \xi^{\nu} \end{pmatrix} \quad (n_r \ge 1)
$$
 (27)

the coefficients of corresponding polynomial are determined by the system of recursive relations ([23](#page-6-0)). All appearance, at the boundary of the hydrogen atom

$$
\lim_{\xi \to 0} R = \begin{pmatrix} \text{Constant} \\ \text{Constant} \end{pmatrix}, \qquad \lim_{\xi \to \infty} R = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.
$$
 (28)

Make use of the definition ([6](#page-3-0)), the probability density of the electron appearing outside the nucleus of the hydrogen atom takes the form

$$
\rho = \left(\frac{e^{-a\xi}}{\xi + \delta} \sum_{\nu=0}^{n_r} b_{\nu} \xi^{\nu}\right)^2 + \left(\frac{e^{-a\xi}}{\xi + \delta} \sum_{\nu=0}^{n_r} d_{\nu} \xi^{\nu}\right)^2 \tag{29}
$$

homoplastically, one has

$$
\lim_{\xi \to 0} \rho = \text{Constant}, \qquad \lim_{\xi \to \infty} \rho = 0. \tag{30}
$$

#### **4 Conclusions**

In this paper we expatiated on that the divergences of the Dirac function and the virtual energies of the Dirac formula of the energy levels for the hydrogen and hydrogen-like atom are due to the traditional rough boundary condition. By using the exact boundary condition one can obtain a new solution of the Dirac equation in the Coulomb field. The new solution without any mathematical difficulty gives a new formula of the energy levels which is different from the distinguished Dirac formula. One can find that in the new solution the *K* values constructed by Dirac have been written in the radius of the atomic nucleus and they are independent of the new formula of the energy levels. Only when looking from point of view for the formula of the energy levels, the new formula is not as exact as the Dirac formula. However, considering the spin-orbit coupling or some new potential parameters, one will obtain the exacter formula.

It is well known that the Dirac equation succeed in many important prognostics [[41](#page-9-0)]. Dirac's equation has an infinite number of solutions with negative energies. It leads to discover the existence of the positron and implies an unexpected relativistic interaction between an electron's translational motion and spin, which leads to a violent oscillation of the particle at very high frequencies and over distances of roughly one Compton wavelength. For Dirac's electrons, zitterbewegung takes place whenever the electron wave function includes <span id="page-8-0"></span>both positive and negative energy components. It takes both sets of states to build up an arbitrary electronic state. The distillate of quantum mechanics is to naturally obtain the formula of the energy levels for the bound state by solving the wave equation with the boundary condition. Disclosing the mathematical and physical difficulty concealing in the Dirac equation with the Coulomb potential does not imply to negative the Dirac theory. Our works wish to clearly vindicate the mathematical logic difficulties for the Dirac equation, at least to eliminate the divergence by using the exact boundary condition to replace the rough boundary condition.

No matter which wave equation is used to describe the quantum system of the bound stage, their eigenvalues set and eigensolutions set must be in agreement with the uniqueness, and the solution must accord with the conditions for the exact solution but not any approximate solution such as cut off potential. In principle, we cannot immolate the mathematical rule to obtain a formula only for agreeing with the experimentally observed hydrogen spectra. Actually the divergence of the original solution for the Dirac equation in the Coulomb field is nonexistent. The Dirac equation is more and more widely applied for various models. One should note that using different mathematical methods and different boundary condition to solve the differential equation will obtain different results  $[42, 43]$  $[42, 43]$  $[42, 43]$  $[42, 43]$  $[42, 43]$ . The rough boundary condition for the Dirac equation with the Coulomb potential brings on so mathematical contradictions. We need to revise all incorrect mathematical methods and search the correct mathematical methods to find the correct and exact solution of the various wave equations. One can find that the classical solution of the plane transverse electromagnetic mode of the Maxwell equation is also incorrect [\[44\]](#page-9-0), because of the incorrect mathematical method for solving the wave equation. For quantum mechanics, only by exactly solving the wave equation can we know if the energy eigenvalues exist. Further research should explore the exacter formula of the energy levels for the hydrogen and hydrogen-like atom by using the exact boundary condition that accords with the structure of the atoms. Here it should be pointed out that the Schrödinger equation and the Klein-Gordon equation in the Coulomb field with the exact boundary condition have the same corresponding formula of the energy levels.

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