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New method for solving the '$Z > 137$' problem and determining hydrogen-like energy levels

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Abstract. A new method for including finite nuclear size effects is suggested to overcome the '$Z > 137$ catastrophe' encountered in solving the Dirac equation for an electron in the field of a point charge Ze. In this method, the boundary condition for the numerical solution of the equations for the Dirac radial wave functions is taken so that the components of the electron current density are zero at the boundary of the nucleus. As a result, for all of the nuclei of the Periodic Table the calculated energy levels practically coincide with those obtained in a standard way from the Dirac equation for a Coulomb pointlike charge potential. For $Z > 105$, the calculated energy level functions $E(Z)$ prove to be smooth and monotonic. The ground energy level reaches $E = -mc^2$ (i.e., the electron drops onto the nucleus) at $Z_c = 178$. The proposed method of accounting for the finite size of nuclei can be useful in numerically simulating the energy levels of many-electron atoms.

1. Introduction

More than a hundred years ago, in 1913, Niels Bohr developed the postulates of a new quantum theory. Just three year later, based on the theory of Bohr's orbits, A Sommerfeld [1] devised a formula describing the fine structure of energy levels in hydrogen-like atoms:

$$E = mc^2\left(1 + \frac{\alpha_{\rm em}^2 Z^2}{\left(n - |\kappa| + \sqrt{\kappa^2 - \alpha_{\rm em}^2 Z^2}\right)^2}\right)^{-1/2}. \qquad (1)$$

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In expression (1), m is the electron mass, c is the speed of light in vacuum, $\alpha_{\rm em} = e^2/(\hbar c)$ is the electromagnetic fine-structure constant, Z is the number of protons, $n = 1, 2....$ is the principal quantum number, and κ is the quantum number of the Dirac equation:

$$\kappa = \pm 1 \pm 2... = \begin{cases} -(l+1), & j = l + \dfrac{1}{2}, \\ l, & j = l - \dfrac{1}{2}, \end{cases} \qquad (2)$$

where j, l, are the quantum numbers of the total and angular momentum of the electron. Following the achievements of the Dirac theory in 1928, Dirac [2, 3], Darwin [4], and Gordon [5] obtained expression (1) as a result of an exact solution of the Dirac equation in the Coulomb field of a pointlike charge $-Ze$.

Formula (1) takes the complex value for

$$Z > \frac{|\kappa|}{\alpha_{\rm em}} \sim 137|\kappa|. \qquad (3)$$

From the viewpoint of the existence of real nuclei in the Periodic Table, as related to inequality (3), the electron states with $|\kappa| = 1$, i.e., the $1S_{1/2}$ and $2P_{1/2}$ states are of interest. For these states, the complexity of energy levels in formula (1) is often called the '$Z > 137$ catastrophe'. It was established fairly quickly that the catastrophe results from the ignorance of the finite size of the nuclei.

In 1945, Pomeranchuk and Smorodinsky [6] considered an atomic system with the electrical potential

$$U = \begin{cases} -\dfrac{Ze^2}{r_{\rm N}} & \text{for} \quad r \leqslant r_{\rm N}, \\ -\dfrac{Ze^2}{r} & \text{for} \quad r > r_{\rm N}, \end{cases} \qquad (4)$$

where $r_{\rm N}$ is the nucleus radius. At the close of the consideration, they estimated the value of Z_c, at which the lower energy

level of the $1S_{1/2}$ state reaches the limiting value of $E = -mc^2$:

$$Z_c = 175 \quad \text{at} \quad r_N = 0.8 \times 10^{-12}\ \text{cm}\,. \tag{5}$$

This led to an important conclusion that in the range of $Z_c \geqslant Z > 137$ a real function $E(Z)$ must exist, and the catastrophe in formula (1) indeed occurs as a result of the ignorance of the finite size of nuclei.

In 1959, Zel'dovich [7] demonstrated that variations in the Coulomb potential near the origin of coordinates produce minor effects on the energy spectrum of the hydrogen atom.

An overview of subsequent papers devoted to the energy level structure of hydrogen-like ions for $Z\alpha > 1$ is presented in Refs [8–10]. In particular, Zeldovich and Popov [8] analyzed the structure of energy levels using in addition to the potential (4) a potential corresponding to that of a uniformly charged sphere:

$$U_1 = \begin{cases} \dfrac{Ze^2}{r_N}\left[-\dfrac{3}{2}+\dfrac{1}{2}\left(\dfrac{r}{r_N}\right)^2\right] & \text{for} \quad r \leqslant r_N\,, \\ -\dfrac{Ze^2}{r} & \text{for} \quad r > r_N\,. \end{cases} \tag{6}$$

The authors of Ref. [11] numerically calculated the energy levels of the first nine states ($1S_{1/2}$, $2S_{1/2}$, ..., $3D_{5/2}$) as a function of Z for potential (6). The value of Z_c determined in Ref. [11] amounted to 169 for $r_N = 9.5 \times 10^{-12}$ cm. This value is close to the values of $Z_c = 170-175$ obtained by other researchers (see Refs [6, 8]).

To date more than 30 electrostatic potentials, which take into account the finite distribution of electric charge in atomic nuclei, have been proposed by various authors. These potentials are tapped in various machine codes for determining the electronic structure of atoms and molecules. A review of the developed potentials and their application in numerical calculations of Dirac and Schrödinger equations can be found in Ref. [9] (see also Ref. [10]). In reviews [9, 10], one can also find a wide circle of literature on analytical and numerical determinations of the electronic structure of atoms and molecules.

The solutions of the Dirac and Schrödinger equations involving the finite electrical potentials of the atomic nucleus are found by the standard method. First, the wave functions of electrons are calculated within a nucleus in a field of the electrostatic potential of interest. Then, the values of these functions at the boundary of the nucleus are equated with similar values of the wave functions of electrons in the Coulomb field. The boundary condition for radial waves at functions as $r \to \infty$ and at $r = 0$ determine the energy spectrum of the atomic and molecular systems.

According to Refs [8, 9, 11], the introduction of different electrostatic potentials of atomic nuclei into equations leads to a relatively little change (tenths of a percent) in both the absolute values of the electron binding energies and the differences between the energy levels. These changes grow as Z increases.

In the present paper, the problem of determining the energy spectrum of hydrogen-like ions, including a nucleus with $Z > 137$, is resolved by a new approach to numerical calculations of the Dirac equation in the Coulomb field by introducing a boundary condition for wave functions at the boundary of the nuclei of interest.

The boundary condition at the nucleus edge is taken by analogy with that in the analysis of the possibility of existence of the stationary bound states in the Schwarzschild gravitational field [12]. It involves zeroing of the φ-component of Dirac's current density at the boundary of the nucleus of interest, which resolves itself into zeroing of one of the two radial Dirac wave functions at the nucleus boundary in the Coulomb field. In this case, the calculations are simplified being made in the range from $r \to \infty$ up to the boundary of the nucleus r_N.

The paper outline is as follows. For completeness of presentation, Section 2 contains the Dirac equation in the Coulomb field, briefly discusses the procedure of separation of variables, and gives a system of equations for radial wave functions. Section 3 explores the behavior of the components of the vector of current density of Dirac particles and introduces the boundary condition for wave functions at the boundary of the nucleus. Section 4 reviews the results of numerical calculations of energy spectra of hydrogen-like ions with various Z. The concluding Section 5 summarizes the results of this study.

2. Dirac equation in the Coulomb field of the charge $(-Ze)$

Below, we take advantage of the system of units $\hbar = c = 1$, and the signature

$$g^{\alpha\beta} = \text{diag}\,[1, -1, -1, -1]\,; \tag{7}$$

β, α^k are 4×4 Dirac matrices in the Dirac–Pauli representation, and σ^k are 2×2 Pauli matrices, with $k = 1, 2, 3$. We consider the stationary case, when the wave function can be written out as $\psi(\mathbf{r}, t) = \psi(\mathbf{r}) \exp(-iEt)$. The Dirac equation in the Coulomb field of the point charge $(-Ze)$ in spherical coordinates (r, θ, φ) can be expressed as

$$E\psi(\mathbf{r}) = \left[\beta m - i\alpha^1\left(\frac{\partial}{\partial r}+\frac{1}{r}\right) - i\alpha^2\,\frac{1}{r}\left(\frac{\partial}{\partial\theta}+\frac{1}{2}\cot\theta\right) - i\alpha^3\,\frac{1}{r\sin\theta}\,\frac{\partial}{\partial\varphi} - \frac{Ze^2}{r}\right]\psi(\mathbf{r})\,. \tag{8}$$

Equation (8) allows the separation of variables, if the bispinor $\psi(\mathbf{r}) = \psi(r, \theta, \varphi)$ is defined as

$$\psi(r, \theta, \varphi) = \begin{pmatrix} F(r)\,\xi(\theta) \\ -iG(r)\,\sigma^3\xi(\theta) \end{pmatrix} \exp(im_\varphi\varphi) \tag{9}$$

and advantage is taken of the following equation (see, e.g., Ref. [13])

$$\left[-\sigma^2\left(\frac{\partial}{\partial\theta}+\frac{1}{2}\cot\theta\right) + i\sigma^1 m_\varphi\,\frac{1}{\sin\theta}\right]\xi(\theta) = i\kappa\xi(\theta)\,. \tag{10}$$

In Eqns (9) and (10), $\xi(\theta)$ are spherical harmonics for spin 1/2, m_φ is the magnetic quantum number, and κ is the quantum number (2); the function $\xi(\theta)$ can be represented as in Ref. [14]:

$$\xi(\theta) = \begin{pmatrix} {}_{-1/2}Y_{jm_\varphi}(\theta) \\ {}_{1/2}Y_{jm_\varphi}(\theta) \end{pmatrix} = (-1)^{m_\varphi+1/2}\sqrt{\frac{1}{4\pi}\,\frac{(j-m_\varphi)!}{(j+m_\varphi)!}} \times \begin{pmatrix} \cos\dfrac{\theta}{2} & \sin\dfrac{\theta}{2} \\ -\sin\dfrac{\theta}{2} & \cos\dfrac{\theta}{2} \end{pmatrix} \begin{pmatrix} \left(\kappa - m_\varphi + \dfrac{1}{2}\right) P_l^{m_\varphi-1/2}(\theta) \\ P_l^{m_\varphi+1/2}(\theta) \end{pmatrix}, \tag{11}$$

where $P_l^{m_\varphi\pm1/2}(\theta)$ are associated Legendre polynomials.

The separation of variables yields a system of equations for real radial functions $F(r)$, $G(r)$. We write out these equations in dimensionless variables $\varepsilon = E/m$, $\rho = r/l_C$, where $l_C = \hbar/(mc)$ is the electron Compton wavelength:

$$\frac{dF}{d\rho} + \frac{1+\kappa}{\rho} F - \left(\varepsilon + 1 + \frac{\alpha_{em} Z}{\rho}\right) G = 0\,,$$
$$\frac{dG}{d\rho} + \frac{1-\kappa}{\rho} G + \left(\varepsilon - 1 + \frac{\alpha_{em} Z}{\rho}\right) F = 0\,. \quad (12)$$

Introducing the definition of the phase through the relation

$$\tan \Phi = \frac{F(\rho)}{G(\rho)}\,, \quad (13)$$

we can obtain the energy spectrum ε_n from the equation for the phase $\Phi = \arctan(F(\rho)/G(\rho)) + k\pi$, $k = 0, \pm 1, \pm 2, \ldots$ in the form proposed by Vronsky [12]:

$$\frac{d\Phi}{d\rho} = \varepsilon + \frac{\alpha_{em} Z}{\rho} + \cos(2\Phi) - \frac{\kappa}{\rho} \sin(2\Phi)\,. \quad (14)$$

For the finite motion of the electron, the asymptotics of solutions to equations (12) in the limit $\rho \to \infty$ are given by

$$F(\rho) = C_1 \exp\left(-\rho\sqrt{1-\varepsilon^2}\right),$$
$$G(\rho) = -\sqrt{\frac{1-\varepsilon}{1+\varepsilon}} F(\rho)\,. \quad (15)$$

The phase Φ for $\rho \to \infty$ takes the form

$$\Phi = -\arctan\sqrt{\frac{1+\varepsilon}{1-\varepsilon}}. \quad (16)$$

3. Electron current density, boundary condition for the wave functions

In the course of separating the variables for the purpose of deriving equations (10), (12) from equation (8), we performed an equivalent replacement of the Dirac matrices:

$$\alpha^1 \to \alpha^3\,, \quad \alpha^2 \to \alpha^1\,, \quad \alpha^3 \to \alpha^2\,. \quad (17)$$

Then, considering formulae (9), (11), the components of the Dirac current density assume the form

$$j^r = \psi^+ \alpha^3 \psi = -iF(\rho)\, G(\rho)\left[\xi^+(\theta)(\sigma^3\sigma^3 - \sigma^3\sigma^3)\,\xi(\theta)\right] = 0, \quad (18)$$

$$j^\theta = \psi^+ \alpha^1 \psi = -2F(\rho)\, G(\rho)\left[\xi^+(\theta)\,\sigma^2 \xi(\theta)\right] = 0\,, \quad (19)$$

$$j^\varphi = \psi^+ \alpha^2 \psi = 2F(\rho)\, G(\rho)\left[\xi^+(\theta)\,\sigma^1 \xi(\theta)\right] \neq 0\,. \quad (20)$$

The equalities (18)–(20) coincide with previously obtained results [15].

Our boundary condition involves zeroing of the current component j^φ at the nucleus boundary ρ_N, which resolves itself into zeroing of one of the two wave functions $F(\rho_N)$ or $G(\rho_N)$:

$$F(\rho_N)\, G(\rho_N) = 0\,. \quad (21)$$

Boundary condition (21) is similar to the condition near the 'event horizon' introduced in the numerical calculations of the solution to the Dirac equation in the Schwarzschild field [12].

As a result, for the values of the gravitational coupling constant $\alpha \approx 1$, calculations [12] yield energy levels close to those in the hydrogen atom.

4. Results of numerical calculations of the energy spectrum of hydrogen-like atoms while effectively taking into account the finite size of nuclei

The sizes of nuclei were calculated based on the relationships

$$r_N = (0.836\, A^{1/3} + 0.57) \times 10^{-13}\ \text{cm}\,, \quad A > 9 \quad [16]\,,$$
$$r_N = 1.3 \times 10^{-13}\, A^{1/3}\ \text{cm}\,, \quad A < 9\,, \quad (22)$$

where A is the atomic weight of the nucleus.

The equation for phase (14) was solved by the fifth-order Runge–Kutta implicit method with a step control [17]. We used the Ehle scheme [18] to obtain the three-stage Rado IIA method.

From two possible variants of implementation of condition (21), we will satisfy it, as in Ref. [12], using the equality

$$G(\rho_N) = 0\,. \quad (23)$$

One of the reasons for making such a choice is the known smallness of function $G(\rho)$ in comparison with function $F(\rho)$ in the nonrelativistic approximation of the Dirac equation. It follows from equality (23) that the condition for the phase assumes the form

$$\Phi(\varepsilon, \kappa, z) = k\,\frac{\pi}{2}\,, \quad k = \pm 1, \pm 3, \pm 5, \ldots\,. \quad (24)$$

Tables 1–3 contain the values of the energy levels for the hydrogen atom ($Z = 1$, $A = 1$), obtained by numerical calculations of equation (14) with the boundary conditions (16), (24) for $\kappa = \pm 1 \pm 2, \pm 3$ and $n = 1-11$. The tables also present corresponding energy values obtained from for-

Table 1. Energy levels of the hydrogen atom for the $S_{1/2}$ and $P_{1/2}$ states ($\kappa = \pm 1$).

n	$1 - \varepsilon_{an}$	$1 - \varepsilon_{num}$	δ, %
1*	2.6640×10^{-5}	2.6641×10^{-5}	-0.004
2	6.6600×10^{-6}	6.6602×10^{-6}	-0.003
3	2.9600×10^{-6}	2.9601×10^{-6}	-0.003
4	1.6650×10^{-6}	1.6651×10^{-6}	-0.006
5	1.0656×10^{-6}	1.0656×10^{-6}	0.000
6	7.4000×10^{-7}	7.3999×10^{-7}	0.001
7	5.4367×10^{-7}	5.4367×10^{-7}	0.000
8	4.1625×10^{-7}	4.1624×10^{-7}	0.002
9	3.2889×10^{-7}	3.2888×10^{-7}	0.002
10	2.6640×10^{-7}	2.6639×10^{-7}	0.003
11	2.2016×10^{-7}	2.2015×10^{-7}	0.006

* No solution available for $\kappa = +1$.

Table 2. Energy levels of the hydrogen atom for the $P_{3/2}$ and $D_{3/2}$ states ($\kappa = \pm 2$).

n	$1 - \varepsilon_{an}$	$1 - \varepsilon_{num}$	δ, %
2*	6.6599×10^{-6}	6.6585×10^{-6}	0.022
3	2.9600×10^{-6}	2.9603×10^{-6}	-0.009
4	1.6650×10^{-6}	1.6653×10^{-6}	-0.016
5	1.0656×10^{-6}	1.0656×10^{-6}	0.004
6	7.3999×10^{-7}	7.3997×10^{-7}	0.004
7	5.4367×10^{-7}	5.4367×10^{-7}	0.001
8	4.1625×10^{-7}	4.1622×10^{-7}	0.007
9	3.2889×10^{-7}	3.2887×10^{-7}	0.006
10	2.6640×10^{-7}	2.6637×10^{-7}	0.012
11	2.2016×10^{-7}	2.2017×10^{-7}	-0.001
* No solution available for $\kappa = +2$.			

Table 3. Energy levels of the hydrogen atom for the $D_{5/2}$ and $F_{5/2}$ states ($\kappa = \pm 3$).

n	$1 - \varepsilon_{an}$	$1 - \varepsilon_{num}$	δ, %
3*	2.9600×10^{-6}	2.9597×10^{-6}	0.011
4	1.6650×10^{-6}	1.6652×10^{-6}	-0.010
5	1.0656×10^{-6}	1.0657×10^{-6}	-0.006
6	7.3999×10^{-7}	7.3997×10^{-7}	0.004
7	5.4367×10^{-7}	5.4367×10^{-7}	0.000
8	4.1625×10^{-7}	4.1622×10^{-7}	0.007
9	3.2889×10^{-7}	3.2887×10^{-7}	0.006
10	2.6640×10^{-7}	2.6637×10^{-7}	0.012
11	2.2016×10^{-7}	2.2017×10^{-7}	-0.001
* No solution available for $\kappa = +3$.			

mula (1) and relative deviations δ of calculated values from analytical ones in percent. It is evident that the numerical and analytical values of energy are in close agreement to within hundredths of a percent [$\delta = (\varepsilon_{num} - \varepsilon_{an})/\varepsilon_{an} \lesssim 10^{-4}$]. Within the above accuracy, the calculations reproduce the degeneration of the energy levels with the same total momentum j (the same value of $|\kappa|$) typical for the fine-structure formula (1).

Next, the energy levels of the one-electron ions were calculated for the following nuclei: B ($Z = 5, A = 10$), Ne ($Z = 10, A = 21$), Mn ($Z = 25, A = 5$), Sn ($Z = 50, A = 119$), U ($Z = 92, A = 238$), and that with $Z = 104$, $A = 261$. For hypothesized nuclei with $Z > 104$, the ratio A/Z was chosen to be equal to 2.9.

The results of the calculations for three lower energy levels and for the values of $\kappa = \pm 1, \pm 2, \pm 3$ are shown in Figs 1–6. For comparison, the same figures present some numerical results [11] and analytical values obtained from the fine-structure formula (1). In calculations [11], the nucleus radii were determined from the relationship $r_N = 1.2 \times 10^{-13} \times A^{1/3}$ cm.

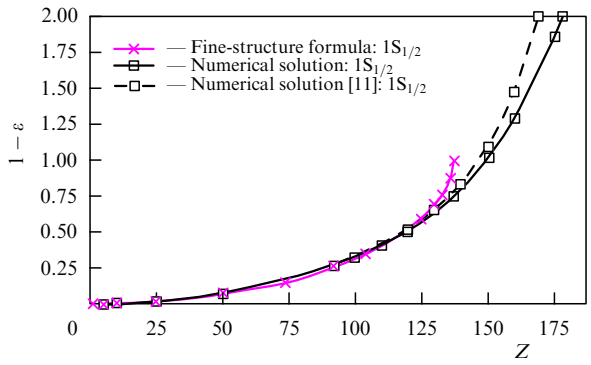

Figure 1. Plots of $E(Z)$ for the $1S_{1/2}$ state.

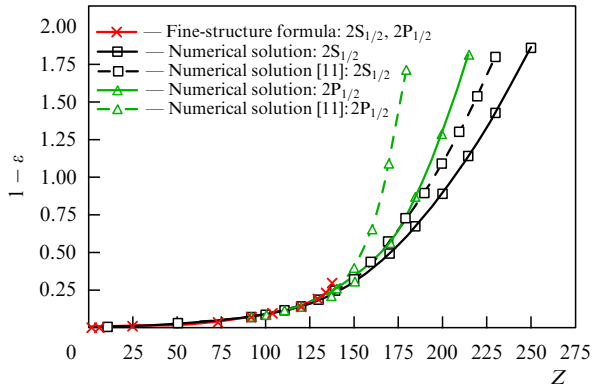

Figure 2. Plots of $E(Z)$ for the $2S_{1/2}$ and $2P_{1/2}$ states.

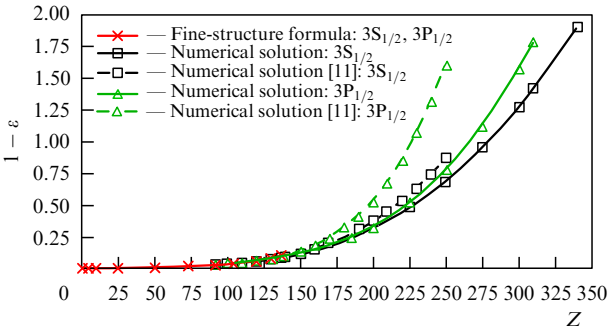

Figure 3. Plots of $E(Z)$ for the $3S_{1/2}$ and $3P_{1/2}$ states.

These data indicate that formula (1) give results being in good agreement with the calculated values of energy levels for all the known elements of the Periodic Table. At $\kappa = -1$ ($1S_{1/2}$), any noticeable discrepancy for the lower level ($> 1\,\%$) occurs for $Z > 105$ (see Fig. 1). The calculated plots of $E(Z)$ are smooth and monotonic. The lower level $1S_{1/2}$ reaches the value of $\varepsilon = -1$ (the electron 'drops' onto a nucleus) at $Z_c \approx 178$.

If the level $1S_{1/2}$ reaches the lower continuum $\varepsilon = -1$ for $Z > 178$, one must move from single-body quantum mechanics to many-body quantum field theory [8].

In this paper, the plots of $E(Z)$ for $Z > 178$ are shown in Figs 2–4 for methodological reasons. These plots have no singularities and are qualitatively similar to the plots of $E(Z)$ for the lower energy level $1S_{1/2}$.

In accordance with the results obtained in Ref. [8], one can see in Figs 2–4 that energy levels with the same j are no longer degenerate for $Z > 137$. As the values of n and κ grow, the

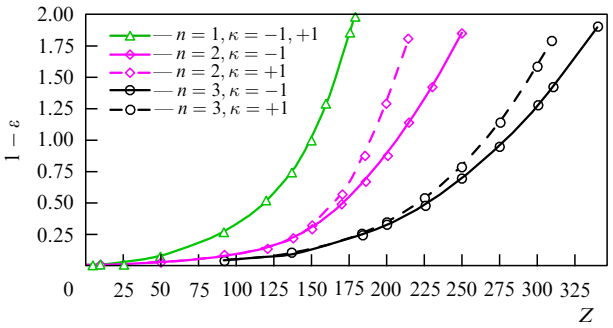

Figure 4. Calculated plots of $E(Z)$ for the states with $n = 1, 2, 3$ and $\kappa = \pm 1$.

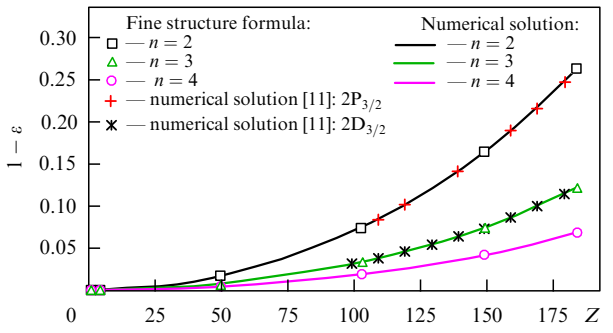

Figure 5. Plots of $E(Z)$ for $P_{3/2}$ and $D_{3/2}$ states and $n = 2, 3, 4$.

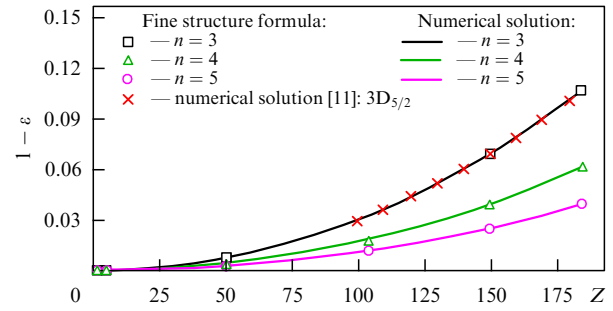

Figure 6. Plots of $E(Z)$ for the $D_{5/2}$ and $F_{5/2}$ states and $n = 3, 4, 5$.

values of Z, at which energy levels with the same j begin to differ, get higher. It follows from Figs 5, 6 that the energy levels $P_{3/2}$, $D_{3/2}$ and $D_{5/2}$, $F_{5/2}$ coincide up to $Z_c = 178$. These levels also demonstrate good agreement with the results obtained from a fine-structure formula.

As a result of effectively accounting for the finite size of nuclei using the boundary condition for the Dirac wave functions (21), (24), energy levels for $Z \leqslant 105$ practically coincide with those from the fine-structure formula (1) and with the results found in Refs [8, 11] using effective nucleus potentials (4), (6). This gives evidence of an absence of an appreciable effect of the electron location probability in a nucleus on the energy spectrum (maximum probability — in the calculations with the use of the singular Coulomb potential; smaller probability — in the calculations with the use of the finite electrostatic potentials of nuclei, and zero probability — in the calculations reported in this paper with the use of a boundary condition (21)).

For $Z > 105$, the plots of $E(Z)$ based on the results of this work are less steep (see Figs 1–6). This leads to a somewhat higher value of $Z_c = 178$ compared with $Z_c \approx 170$ found in Refs [8, 11]. The difference between the plots of $E(Z)$ decreases as the quantum numbers n and κ grow.

A single-electron quantum-mechanical consideration becomes more approximate when Z increases. It is necessary to take into account the effects of quantum electrodynamics and take advantage of a many-body relativistic quantum theory of heavy and superheavy nuclei. Considering this fact, the value of $Z_c = 178$ derived in this paper with the boundary condition (21), which provides a zero probability of electron location within a nucleus, should be considered as the upper limit of the true value of Z_c. A formulation of conditions which must be fulfilled to determine Z_c in future experiments may be found in review [10].

5. Conclusion

The calculations aimed to determine energy levels of hydrogen-like atoms with effectively accounting (21) for the finite size of nuclei allow us to draw the following conclusions:

(1) Calculated results with $Z = 1$, $A = 1$ reproduce the fine-structure formula (1) for the hydrogen atom to within $\sim 10^{-4}$.

(2) Calculated results are in a good agreement with the fine-structure formula for all the known nuclei of the Periodic Table. For the lower energy level, any noticeable discrepancy occurs for $Z > 105$.

(3) The calculated plots of $E(Z)$ are smooth and monotonic.

(4) The lower level $1S_{1/2}$ reaches the value of $\varepsilon = -1$ ($E = -mc^2$ is the electron 'drop' onto a nucleus) at $Z_c = 178$.

(5) To account for the finite size of nuclei, the boundary condition (21), which works well for the one-electron case, can be easily applied to calculations of many-electron atoms using solutions of the Dirac equation for radial wave functions.

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