Electronic Structure of Super Heavy Atoms. Revisited.

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The electronic structure of an atom with $Z \leq Z_c = 137$ can be described by the Dirac equation with the Coulomb field of a point charge $Ze$. It was believed that the Dirac equation with $Z > Z_c$ meets difficulties because the formula for the lower energy level of the Dirac Hamiltonian formally gives imaginary eigenvalues. But a strict mathematical consideration shows that difficulties with the electronic spectrum for $Z > Z_c$ do not arise if the Dirac Hamiltonian is correctly defined as a self-adjoint operator. In this article, we briefly summarize the main physical results of that consideration in a form suitable for physicists with some additional new details and numerical calculations of the electronic spectra.

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1. INTRODUCTION

The question of electronic structure of an atom with large charge number $Z$ of the nucleus, especially with $Z$ that is more than the critical value $Z_c = \alpha^{-1} \approx 137.04$, where $\alpha$ is the finite structure constant, is of fundamental importance. The formulation of QED cannot be considered really completed until an exhaustive answer to this question is given. Although nuclei with overcritical charges can hardly be synthesized (at present, the maximum is $Z = 118$), the existing heavy nuclei can imitate the supercritical Coulomb fields at collision. Nuclear forces can hold the colliding nuclei together for $10^{-19}$ s or more. This time is enough to effectively reproduce the experimental situation where the electron experiences the supercritical Coulomb field [2].

The electronic structure of an atom with $Z \leq Z_c$ can be described by the Dirac equation, which gives relativistic electronic spectra in agreement with experiment [3]. For such $Z$ a complete set of solutions of the Dirac equation exists; the corresponding Coulomb field does not violate the vacuum stability, therefore, the Furry picture in QED can be constructed, and the relativistic quantum mechanics of an electron in such a Coulomb field based on the Dirac equation is self-consistent. It was believed that the Dirac equation with $Z > Z_c$ meets difficulties [4–6]. One of the standard arguments is that the formula for the lower energy level,

$$E = mc^2 \sqrt{1 - \left(\frac{Z\alpha}{\sqrt{1 - (Z\alpha)^2}}\right)^2},$$

formally gives imaginary result for $Z > Z_c$. This difficulty of the imaginary spectrum was attributed to an inadmissible singularity of the supercritical Coulomb field at the origin for a relativistic electron, see [7]. It was believed that this difficulty can be eliminated if a nucleus of some finite radius $R$ is considered. It was shown that with cutting off the Coulomb potential with $Z < 173$ at a radius $R \sim 1.2 \times 10^{-12}$ cm, the Dirac Hamiltonian has physically meaningful spectrum and eigenstates [8, 9]. But even in the presence of the cutoff, another difficulty arises at $Z \sim 173$. Namely, the lower bound state energy descends to the upper boundary $E = -mc^2$ of the lower continuum, and it is generally agreed that in such a situation, the problem can no longer be considered a one-particle one because of the electron-positron pair production, which, in particular, results in a screening of the Coulomb potential of the nucleus. Probabilities of the particle production in the heavy-ion collisions were calculated within the framework of this conception [2]. Unfortunately, experimental conditions for verifying the corresponding predictions are unavailable at present.

Not disputing the fact that taking account of a finite size of the nucleus corresponds to a more realistic setting up the problem, we do not agree with the assertion that the Dirac Hamiltonian with the Coulomb field of overcritical point-like nucleus charge is inconsistent. The above-mentioned difficulties with the spectrum for $Z > Z_c$ do not arise if the Dirac Hamiltonian is correctly defined as a self-adjoint (s.a.) operator. A first heuristic attempt in this direction is due to [10]. A rigorous mathematical treatment of all the aspects of this problem including a spectral analysis of the Hamiltonian based on the theory of s.a. extensions of symmetric operators and the Krein method of guiding functionals was presented in [1, 11, 12]. It was demonstrated that from a mathematical standpoint, a...
definition of the Dirac Hamiltonian as a s.a. operator presents no problem for arbitrary \( Z \). A specific feature of the overcritical charges is a nonuniqueness of the s.a. Dirac Hamiltonian, but this nonuniqueness is characteristic even for \( Z > Z_0 = (\sqrt{3}/2) \alpha^{-1} \approx 118.68 \). For each \( Z \geq Z_0 \), there exist a family of s.a. Dirac Hamiltonians parametrized by a finite number of extra parameters (and specified by additional boundary conditions at the origin). The existence of these parameters is a manifestation of a nontrivial physics inside the nucleus. A real spectrum and a complete set of eigenstates can be evaluated for each Hamiltonian, so that a relativistic quantum mechanics for an electron in such a Coulomb field can be constructed.

In the present article, we briefly summarize all the previously obtained formal results in a form more suitable for physicists with some additional new important details and numerical calculations of the electronic spectra. The spectrum of each Hamiltonian consists of a universal continuous part that is a union of two intervals \((-\infty, m)\) and \([m, \infty)\) and a specific discrete spectrum located in the interval \([-m, m)\). We concentrate on the discrete spectrum.

2. DIRAC HAMILTONIAN WITH COULOMB FIELD

We consider an electron of charge \(-e < 0\) and mass \( m \) moving in the Coulomb field of charge \( Ze > 0 \). We describe this field by a scalar electromagnetic potential of the form \( A_0 = Zev^{-1} \), we set \( \hbar = c = 1 \) in what follows. A behavior of the electron in the Coulomb field is governed by the Dirac Hamiltonian \( \hat{H}(Z) \) that is a s.a. operator in the Hilbert space \( \mathfrak{H} \) of square-integrable bispinors \( \Psi(r) \). On its domain which must be properly specified, \( \hat{H}(Z) \) acts by the differential operation

\[
\hat{H}(Z) = \gamma^0 (\gamma \hat{p} + m) - q r^{-1}, \quad \hat{p} = -i \nabla, \quad r = |r|, \quad q = Z \alpha
\]

(2)

(in what follows, we use \( \gamma \)-matrices in the standard representation). In the problem under consideration, there are three commuting s.a. operators \( \hat{J}^2, \hat{J}_z, \) and \( \hat{K} \), where \( \hat{J} \) is the total angular momentum and \( \hat{K} \) is the so-called spin operator

\[
\hat{J} = \hat{L} + \Sigma/2, \quad \hat{L} = [r \times \hat{p}], \quad \hat{K} = \gamma^0 \left[ 1 + \left( \Sigma \hat{L} \right) \right].
\]

All they commute with \( \hat{H}(Z) \). Any bispinor \( \Psi(r) \) can be represented as \( \Psi(r) = \sum_{j, M, \zeta} \Psi_{j, M, \zeta} (r) \), where \( \Psi_{j, M, \zeta} \) are bispinors of the form

\[
\Psi_{j, M, \zeta} (r) = \frac{1}{r} \left( \frac{\Omega_{j, M, \zeta}(\theta, \varphi)f(r)}{i \Omega_{j, M, -\zeta}(\theta, \varphi)g(r)} \right),
\]

(3)

\( \Omega_{j, M, \zeta} \) are normalized spherical spinors, \( f(r) \) and \( g(r) \) are radial functions, and \( j = 1/2, 3/2, \ldots, M = -j, -j+1, \ldots, j, \zeta = \pm \). Bispinors \( \Psi_{j, M, \zeta} \) are eigenvectors of \( \hat{J}^2, \hat{J}_z, \) and \( \hat{K} \),

\[
\hat{J}^2 \Psi = j(j+1) \Psi, \quad \hat{J}_z \Psi = M \Psi, \quad \hat{K} \Psi = -\zeta (j+1/2) \Psi.
\]

Let \( L^2 (\mathbb{R}_+) = L^2 (\mathbb{R}_+) \oplus L^2 (\mathbb{R}_+) \) (where \( L^2 (\mathbb{R}_+) \) is the space of functions of \( r \) square-integrable on the semiaxis \( \mathbb{R}_+ = [0, \infty) \)) be the Hilbert space of doublets \( F(r) \),

\[
F(r) = \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = (f(r)/g(r)),
\]

with the scalar product

\[
(F_1, F_2) = \int_{\mathbb{R}_+} dr F_1^+ (r) F_2 (r) = \int_{\mathbb{R}_+} dr \left[ f_1 (r)f_2 (r) + g_1 (r)g_2 (r) \right].
\]

Then rep. (2) and the relation

\[
||\Psi_{j, M, \zeta}||^2 = \int_{\mathbb{R}_+} dr [ |f(r)|^2 + |g(r)|^2 ]
\]

show that any subspace of bispinors \( \Psi_{j, M, \zeta} \) with fixed \( j, M, \zeta \) is unitary equivalent to \( L^2 (\mathbb{R}_+) \), an explicit form of this equivalence is

\[
\Psi_{j, M, \zeta}(r) = r^{-1} \Pi_{j, M, \zeta}(\theta, \varphi)F(r), \quad F(r) = r \int \sin \theta d\theta d\varphi \Pi_{j, M, \zeta}^+(\theta, \varphi) \Psi_{j, M, \zeta}(r).
\]

(4)
Here, $\Pi_{j,M,\zeta}$ and $\Pi_{j,M,\zeta}^+$ are the respective $(4 \times 4)$- and $(2 \times 4)$-matrices,

$$
\Pi_{j,M,\zeta} = \begin{pmatrix} \Omega_{j,M,\zeta} & 0 \\
0 & i\Omega_{j,M,\zeta}\end{pmatrix},
\Pi_{j,M,\zeta}^+ = \begin{pmatrix} \Omega_{j,M,\zeta}^+ & 0^T \\
0^T & -i\Omega_{j,M,\zeta}^+\end{pmatrix},
$$

$$
\int \sin \theta d\theta d\varphi \left[ \Pi_{j,M,\zeta}^+(\theta,\varphi)\Pi_{j,M,\zeta}(\theta,\varphi) \right]_{ab} = \delta_{ab}, \ a, b = 1, 2,
$$

where $0 = (0/0)$ is a two-column and $0^T = (0, 0)$ is a two-row. The stationary Schrödinger equation $\hat{H}(Z)\Psi(r) = E\Psi(r)$ in the Hilbert space $\mathcal{H}$ is reduced to radial equations

$$
\hat{h}(Z,j,\zeta)F(r) = EF(r), \quad F \in L^2(\mathbb{R}^+_+),
$$

in the Hilbert space $L^2(\mathbb{R}^+_+)$, where $\hat{h}(Z,j,\zeta)$ are s.a. partial radial Hamiltonians acting on the doublets $F(r)$ by radial differential operations

$$
\hat{h}(Z,j,\zeta) = -i\sigma_2d_r + \zeta(j + 1/2)r^{-1}\sigma_1 - qr^{-1} + m\sigma_3.
$$

The problem of constructing a rotationally invariant s.a. Dirac Hamiltonian $\hat{H}(Z)$ is reduced to the problem of constructing s.a. partial radial Hamiltonians $\hat{h}(Z,j,\zeta)$. We construct all possible s.a. partial radial Hamiltonians $\hat{h}(Z,j,\zeta)$ using the theory of s.a. extensions of symmetric operators, which is reduced to specifying their domains of definition $D_{\hat{h}(Z,j,\zeta)} \subset L^2(\mathbb{R}^+_+)$. By construction, each operator $\hat{h}(Z,j,\zeta)$ is a s.a. extension of the so-called initial symmetric operator $\hat{h}_{in}(Z,j,\zeta)$ with the domain $D_{\hat{h}_{in}(Z,j,\zeta)} = D(\mathbb{R}^+_+) \oplus D(\mathbb{R}^+_+)$, where $D(\mathbb{R}^+_+)$ is a space of smooth compactly supported functions on the semiaxis $\mathbb{R}^+$, and (simultaneously) is, generally, a s.a. restriction of the adjoint operator $\hat{h}_{in}^+(Z,j,\zeta)$ defined on the so-called natural domains $D_{\hat{h}(Z,j,\zeta)}^*(\mathbb{R}^+_+) \subset D_{\hat{h}(Z,j,\zeta)}(\mathbb{R}^+_+)$ of doublets $F \in L^2(\mathbb{R}^+_+)$ that are absolutely continuous in $\mathbb{R}^+$ and such that $\hat{h}(Z,j,\zeta)F \in L^2(\mathbb{R}^+_+)$. Thus, $D_{\hat{h}(Z,j,\zeta)} \subset D_{\hat{h}(Z,j,\zeta)} \subset D_{\hat{h}(Z,j,\zeta)}^*(\mathbb{R}^+_+)$, and if $D_{\hat{h}(Z,j,\zeta)}$ does not coincide with $D_{\hat{h}(Z,j,\zeta)}^*(\mathbb{R}^+_+)$, it is specified by some additional asymptotic boundary conditions at the origin, which are defined not uniquely.

A result of constructing s.a. radial Hamiltonians $\hat{h}(Z,j,\zeta)$ essentially depends on the values of the parameters $Z$ and $j$.

There are two regions in the first quadrant of the $j, Z$ plane, we call them the nonsingular and singular ones, where the problem of s.a. extensions has principally different solutions. These regions are separated by the singular curve $Z = Z_s(j)$, where

$$
Z_s(j) = \sqrt{j(j + 1)}\alpha^{-1},
$$

so that the nonsingular and singular regions are defined by the respective inequalities $Z \leq Z_s(j)$ and $Z > Z_s(j)$. The values

$$
Z_s(1/2) = 118, 68; \quad Z_s(3/2) = 265, 37; \quad Z_s(5/2) = 405, 36; \quad \ldots,
$$

can be called the singular values of $Z$ for a given $j$, see FIG. 1.

In what follows, we describe s.a. radial Hamiltonians $\hat{h}(Z,j,\zeta)$ and their spectra in the nonsingular and singular regions separately. The consideration in the non-singular and singular regions is true for the whole set of all quantum numbers.

All the mathematical details concerning s.a. extensions and a spectral analysis of Hamiltonians (including complete sets of eigenfunctions) based on the Krein method of guiding functionals can be found in $[1, 11, 12]$.

3. NONSINGULAR REGION

In the nonsingular region, $Z \leq Z_s(j)$, the partial radial Hamiltonian $\hat{h}(Z,j,\zeta)$ is defined uniquely, $\hat{h}(Z,j,\zeta) = \hat{h}_{in}^+(Z,j,\zeta)$, and its domain is $D_{\hat{h}(Z,j,\zeta)} = D_{\hat{h}(Z,j,\zeta)}^*(\mathbb{R}^+_+)$. The functions belonging to $D_{\hat{h}(Z,j,\zeta)}^*(\mathbb{R}^+_+)$ have the following asymptotic behavior

$$
F(r) = O(r^{1/2}), \quad r \to 0; \quad F(r) \to 0, \quad r \to \infty.
$$
A discrete spectrum \( \{ E_{n(\zeta)}(Z,j,\zeta) \} \) of each Hamiltonian \( \hat{h}(Z,j,\zeta) \) is given by

\[
E_{n(\zeta)}(Z,j,\zeta) = \frac{m(n(\zeta) + \gamma)}{\sqrt{q^2 + (n(\zeta) + \gamma)^2}}; \quad \gamma = \sqrt{(j + 1/2)^2 - q^2}.
\]

(6)

The quantum numbers \( n(\zeta) \) take the values

\[
n(+) \in \mathbb{N} = \{1, 2, \ldots\}; \quad n(+) \in \mathbb{Z}_+ = \{0, 1, 2, \ldots\}.
\]

(7)

The expression (6) coincides with the well-known Sommerfeld formula for the spectrum of the Dirac electron in the Coulomb field. This result justifies the standard formal treatment of the Dirac Hamiltonian with \( Z \) in the nonsingular region in the physical literature where the Dirac Hamiltonian is identified with the differential operation \( \hat{H}_D(Z) \) and the natural domain is implicitly assumed.

4. SINGULAR REGION

In the singular region, \( Z > Z_s(j) \), the s.a. radial Hamiltonian \( \hat{h}(Z,j,\zeta) \) with given \( Z,j,\zeta \) is defined not uniquely (the deficiency indices of the operator \( \hat{h}_{\text{in}}(Z,j,\zeta) \) are \((1,1))\). There exists a one-parameter family \( \{ \hat{h}_\nu(Z,j,\zeta), \nu \in [\pi/2, \pi/2], -\pi/2 \sim \pi/2 \} \) of Hamiltonians defined on different domains \( D_{\hat{h}_\nu(Z,j,\zeta)} \subset D_{\hat{h}(q,\kappa)}(\mathbb{R}_+^+) \) specified by different asymptotic s.a. boundary conditions at the origin, which are parametrized by the parameter \( \nu \).

The position of the discrete energy levels \( E_{n(\nu)}^{(\nu)}(Z,j,\zeta) \) essentially depends on \( \nu \), in particular, there exists a value \( \nu = \nu_m \), for which the lower energy level coincides with the boundary \( E = -m \) of the lower continuous spectrum.

Technically, it is convenient to divide the singular region into three subregions, we call them subcritical, critical, and overcritical regions. The subregions are distinguished by a character of asymptotic boundary conditions at the origin.

The boundary conditions are similar in each subregion, which provides similar solutions of the corresponding spectral problems. In what follows, we describe these subregions, the domains \( D_{\hat{h}_\nu(Z,j,\zeta)} \) in these subregions, and some details of discrete spectra.

4.1. Subcritical regions

The subcritical region is defined by the inequalities \( Z_s(j) < Z < Z_c(j) \), where

\[
Z_c(j) = (j + 1/2)\alpha^{-1},
\]

(8)
can be found explicitly. For \( \nu \) are equivalent and therefore the Hamiltonians \( \hat{h}_\nu (Z, j, \zeta) \) are specified by s.a. boundary conditions,

\[
F(r) = c((mr)^\gamma d_+ \cos \nu + (mr)^{-\gamma} d_- \sin \nu) + O(r^{1/2}), \quad r \to 0,
\]

where \( \gamma = \sqrt{(j + 1/2)^2 - q^2}, \) \( 0 < \gamma < 1/2, \) \( c \) is an arbitrary complex number, and \( d_\pm \) are some constant doublets.

The spectrum of each \( \hat{h}_\nu (Z, j, \zeta) \) is simple (nondegenerate) and consists of a continuous part that is the set \((-\infty, -m] \cup [m, \infty)\) and a discrete part located in the interval \([-m, m)\). The discrete spectrum is a growing infinite sequence \( \{E^{(\nu)}_{n_0(\zeta)} (Z, j, \zeta)\} \) of the energy levels that are the roots of the equation

\[
\frac{f(E) \cos \nu + \Gamma(1 - 2\gamma) \sin \nu}{f(E) \sin \nu - \Gamma(1 - 2\gamma) \cos \nu} = 0,
\]

\[
f(E) = \frac{\Gamma(1 + 2\gamma)(\gamma - qE\tau^{-1})[\gamma(m - E) - (\zeta + \gamma)\tau]}{\Gamma(\gamma - qE/\tau)(\gamma(m - E) - (\zeta - \gamma)\tau)(2\tau/m)^{2\gamma}} = 0,
\]

\[
\nu = \zeta(j + 1/2), \quad \tau = \sqrt{m^2 - E^2},
\]

the integers \( n_0(\zeta) \) take the previous values \( [5] \).

We outline the most important features of the discrete spectrum. For each \( Z, j, \zeta \), there exists \( \nu = \nu_m = \nu_m(Z, j) \) (independent of \( \zeta \)) such that the lowest energy level is equal to \(-m\). This \( \nu_m \) is determined from eq. \( [10] \) by setting \( E = -m \) and noting that \( f(-m) = \Gamma(1 + 2\gamma)(2q)^{-2\gamma} \) to yield

\[
\tan \nu_m = -\frac{\Gamma(1 + 2\gamma)}{\Gamma(1 - 2\gamma)} (2q)^{-2\gamma}
\]

For fixed \( n_0(\zeta) \), \( E^{(\nu)}_{n_0(\zeta)} (Z, j, \zeta) \) as functions of \( \nu \) are monotonically decreasing functions with the properties

\[
\lim_{\nu \to -\pi/2 + 0} E^{(\nu)}_{n_0(\zeta)} (Z, j, \zeta) = \lim_{\nu \to -\pi/2 - 0} E^{(\nu)}_{n_0(\zeta) + 1} (Z, j, \zeta) = E_{n_0(\zeta)}.
\]

Let

\[
n_0(\zeta) = n_0(\zeta)_{\text{min}} = \begin{cases} 1, & \zeta = + \\
0, & \zeta = -. \end{cases}
\]

A subtlety is that the function \( E^{(\nu)}_{n_0(\zeta)} (Z, j, \zeta) \) is defined only for \( \nu \in [-\pi/2, \nu_m) \), which implies that in the energy interval \([-m, E_{n_0(\zeta)}]\), there are no energy level for \( \nu \in (\nu_m, \pi/2) \), while for each \( \nu \in [-\pi/2, \nu_m) \), there is one level \( E^{(\nu)}_{n_0(\zeta)} (Z, j, \zeta) \) monotonically growing from \(-m\) to \( E_{n_0(\zeta)} \) when \( \nu \) changes from \( \nu_m \) to \(-\pi/2\).

The functions \( E^{(\nu)}_{n_0(\zeta)} (Z, j, \zeta) \) with \( n_0(\zeta) > n_0(\zeta) \) are defined for all \( \nu \in [-\pi/2, \pi/2] \). In each energy interval \([E_{n_0(\zeta)}, E_{n_0(\zeta) + 1}]\), there is one level \( E^{(\nu)}_{n_0(\zeta) + 1} (Z, j, \zeta) \) monotonically growing from \( E_{n_0(\zeta)} \) to \( E_{n_0(\zeta) + 1} \) when \( \nu \) changes from \( \pi/2 \) to \(-\pi/2\). We note that the states with the energies \( E^{(\nu)}_{n_0(\zeta) + 1} (Z, j, \zeta) \) and \( E^{(\nu)}_{n_0(\zeta) + 1} (Z, j, \zeta) = E^{(\nu)}_{n_0(\zeta) + 1} (Z, j, \zeta) = E_{n_0(\zeta)} \) represent the same eigenstate. It follows from the fact that according to eq. \([9]\), the values \( \nu = \pi/2 \) and \( \nu = -\pi/2 \) are equivalent and therefore the Hamiltonians \( \hat{h}_{\pi/2} (Z, j, \zeta) \) and \( \hat{h}_{-\pi/2} (Z, j, \zeta) \) are the same. The eigenvalues \( E_{n_0(\zeta)} \) can be found explicitly. For \( \nu = \pm\pi/2 \), eq. \([10]\) is reduced to the equation \( 1/f(E) = 0 \), and we find

\[
E_{n_0(\zeta)} = \frac{(n_0(\zeta) - \gamma)m}{\sqrt{q^2 + (n_0(\zeta) - \gamma)^2}}.
\]

In particular, we see that the discrete spectrum \( E^{(0)}_{n_0(\zeta)} (Z, j, \zeta) \) is given by eq. \([6]\) with \( Z \) corresponding to the region under consideration.

For illustration, we give graphs of five low energy levels \( (Z = 121, j = 1/2) \) as functions of \( \nu \) for \( \zeta = + \) (FIG. [2a]), for \( \zeta = - \) (FIG. [2b]), and also a graph of the parameter \( \nu_m \) \( j = 1/2 \) as a function of \( Z \), see FIG. [3].

In addition, to give an idea of energy scale, we give Table 1 of numerical values of some energy levels.
For fixed \( \alpha = \varepsilon \) where (independent of \( \zeta \))

\[
\text{the critical region, the s.a. radial Hamiltonian } \hat{h}_\nu (Z, j, \zeta) \text{ is specified by s.a. boundary conditions at the origin of the form}
\]

\[
F(r) = c [d_0(r) \cos \nu + d_+ \sin \nu] + O(r^{1/2} \ln r), \quad r \to 0,
\]

where \( d_0(r) \) are some doublet with the asymptotic behavior \( d_0(r) = O(\ln nr) \) as \( r \to 0 \).

The spectrum of each \( \hat{h}_\nu (Z, j, \zeta) \) is simple (nondegenerate) and consists of a continuous part that is the set \((-\infty, -m] \cup [m, \infty)\) and a discrete part located in the interval \([-m, m)\). The discrete spectrum is a growing infinite sequence \( \{E_{n(\zeta)}^{(\nu)} (Z, j, \zeta)\} \) of energy levels that are the roots of the equation

\[
\frac{g(E) \cos \nu - \sin \nu}{g(E) \sin \nu + \cos \nu} = 0, \quad g(E) = \ln(2\tau/m) + \psi(- (j + 1/2) E/\tau) + \frac{\zeta - (\tau + \zeta m) / E}{2(j + 1/2)} - 2\psi(1),
\]

where \( \psi(x) = \Gamma'(x)/\Gamma(x) \).

We outline the most important features of the discrete spectrum. For each \( Z, j, \zeta, \) there exists \( \nu = \nu_m = \nu_m (Z, j) \) (independent of \( \zeta \)) such that the lowest energy level is equal to \(-m\). This \( \nu_m \) is determined from eq. (12) by setting \( E = -m \) and noting that \( g(-m) = \ln(2q_c) - 2\psi(1) + \zeta/q_c \) to yield

\[
\tan \nu_m = \ln(2q_c) - 2\psi(1) + \zeta/q_c.
\]

For fixed \( n(\zeta) \), \( E_{n(\zeta)}^{(\nu)} (Z, j, \zeta) \) as functions of \( \nu \) are monotonically decreasing functions with the properties

\[
\lim_{\nu \to -\pi/2+0} E_{n(\zeta)}^{(\nu)} (Z, j, \zeta) = \lim_{\nu \to \pi/2-0} E_{n(\zeta)+1}^{(\nu)} (Z, j, \zeta) \equiv E_{n(\zeta)}.
\]
A subtlety is that the function $E_{n_0}^{(\nu)}(Z, j, \zeta)$ is defined only for $\nu \in [-\pi/2, \nu_{-m}]$, which implies that in the energy interval $[-m, E_{n_0}^{(\nu)}]$, there are no energy level for $\nu \in (\nu_{-m}, \pi/2]$, while for each $\nu \in [-\pi/2, \nu_{-m}]$, there is one level $E_{n_0}^{(\nu)}(Z, j, \zeta)$ monotonically growing from $-m$ to $E_{n_0}^{(\nu)}$ when $\nu$ changes from $\nu_{-m}$ to $-\pi/2$. The functions $E_{n_0}^{(\nu)}(Z, j, \zeta)$ are defined for all $\nu \in [-\pi/2, \pi/2]$. In each energy interval $[E_{n_0}^{(\nu)}, E_{n_0}^{(\nu)+1}]$, there is one level $E_{n_0}^{(\nu)}(Z, j, \zeta)$ monotonically growing from $E_{n_0}^{(\nu)}$ to $E_{n_0}^{(\nu)+1}$ when $\nu$ changes from $\pi/2$ to $-\pi/2$. We note that the states with the energies $E_{n_0}^{(-\pi/2)}(Z, j, \zeta)$ and $E_{n_0}^{(\pi/2)}(Z, j, \zeta) = E_{n_0}^{(-\pi/2)}(Z, j, \zeta) = E_{n_0}^{(\pi/2)}(Z, j, \zeta)$ are the same. The eigenvalues $E_{n_0}^{(\nu)}$ can be found explicitly. For $\nu = \pm\pi/2$, eq. (12) is reduced to the equation $1/g(E) = 0$, and we find

$$E_{n_0}^{(\nu)} = \frac{m n_0^{(\nu)}}{\sqrt{(j + 1/2)^2 + (n_0^{(\nu)})^2}}.$$ (13)

For illustration, we give graphs of five low energy levels $(j = 1/2)$ as functions of $\nu$, for $\zeta = +$ (FIG. 3a), for $\zeta = -$ (FIG. 3b). In addition, to give an idea of energy scale, we give Table 2 of numerical values of some energy levels.

![Graph of energy levels](image)

**FIG. 3:** $\nu$-dependence of energy levels $E_{n_0}^{(\nu)}(Z_c, 1/2, \zeta = \pm)$.

| $\nu$ | $E_0$ | $E_1$ | $E_2$ | $E_3$ | $E_4$ |
|-------|-------|-------|-------|-------|-------|
| $+$   | 0.1071707 | 0.707107 | 0.894427 | 0.894427 | 0.948680 | 0.948680 | 0.970143 | 0.970143 |
| $-$   | 0.7071707 | 0.894404 | 0.894404 | 0.948680 | 0.948680 | 0.970143 | 0.970143 |
| $0$   | 0.476777 | 0.548204 | 0.581750 | 0.864408 | 0.939071 | 0.983920 | 0.983944 | 0.985919 | 0.978405 |
| $+$   | 0.036533 | 0.466006 | 0.359245 | 0.854926 | 0.856797 | 0.936069 | 0.936298 | 0.960727 | 0.960788 |
| $0$   | 0.476777 | 0.548204 | 0.581750 | 0.864408 | 0.939071 | 0.983920 | 0.983944 | 0.985919 | 0.978405 |
| $-$   | 0.036533 | 0.466006 | 0.359245 | 0.854926 | 0.856797 | 0.936069 | 0.936298 | 0.960727 | 0.960788 |

**Table 2. Energy levels for $Z_c$, $j = 1/2$.**

4.3. **Overscritical region**

The overscritical region is defined by the inequality $Z > Z_c (j)$, $Z_c (j) = (j + 1/2) \alpha^{-1}$. In this region, the s.a. radial Hamiltonians $\hat{h}_\nu (Z, j, \zeta)$ are specified by s.a. boundary conditions

$$F(r) = c [ie^{i\nu}(mr)^{i\sigma}\rho_+ - ie^{-i\nu}(mr)^{-i\sigma}\rho_-] + O(r^{1/2}), \quad r \to 0,$$ (14)

where $\sigma = \sqrt{q^2 - (j + 1/2)^2}$, $c$ is an arbitrary complex number, and $\rho_{\pm}$ are some constant doublets.

The spectrum of each $\hat{h}_\nu (Z, j, \zeta)$ is simple (nondegenerate) and consists of a continuous part that is the set $(-\infty, -m] \cup [m, \infty)$ and a discrete part located in the interval $[-m, m)$. The discrete spectrum is a growing
infinite sequence \( \{E_n^{(v)}(Z, j, \zeta)\}, n \in \mathbb{Z}_+ \), of energy levels that are the roots of the equation

\[
\cos(\Theta(E) - \nu) = 0,
\]

(15)

\[
\Theta(E) = \frac{1}{2i} \sum_{a=1}^{3} \left[ \ln B_a - (\ln B_a)^* \right] + \sigma \ln \frac{2\tau}{m},
\]

where \( B_1 = -2i\sigma, B_2(E) = i\sigma - Eq\tau^{-1}, \) and \( B_3(E) = \tau(j + 1/2 - i\zeta\sigma) - \zeta q(m - E). \)

We outline the most important features of the discrete spectrum. For each \( Z, j, \zeta, \) there exists \( \nu = \nu_{-m} = \nu_{-m}(Z, j) \) (independent of \( \zeta \)) such that the lowest energy level is equal to \( -m \). This \( \nu_{-m} \) is determined from eq. (13) by setting \( E = -m \) which yields

\[
e^{\frac{2i(\nu_{-m} - \pi/2)}{m}} = \frac{\Gamma(-2i\sigma)}{\Gamma(2i\sigma)} (2q)^{2i\sigma}.
\]

The energy levels are determined by

\[
\Theta(-m) - \Theta(E_n^{(v)}(Z, j, \zeta)) = \pi n + \nu_{-m} - \nu.
\]

For fixed \( n, E_n^{(v)}(Z, j, \zeta) \) as functions of \( \nu \) are monotonically decreasing functions with the properties

\[
\lim_{\nu \to -\pi/2 + 0} E_n^{(v)}(Z, j, \zeta) = \lim_{\nu \to -\pi/2 - 0} E_n^{(v)}(Z, j, \zeta).
\]

A subtlety is that the function \( E_0^{(v)}(Z, j, \zeta) \) is defined only for \( \nu \in [-\pi/2, \nu_{-m}] \), which implies that in the energy interval \([-m, E_0^{(-\pi/2)}(Z, j, \zeta)]\), there are no energy level for \( \nu \in (\nu_{-m}, \pi/2) \), while for each \( \nu \in [-\pi/2, \nu_{-m}] \), there is one level \( E_n^{(v)}(Z, j, \zeta) \) monotonically growing from \(-m\) to \( E_0^{(-\pi/2)}(Z, j, \zeta) \) when \( \nu \) changes from \( \nu_{-m} \) to \(-\pi/2\).

The functions \( E_n^{(v)}(Z, j, \zeta) \) with \( n \geq 1 \) are defined for all \( \nu \in [-\pi/2, \pi/2] \). In each energy interval \([E_n^{(v)}(Z, j, \zeta), E_{n+1}^{(-\pi/2)}(Z, j, \zeta)]\), there is one level \( E_n^{(v)}(Z, j, \zeta) \) monotonically growing from \( E_n^{(v)}(Z, j, \zeta) \) to \( E_{n+1}^{(-\pi/2)}(Z, j, \zeta) \) when \( \nu \) changes from \(-\pi/2\) to \(-\pi/2\). We note that the states with the energies \( E_n^{(v)}(Z, j, \zeta) \) and \( E_{n+1}^{(-\pi/2)}(Z, j, \zeta) \) are the same eigenstate. It follows from the fact that according to eq. (14), the values \( \nu = \pi/2 \) and \( \nu = -\pi/2 \) are equivalent and therefore the Hamiltonians \( \hat{h}_{\pi/2}(Z, j, \zeta) \) and \( \hat{h}_{-\pi/2}(Z, j, \zeta) \) are the same.

We note that in contrast to previous regions, the integers \( n \) take the same values for both \( \zeta = + \) and \( \zeta = - \) because there is no the Sommerfeld degeneracy.

For illustration, we give graphs of five low energy levels (\( Z = 138, j = 1/2 \)) as functions of \( \nu \), for \( \zeta = + \) (FIG. 4b), and also a graph of the parameter \( \nu_{-m} \) as a function of \( Z \), see FIG. 3. In addition, to give an idea of energy scale, we give Table 3 of numerical values of some energy levels

| \( \nu \) | \( E_0 \) | \( E_1 \) | \( E_2 \) | \( E_3 \) | \( E_4 \) |
|---|---|---|---|---|---|
| \( \frac{-1}{2} \) | 0.705525 | 0.024086 | 0.893927 | 0.717081 | 0.948327 | 0.89653 | 0.969889 | 0.949229 | 0.983959 | 0.970294 |
| \( \frac{-1}{2} \) | 0.663227 | 0.075165 | 0.884039 | 0.682941 | 0.949152 | 0.887947 | 0.968399 | 0.946323 | 0.97355 | 0.96083 |
| 0 | 0.281658 | -0.42021 | 0.839196 | 0.584005 | 0.93119 | 0.865425 | 0.93119 | 0.865425 | 0.93119 | 0.865425 | 0.93119 |
| \( \frac{1}{2} \) | 0.742474 | 1.015125 | 0.903701 | 0.764449 | 0.951885 | 0.900914 | 0.971521 | 0.95389 |
| \( \frac{1}{2} \) | 0.705525 | 0.024086 | 0.893927 | 0.717081 | 0.948327 | 0.89653 | 0.969889 | 0.949229 | 0.983959 | 0.970294 |

| \( \zeta \) | + | - | + | - | + | - | + | - | + | - |

| \( \nu \) | \( E_0 \) | \( E_1 \) | \( E_2 \) | \( E_3 \) | \( E_4 \) |
|---|---|---|---|---|---|
| \( \frac{-1}{2} \) | 0.552275 | 0.233229 | 0.83542 | 0.742113 | 0.917366 | 0.883988 | 0.95099 | 0.936012 | 0.967737 | 0.959912 |
| \( \frac{-1}{2} \) | 0.364392 | -0.033728 | 0.796957 | 0.670614 | 0.90180 | 0.861427 | 0.941832 | 0.92676 | 0.964789 | 0.955329 |
| 0 | -0.005926 | -0.384817 | 0.743034 | 0.572097 | 0.886487 | 0.832513 | 0.937384 | 0.91555 | 0.960658 | 0.967177 |
| \( \frac{1}{2} \) | -0.83722 | -0.91167 | 0.660155 | 0.43226 | 0.86421 | 0.794284 | 0.928325 | 0.901662 | 0.956183 | 0.946368 |
| \( \frac{1}{2} \) | 0.552275 | 0.233229 | 0.83542 | 0.742113 | 0.917366 | 0.883988 | 0.95099 | 0.936012 | 0.967737 | 0.959912 |

| \( \zeta \) | + | - | + | - | + | - | + | - | + | - |

For comparison, we give graphs of five low energy levels (\( Z = 180, j = 1/2 \)) as functions of \( \nu \), for \( \zeta = + \) (FIG. 5b), for \( \zeta = - \) (FIG. 5b). In addition, to give an idea of energy scale, we give Table 4 of numerical values of some energy levels.
5. CONCLUDING REMARKS

Here, we list the properties of all the radial s.a. Hamiltonians which are common to both nonsingular and singular regions.

i) The spectrum of each s.a. Hamiltonian $\hat{h}(Z,j,\zeta)$ is simple (nondegenerate) and contains a continuous part that is the set $(-\infty, -m] \cup [m, \infty)$ and a discrete part $\{E_n(Z,j,\zeta)\}$ located in the interval $[-m, m]$; for a precise meaning of a nonnegative integer $n$, see the corresponding subsection.

ii) The discrete spectrum is always accumulated at the point $E = m$, and the asymptotic form of the difference $E_{n}^{\text{nonrel}} = E_n(Z,j,\zeta) - m$ as $n \to \infty$ is given by the well-known nonrelativistic formula

$$E_{n}^{\text{nonrel}} = -mq^2 \left(\frac{2n^2}{m} \right)^{-1},$$

the nonrelativistic spectrum does not depend on the extension parameter, $j$ and $\zeta$ (is degenerate in $j$ and $\zeta$).

iii) Eigenfunctions of the discrete spectrum and generalized eigenfunctions of the continuous spectrum form a complete orthonormalized system in $L^2(\mathbb{R}_+)$. As soon as all s.a. radial Hamiltonians $\hat{h}(Z,j,\zeta)$ are fixed unambiguously, a corresponding total s.a. Dirac Hamiltonian $\hat{H}(Z)$ is defined in a unique way.

Because s.a. radial Hamiltonians $\hat{h}(Z,j,\zeta)$ are unique for $Z \leq 118$, the total Dirac Hamiltonian $\hat{H}(Z)$ with $Z \leq 118$ is defined uniquely. For $Z \geq 119$, there is a family $\{\hat{H}_{\nu_1,\ldots,\nu_{\Delta}}(Z)\}$ of possible total s.a. Dirac Hamiltonians. The family is parametrized by the parameters $\nu_i \in [-\pi/2, \pi/2], -\pi/2 < \pi/2, i = 1, \ldots, \Delta$. The number $\Delta$ of the parameters is given by $\Delta = 2k(Z)$, where the integer $k(Z)$ is given by $k(Z) = (1/4 + Z^2\alpha^2)^{1/2} - \delta$, $0 < \delta \leq 1$. Any specific s.a. Dirac Hamiltonian $\hat{H}_{\nu_1,\ldots,\nu_{\Delta}}(Z)$ corresponds to a certain prescription for a behavior of an electron at the origin.
The general theory thus describes all the possibilities that can be offered to a physicist for his choice. This choice is a completely physical problem. We believe that each s.a. Dirac Hamiltonian with superstrong Coulomb field can be understood through an appropriate regularization of the potential and a subsequent limit process of removing the regularization. We recall that a physical interest in the electronic structure of superheavy atoms was mainly motivated by a possible pair creation in the superstrong Coulomb field. Consideration of this effect in the framework of the most simplest model of a point-like nucleus was accepted to be impossible due to the conclusion (which is wrong as it is clear now) that this model is mathematically inconsistent. We believe that a rehabilitation of the model allows returning to a consideration of the particle creation in this model providing considerable scope for analytical studies.

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