COMMENT

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Electronic structure of super heavy atoms revisited

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Abstract

The electronic structure of an atom with $Z \leqslant Z_c = 137$ can be described by the Dirac equation with the Coulomb field of a point charge Ze. It was believed that the Dirac equation with $Z > Z_c$ poses 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 paper, 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 a large charge number Z of the nucleus, especially with Z that is more than the critical value $Z_c = \alpha^{-1} \simeq 137.04$, where α is the finite structure constant, is of fundamental importance. The formulation of QED cannot be considered as really complete 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 $Z \leqslant Z_c$ can be described by the Dirac equation, which gives relativistic electronic spectra in agreement with experiment [3]. For such a 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 $Z > Z_c$ poses difficulties [4–6]. One of the standard arguments is that the formula for the lower energy level,

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

formally gives an 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 the cutting off of the Coulomb potential with $Z < 173$ at a radius $R \sim 1.2 \times 10^{-12}$ cm, the Dirac Hamiltonian has a 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 problem 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 into account a finite size of the nucleus corresponds to a more realistic setting up of 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 $Z > Z_s = (\sqrt{3}/2)\alpha^{-1} \simeq 118.68$. For each $Z \geqslant Z_s$, 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 paper, 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 a 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 $A_0 = Zer^{-1}$; we set $\hbar = c = 1$ in what follows. The behavior of the electron in the Coulomb field is governed by the Dirac Hamiltonian $\hat{H}(Z)$ that is an s.a. operator in the Hilbert space $\mathfrak{H}$ of square-integrable bispinors $\Psi(\mathbf{r})$. On its domain which must be properly specified, $\hat{H}(Z)$ acts by the differential operation

$$\check{H}(Z) = \gamma^0 \left(\boldsymbol{\gamma}\check{\mathbf{p}} + m \right) - qr^{-1}, \quad \check{\mathbf{p}} = -i\nabla,$$
$$r = |\mathbf{r}|, \quad q = Z\alpha \tag{2}$$

(in what follows, we use γ-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 $\hat{\boldsymbol{J}}$ is the total angular momentum and $\hat{K}$ is the so-called spin operator

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

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

$$\Psi_{j,M,\zeta}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} \Omega_{j,M,\zeta}(\theta,\varphi) f(r) \\ i\Omega_{j,M,-\zeta}(\theta,\varphi) g(r) \end{pmatrix}, \tag{3}$$

$\Omega_{j,M,\zeta}$ 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 $\hat{K}$,

$$\hat{J}^2\Psi = j(j+1)\Psi, \quad \hat{J}_z\Psi = M\Psi, \quad \hat{K}\Psi = -\zeta(j+1/2)\Psi. \tag{4}$$

Let $\mathbb{L}^2(\mathbb{R}_+) = L^2(\mathbb{R}_+) \oplus L^2(\mathbb{R}_+)$ (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 $F(r)$,

$$F(r) = \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} = (f(r) \diagup g(r)),$$

with the scalar product

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

Then representation (3) and the relation

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

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

$$\Psi_{j,M,\zeta}(\mathbf{r}) = r^{-1}\boldsymbol{\Pi}_{j,M,\zeta}(\theta,\varphi) F(r),$$
$$F(r) = r \int \sin\theta\, d\theta\, d\varphi\, \boldsymbol{\Pi}_{j,M,\zeta}^+(\theta,\varphi)\Psi_{j,M,\zeta}(\mathbf{r}). \tag{5}$$

Here, $\boldsymbol{\Pi}_{j,M,\zeta}$ and $\boldsymbol{\Pi}_{j,M,\zeta}^+$ are the respective (4×2)- and (2×4)-matrices,

$$\boldsymbol{\Pi}_{j,M,\zeta} = \begin{pmatrix} \Omega_{j,M,\zeta} & \mathbf{0} \\ \mathbf{0} & i\Omega_{j,M,-\zeta} \end{pmatrix},$$

$$\boldsymbol{\Pi}_{j,M,\zeta}^+ = \begin{pmatrix} \Omega_{j,M,\zeta}^+ & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0}^{\mathrm{T}} & -i\Omega_{j,M,-\zeta}^+ \end{pmatrix},$$

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

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

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

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

$$\check{h}(Z, j, \zeta) = -i\sigma_2 d_r + \zeta(j+1/2)r^{-1}\sigma_1 - qr^{-1} + m\sigma_3. \tag{6}$$

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
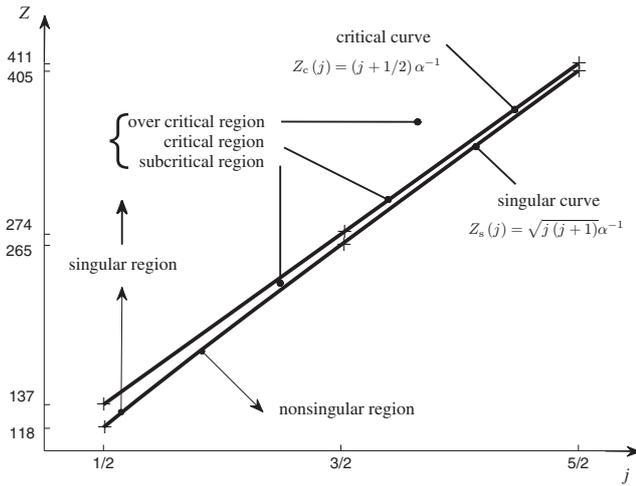
Figure 1. Regions in the j, Z plane. Singular and critical curves.

reduced to specifying their domains of definition $D_{\hat{h}(Z,j,\zeta)} \subset \mathbb{L}^2(\mathbb{R}_+)$. 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 $D_{\hat{h}_{in}(Z,j,\zeta)} = \mathcal{D}(\mathbb{R}_+) \oplus \mathcal{D}(\mathbb{R}_+)$, where $\mathcal{D}(\mathbb{R}_+)$ 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 $D_{\check{h}(Z,j,\zeta)}^*(\mathbb{R}_+)$ of doublets $F \in \mathbb{L}^2(\mathbb{R}_+)$ that are absolutely continuous in $\mathbb{R}_+$ and such that $\check{h}(Z, j, \zeta)F \in \mathbb{L}^2(\mathbb{R}_+)$. Thus, $D_{\hat{h}_{in}(Z,j,\zeta)} \subset D_{\hat{h}(Z,j,\zeta)} \subseteq D_{\check{h}(Z,j,\zeta)}^*(\mathbb{R}_+)$, and if $D_{\hat{h}(Z,j,\zeta)}$ does not coincide with $D_{\check{h}(Z,j,\zeta)}^*(\mathbb{R}_+)$, 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 $Z \leqslant Z_s(j)$ and $Z > Z_s(j)$. The values

$$Z_s(1/2) = 118.68, \quad Z_s(3/2) = 265.37,$$
$$Z_s(5/2) = 405.36, \ \ldots$$

can be called the singular values of Z for a given j, see figure 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 nonsingular 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, $Z \leqslant Z_s(j)$, 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 $D_{\hat{h}(Z,j,\zeta)} = D_{\check{h}(Z,j,\zeta)}^*(\mathbb{R}_+)$. The functions belonging to $D_{\check{h}(Z,j,\zeta)}^*(\mathbb{R}_+)$ 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

$$E_{n^{(\zeta)}}(Z, j, \zeta) = \frac{m(n^{(\zeta)} + \gamma)}{\sqrt{q^2 + (n^{(\zeta)} + \gamma)^2}},$$

$$\gamma = \sqrt{(j + 1/2)^2 - q^2}.$$

$$(7)$$

The quantum numbers $n^{(\zeta)}$ take the values

$$n^{(+)} \in \mathbb{N} = \{1, 2, \ldots\}, \quad n^{(-)} \in \mathbb{Z}_+ = \{0, 1, 2, \ldots\}. \quad (8)$$

Expression (7) 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 $\check{H}_D(Z)$ (2) 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 a given Z, j, ζ is defined not uniquely (the deficiency indices of the operator $\hat{h}_{in}(Z, j, \zeta)$ 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 $D_{\hat{h}_\nu(Z,j,\zeta)} \subset D_{\check{h}(q,\varkappa)}^*(\mathbb{R}_+)$ specified by different asymptotic s.a. boundary conditions at the origin, which are parametrized by the parameter ν.

The position of the discrete energy levels $E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta)$ essentially depends on ν; 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 the 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

$$Z_c(j) = (j + 1/2)\alpha^{-1}, \quad (9)$$

see figure 1. The values

$$Z_c(1/2) = Z_c = 137.04, \quad Z_c(3/2) = 274.08,$$
$$Z_c(5/2) = 411.12, \ldots$$

can be called the critical Z-value for a given j. In the subcritical region, the s.a. radial Hamiltonians $\hat{h}_\nu(Z, j, \zeta)$ are specified by s.a. boundary conditions

$$F(r) = c\left[(mr)^\gamma d_+ \cos \nu + (mr)^{-\gamma} d_- \sin \nu\right] + O(r^{1/2}),$$
$$r \to 0, \tag{10}$$

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 $\{E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta)\}$ of the energy levels that are the roots of the equation

$$\frac{f(E)\cos\nu + \Gamma(1 - 2\gamma)\sin\nu}{f(E)\sin\nu - \Gamma(1 - 2\gamma)\cos\nu} = 0, \tag{11}$$

$$f(E) = \frac{\Gamma(1 + 2\gamma)\Gamma(-\gamma - qE\tau^{-1})[q(m - E) - (\varkappa + \gamma)\tau]}{\Gamma(\gamma - qE/\tau)[q(m - E) - (\varkappa - \gamma)\tau](2\tau/m)^{2\gamma}},$$
$$\varkappa = \zeta(j + 1/2), \quad \tau = \sqrt{m^2 - E^2},$$

and the integers $n^{(\zeta)}$ take the previous values (8).

We outline the most important features of the discrete spectrum. For each Z, j, ζ, there exists $\nu = \nu_{-m} = \nu_{-m}(Z, j)$ (independent of ζ) such that the lowest energy level is equal to $-m$. This ν_{-m} is determined from equation (11) 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 $n^{(\zeta)}$, $E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta)$ as functions of ν are monotonically decreasing functions with the properties
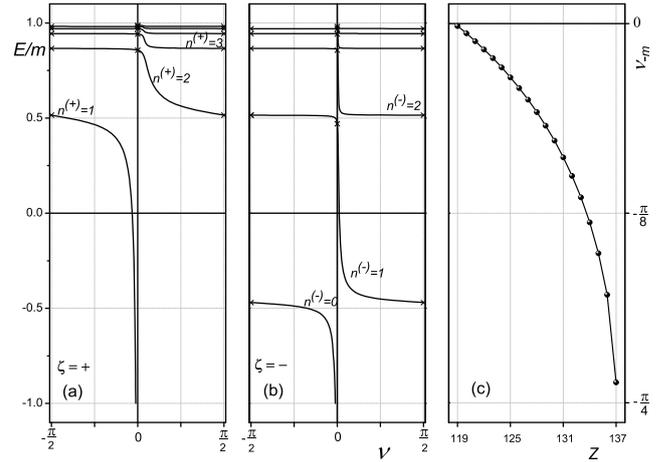
$$\lim_{\nu \to -\pi/2+0} E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta) = \lim_{\nu \to \pi/2-0} E_{n^{(\zeta)}+1}^{(\nu)}(Z, j, \zeta) \equiv \mathcal{E}_{n^{(\zeta)}}.$$

Let

$$n_0^{(\zeta)} = n_{\min}^{(\zeta)} = \begin{cases} 1, & \zeta = +, \\ 0, & \zeta = -. \end{cases}$$

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

The functions $E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta)$ with $n^{(\zeta)} > n_0^{(\zeta)}$ are defined for all $\nu \in [-\pi/2, \pi/2]$. In each energy interval $[\mathcal{E}_{n^{(\zeta)}}, \mathcal{E}_{n^{(\zeta)}+1}]$, there is one level $E_{n^{(\zeta)}+1}^{(\nu)}(Z, j, \zeta)$ monotonically growing from $\mathcal{E}_{n^{(\zeta)}}$ to $\mathcal{E}_{n^{(\zeta)}+1}$ when ν changes from $\pi/2$ to $-\pi/2$. We note that the states with the energies $E_{n^{(\zeta)}}^{(-\pi/2)}(Z, j, \zeta)$

Figure 2. The ν-dependence of energy levels $E_{n^{(\zeta)}}^{(\nu)}(121, 1/2, \zeta = \pm)$ and the Z-dependence of $\nu_{-m}|_{j=1/2}$.

and $E_{n^{(\zeta)}+1}^{(\pi/2)}(Z, j, \zeta) = E_{n^{(\zeta)}}^{(-\pi/2)}(Z, j, \zeta) = \mathcal{E}_{n^{(\zeta)}}$ represent the same eigenstate. It follows from the fact that according to equation (10), the values $\nu = \pi/2$ and $-\pi/2$ 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 $\mathcal{E}_{n^{(\zeta)}}$ can be found explicitly. For $\nu = \pm\pi/2$, equation (11) is reduced to the equation $1/f(E) = 0$, and we find that

$$\mathcal{E}_{n^{(\zeta)}} = \frac{(n^{(\zeta)} - \gamma)m}{\sqrt{q^2 + (n^{(\zeta)} - \gamma)^2}}.$$

In particular, we see that the discrete spectrum $E_{n^{(\zeta)}}^{(0)}(Z, j, \zeta)$ is given by equation (7) 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 ν, for $\zeta = +$ (figure 2(a)), for $\zeta = -$ (figure 2(b)), and also a graph of the parameter $\nu_{-m}|_{j=1/2}$ as a function of Z, see figure 2(c).

In addition, to give an idea of energy scale, we give in table 1 the numerical values of some energy levels.

4.2. Critical region

The critical region is the critical curve $Z = Z_c(j)$, see figure 1. For integer Z, this region does not exist if the fine structure constant α is an irrational number, see (9). In particular, this region is certainly absent for $j = 1/2$. In the critical region, the s.a. radial Hamiltonian $\hat{h}_\nu(Z, j, \zeta)$ is specified by s.a. boundary conditions at the origin of the form

$$F(r) = c[d_0(r)\cos\nu + d_+ \sin\nu] + O(r^{1/2}\ln r), \quad r \to 0, \tag{12}$$

where $d_0(r)$ are some doublet with the asymptotic behavior $d_0(r) = O(\ln mr)$ 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

Table 1. Energy levels for $Z = 121$, $j = 1/2$.

ν	$\mathbf{E_0}$		$\mathbf{E_1}$		$\mathbf{E_2}$		$\mathbf{E_3}$		$\mathbf{E_4}$	
$-\frac{\pi}{2}$	$-0.469\,411$	$0.515\,067$	$0.515\,067$	$0.866\,198$	$0.866\,198$	$0.944\,175$	$0.944\,175$	$0.970\,121$	$0.970\,121$	
$-\frac{\pi}{4}$	$-0.487\,899$	$0.465\,810$	$0.514\,264$	$0.865\,181$	$0.866\,078$	$0.943\,927$	$0.944\,142$	$0.970\,026$	$0.970\,108$	
0		$0.469\,41$	$0.857\,15$	$0.857\,15$	$0.941\,615$	$0.941\,615$	$0.969\,107$	$0.941\,615$		
$\frac{\pi}{4}$		$-0.450\,991$	$0.563\,241$	$0.515\,898$	$0.867\,497$	$0.866\,322$	$0.944\,482$	$0.944\,209$		
$\frac{\pi}{2}$		$-0.469\,411$	$0.515\,067$	$0.515\,067$	$0.866\,198$	$0.866\,198$	$0.944\,175$	$0.944\,175$		
ζ	$+$	$-$	$+$	$-$	$+$	$-$	$+$	$-$	$+$	$-$

of the equation

$$\frac{g(E)\cos \nu - \sin \nu}{g(E)\sin \nu + \cos \nu} = 0,$$

$$g(E) = \ln(2\tau/m) + \psi(-(j+1/2)\,E/\tau) \qquad (13)$$

$$+ \frac{\zeta - (\tau + \zeta m)/E}{2(j+1/2)} - 2\psi(1),$$

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

We now outline the most important features of the discrete spectrum. For each Z, j, ζ, there exists $\nu = \nu_{-m} = \nu_{-m}(Z, j)$ (independent of ζ) such that the lowest energy level is equal to $-m$. This ν_{-m} is determined from equation (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 a fixed $n^{(\zeta)}$, $E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta)$ as functions of ν are monotonically decreasing functions with the properties

$$\lim_{\nu \to -\pi/2+0} E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta) = \lim_{\nu \to \pi/2-0} E_{n^{(\zeta)}+1}^{(\nu)}(Z, j, \zeta) \equiv \mathcal{E}_{n^{(\zeta)}}.$$

A subtlety is that the function $E_{n_0^{(\zeta)}}^{(\nu)}(Z, j, \zeta)$ is defined only for $\nu \in [-\pi/2, \nu_{-m}]$, which implies that in the energy interval $[-m, \mathcal{E}_{n_0^{(\zeta)}})$, there are no energy levels for $\nu \in (\nu_{-m}, \pi/2]$, while for each $\nu \in [-\pi/2, \nu_{-m}]$, there is one level $E_{n_0^{(\zeta)}}^{(\nu)}(Z, j, \zeta)$ monotonically growing from $-m$ to $\mathcal{E}_{n_0^{(\zeta)}}$ when ν changes from ν_{-m} to $-\pi/2$. The functions $E_{n^{(\zeta)}}^{(\nu)}(Z, j, \zeta)$ with $n^{(\zeta)} > n_0^{(\zeta)}$ are defined for all $\nu \in [-\pi/2, \pi/2]$. In each energy interval $[\mathcal{E}_{n^{(\zeta)}}, \mathcal{E}_{n^{(\zeta)}+1}]$, there is one level $E_{n^{(\zeta)}+1}^{(\nu)}(Z, j, \zeta)$ monotonically growing from $\mathcal{E}_{n^{(\zeta)}}$ to $\mathcal{E}_{n^{(\zeta)}+1}$ when ν changes from $\pi/2$ to $-\pi/2$. We note that the states with the energies $E_{n^{(\zeta)}}^{(-\pi/2)}(Z, j, \zeta)$ and $E_{n^{(\zeta)}+1}^{(\pi/2)}(Z, j, \zeta) = E_{n^{(\zeta)}}^{(-\pi/2)}(Z, j, \zeta) = \mathcal{E}_{n^{(\zeta)}}$ represent the same eigenstate. It follows from the fact that according to equation (11), the values $\nu = \pi/2$ and $-\pi/2$ 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 $\mathcal{E}_{n^{(\zeta)}}$ can be found explicitly. For $\nu = \pm\pi/2$, equation (12) is reduced to the equation $1/g(E) = 0$, and we find that

$$\mathcal{E}_{n^{(\zeta)}} = \frac{mn^{(\zeta)}}{\sqrt{(j+1/2)^2 + (n^{(\zeta)})^2}}. \qquad (14)$$

For illustration, we give graphs of five low energy levels ($j = 1/2$) as functions of ν, for $\zeta = +$ (figure 3(a)), and for
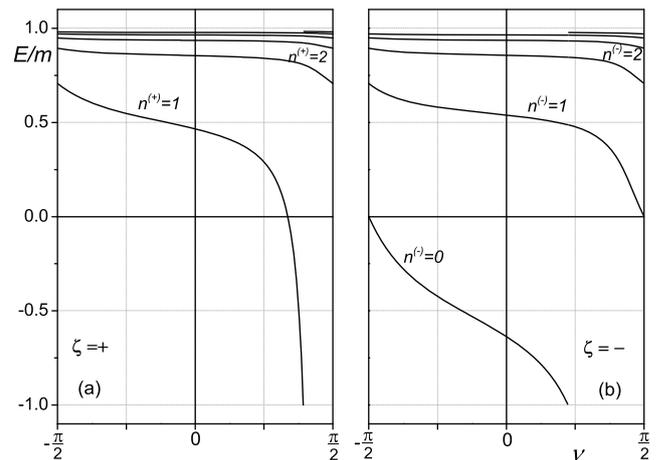
Figure 3. The ν-dependence of energy levels $E_{n^{(\zeta)}}^{(\nu)}(Z_c, 1/2, \zeta = \pm)$.

$\zeta = -$ (figure 3(b)). In addition, to give an idea of energy scale, we give in table 2 the numerical values of some energy levels.

4.3. Overcritical region

The overcritical 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

$$F(r) = c\left[\mathrm{ie}^{\mathrm{i}\nu}(mr)^{\mathrm{i}\sigma}\rho_+ - \mathrm{ie}^{-\mathrm{i}\nu}(mr)^{-\mathrm{i}\sigma}\rho_-\right] + O(r^{1/2}),$$
$$r \to 0, \qquad (15)$$

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 $\{E_n^{(\nu)}(Z, j, \zeta)\}$, $n \in \mathbb{Z}_+$, of energy levels that are the roots of the equation

$$\cos[\Theta(E) - \nu] = 0, \qquad (16)$$

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

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

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

ν	E_0		E_1		E_2		E_3		E_4	
$-\frac{\pi}{2}$	0		0.707107	0.707107	0.894427	0.894427	0.948683	0.948683	0.970143	0.970143
$-\frac{\pi}{4}$	0.476777		0.548043	0.581793	0.864486	0.939071	0.938 92	0.965944	0.965 91	0.978405
0	−0.636533		0.466006	0.539248	0.854923	0.856797	0.936069	0.936298	0.964727	0.964778
$\frac{\pi}{4}$			0.290246	0.476777	0.843971	0.803545	0.932388	0.920568	0.96309	0.963161
$\frac{\pi}{2}$			0	0.707107	0.707107	0.894427	0.894427	0.948683	0.948683	
ζ	+	−	+	−	+	−	+	−	+	−

We outline the most important features of the discrete spectrum. For each Z, j, ζ, there exists $\nu = \nu_{-m} = \nu_{-m}(Z, j)$ (independent of ζ) such that the lowest energy level is equal to $-m$. This ν_{-m} is determined from equation (16) by setting $E = -m$, which yields

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

The energy levels are determined by

$$\Theta(-m) - \Theta\left(E_n^{(\nu)}(Z, j, \zeta)\right) = \pi n + \nu_{-m} - \nu.$$

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

$$\lim_{\nu \to -\pi/2+0} E_n^{(\nu)}(Z, j, \zeta) = \lim_{\nu \to \pi/2-0} E_{n+1}^{(\nu)}(Z, j, \zeta).$$

A subtlety is that the function $E_0^{(\nu)}(Z, j, \zeta)$ 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 $E_0^{(\nu)}(Z, j, \zeta)$ monotonically growing from $-m$ to $E_0^{(-\pi/2)}(Z, j, \zeta)$ when ν changes from ν_{-m} to $-\pi/2$.

The functions $E_n^{(\nu)}(Z, j, \zeta)$ with $n \geqslant 1$ are defined for all $\nu \in [-\pi/2, \pi/2]$. In each energy interval $[E_n^{(\pi/2)}(Z, j, \zeta) = E_{n-1}^{(-\pi/2)}(Z, j, \zeta), E_n^{(-\pi/2)}(Z, j, \zeta)]$, there is one level $E_n^{(\nu)}(Z, j, \zeta)$ monotonically growing from $E_n^{(\pi/2)}(Z, j, \zeta) = E_{n-1}^{(-\pi/2)}(Z, j, \zeta)$ to $E_n^{(-\pi/2)}(Z, j, \zeta)$ when ν changes from $\pi/2$ to $-\pi/2$. We note that the states with the energies $E_n^{(-\pi/2)}(Z, j, \zeta)$ and $E_{n+1}^{(\pi/2)}(Z, j, \zeta)$ represent the same eigenstate. It follows from the fact that according to equation (14), the values $\nu = \pi/2$ and $-\pi/2$ 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 $-$ because there is no Sommerfeld degeneracy.

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

For comparison, we give graphs of five low energy levels ($Z = 180$, $j = 1/2$) as functions of ν, for $\zeta = +$ (figure 5(a)) and for $\zeta = -$ (figure 5(b)). In addition, to give an idea of energy scale, we give in table 4 the numerical values of some energy levels.
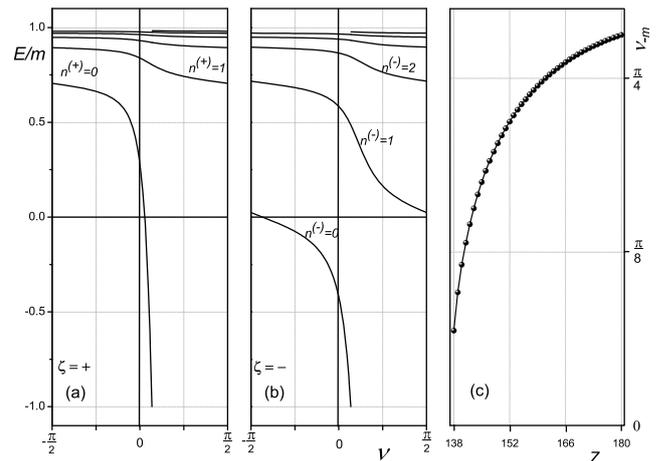
Figure 4. The ν-dependence of energy levels $E_n^{(\nu)}(138, 1/2, \zeta = \pm)$ and the Z-dependence of $\nu_{-m}|_{j=1/2}$.

5. Concluding remarks

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

1. 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.

2. 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 $\to \infty$ is given by the well-known nonrelativistic formula

$$E_n^{\text{nonrel}} = -mq^2(2n^2)^{-1},$$

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

3. Eigenfunctions of the discrete spectrum and generalized eigenfunctions of the continuous spectrum form a complete orthonormalized system in $\mathbb{L}^2(\mathbb{R}_+)$.

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 $Z \leqslant 118$, the total Dirac Hamiltonian $\hat{H}(Z)$ with $Z \leqslant 118$ is defined uniquely. For $Z \geqslant 119$, there is a family $\{\hat{H}_{\nu_1,\ldots,\nu_\Delta}(Z)\}$ of possibletotal s.a. Dirac Hamiltonians. The family is parametrized by the parameters $\nu_i \in [-\pi/2, \pi/2]$, $-\pi/2 \sim \pi/2$, $i = 1, \ldots, \Delta$. The number

Table 3. Energy levels for $Z = 138$, $j = 1/2$.

ν	E_0		E_1		E_2		E_3		E_4	
$-\frac{\pi}{2}$	0.705 525	0.024 086	0.893 927	0.717 081	0.948 327	0.896 53	0.969 889	0.949 229	0.980 395	0.970 294
$-\frac{\pi}{4}$	0.663 242	−0.075 165	0.884 039	0.682 943	0.944 912	0.887 947	0.968 366	0.946 203	0.979 595	0.968 93
0	0.281 658	−0.420 01	0.839 196	0.584 008	0.931 198	0.865 425	0.931 198	0.938 723	0.976 677	0.965 675
$\frac{\pi}{4}$			0.742 474	0.165 125	0.903 704	0.764 448	0.951 885	0.909 191	0.971 521	0.953 89
$\frac{\pi}{2}$			0.705 525	0.024 086	0.893 927	0.717 081	0.948 327	0.896 53	0.969 889	0.949 229
ζ	+	−	+	−	+	−	+	−	+	−

Table 4. Energy levels for $Z = 180$, $j = 1/2$.

ν	E_0		E_1		E_2		E_3		E_4	
$-\frac{\pi}{2}$	0.552 275	0.233 202	0.835 423	0.742 113	0.917 366	0.883 988	0.950 98	0.936 032	0.967 737	0.959 912
$-\frac{\pi}{4}$	0.363 492	−0.033 728	0.796 897	0.670 614	0.903 801	0.861 427	0.944 832	0.926 76	0.964 478	0.955 329
0	−0.005 928	−0.384 837	0.743 034	0.572 097	0.886 487	0.832 513	0.937 382	0.915 55	0.960 658	0.967 177
$\frac{\pi}{4}$	−0.837 22	−0.911 674	0.666 155	0.432 269	0.864 211	0.794 284	0.928 328	0.901 662	0.956 183	0.943 688
$\frac{\pi}{2}$			0.552 275	0.233 202	0.835 423	0.742 113	0.917 366	0.883 988	0.950 98	0.936 032
ζ	+	−	+	−	+	−	+	−	+	−
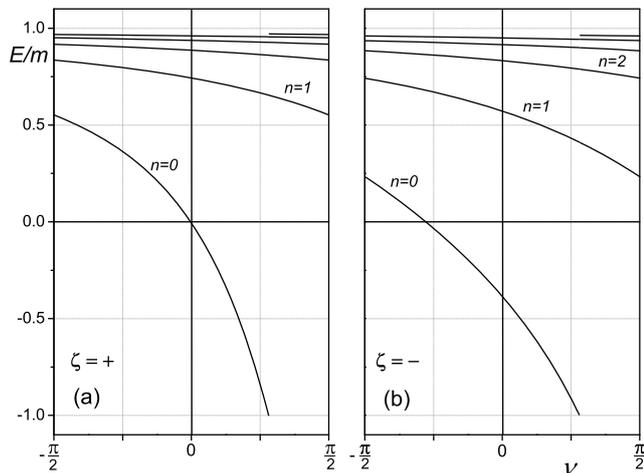
Figure 5. The ν-dependence of energy levels $E_n^{(\nu)}(180, 1/2, \zeta = \pm)$.

Δ of the parameters is given by $\Delta = 2k(Z)$, where the integer $k(Z)$ is given by $k(Z) = (1/4 + Z^2\alpha^2)^{1/2} - \delta$, $0 < \delta \leqslant 1$. Any specific s.a. Dirac Hamiltonian $\hat{H}_{\nu_1,\ldots,\nu_\Delta}(Z)$ corresponds to a certain prescription for the 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 a 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 the 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 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 [7]. 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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