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Dirac Hamiltonian with superstrong Coulomb field

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Abstract

We consider the quantum-mechanical problem of a relativistic Dirac particle moving in the Coulomb field of a point charge Ze . In the literature, it is often declared that a quantum-mechanical description of such a system does not exist for charge values exceeding the so-called critical charge with $Z = \alpha^{-1} = 137$ based on the fact that the standard expression for the lower bound state energy yields complex values at overcritical charges. We show that from the mathematical standpoint, there is no problem in defining a self-adjoint Hamiltonian for any value of charge. What is more, the transition through the critical charge does not lead to any qualitative changes in the mathematical description of the system. A specific feature of overcritical charges is a non uniqueness of the self-adjoint Hamiltonian, but this non uniqueness is also characteristic for charge values less than the critical one (and larger than the subcritical charge with $Z = (\sqrt{3}/2)\alpha^{-1} = 118$). We present the spectra and (generalized) eigenfunctions for all self-adjoint Hamiltonians. The methods used are the methods of the theory of self-adjoint extensions of symmetric operators and the Krein method of guiding functionals. The relation of the constructed one-particle quantum mechanics to the real physics of electrons in superstrong Coulomb fields where multiparticle effects may be of crucial importance is an open question.

Keywords: Dirac Hamiltonian, Coulomb field, self-adjoint extensions, spectral analysis.

1 Introduction

It is common knowledge that the complete sets of solutions of relativistic wave equations (like Klein-Gordon equation, Dirac equation, and so on) when used in quantizing the corresponding (scalar, spinor, and so on) free fields allow interpreting the corresponding quantum theories in terms of particles and antiparticles [1]. The space of quantum states of each such a field is decomposed into sectors with a definite number of particles (the vacuum, one-particle sector, and so on), each sector is stable under time evolution. A description of the one-particle sector of a free QFT can be formulated as a relativistic quantum mechanics where the corresponding relativistic wave equations play the role of the Schrödinger equation

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and their solutions are interpreted as wave functions of particles and antiparticles. In QED (and some other models), the concept of the external electromagnetic field is widely and fruitfully used. It can be considered an approximation in which a “very intensive” part of the electromagnetic field is treated classically and is not subjected to any back reaction of the rest of the system. The Dirac equation with such a field plays an important role in QED with an external field. Of special interest are the cases where an external field allows exactly solving the Dirac equation. There are a few of such exactly solvable cases of physically interesting external electromagnetic fields, see, e.g., [2]. They can be classified into groups such that the Dirac equations with fields of each group have a similar interpretation.

The constant uniform magnetic field, the plane-wave field, and their parallel combination form a first group, the fields of this group do not violate the vacuum stability (do not create particles from the vacuum). The exact solutions of the Dirac equation with such fields form complete systems and can be used in the quantization procedure providing a particle interpretation for a quantum spinor field in the corresponding external background. This allows constructing an approximation where the interaction with the external field is taken into account exactly, while the interaction with the quantized electromagnetic field is treated perturbatively. Such an approach to QED with external fields of the first group is known as the Furry picture, see, e.g., [3, 1]. In the Furry picture, the state space of the quantum theory of the spinor field with the external fields is decomposed into sectors with a definite number of particles, each sector is stable under time evolution similarly to the zero external-field case. The description of the one-particle sector also can be formulated as a relativistic quantum mechanics [4]. We note that the solutions of the Dirac equation with an uniform magnetic field provide a basis for the quantum synchrotron radiation theory [5], and the solutions of the Dirac equation with the plane-wave field are widely used for calculating the quantum effects when electrons and other particles of spin one-half move in laser beams [6].

A uniform electric field and some other electromagnetic fields violate the vacuum stability. A literal application of the above approach to constructing the Furry picture in QED with such fields fails. However, it was demonstrated that existing exact solutions of the Dirac equation with electric-type fields form complete sets and can be used for describing a variety of quantum effects in such fields, in particular, the electron-positron pair production from the vacuum [7]. Moreover, these sets of solutions form a basis for constructing a generalized Furry picture in QED with external fields violating the vacuum stability, see [8]. It should be noted that the one-particle sector in such external fields is unstable under time evolution, and therefore, the corresponding quantum mechanics of a spinning particle cannot be constructed in principle.

A study of the Dirac equation with a singular external Aharonov-Bohm field, and with some additional fields revealed problems of a new type. Although some sets of exact solutions of the Dirac equation with such fields can be found, the problem of the completeness of these sets arises. This problem is related to the fact that the Dirac Hamiltonian with the singular external Aharonov-Bohm field should be additionally specified for it can be treated as a self-adjoint (s.a. in what follows) quantum-mechanical operator. It can be shown (for a review, see [9]) that in this case, there exists a family of s.a. Hamiltonians which are constructed by methods of the theory of s.a. extensions of symmetric operators dating back to von Neumann [10]. Each s.a. Hamiltonian yields a complete set of solutions which can be used for constructing the Furry picture in QED with the singular external Aharonov-Bohm field

(this field does not violate the vacuum stability).

The Dirac equation with the Coulomb field, and with some additional fields, has always been of particular interest. The Coulomb field is even referred to as a "microscopic external field" to underline its qualitative distinction from the above-mentioned external fields which are sometimes referred to as "macroscopic" ones. Until recently, the commonly accepted view on the situation in the theory was the following. The Dirac equation for an electron of charge¹ $-e$ in an external Coulomb field created by a positive point-like electric charge Ze of a nucleus of atomic number² $Z \leq 1/\alpha = 137$ is solved exactly, has a complete set of solutions, and allows constructing a relativistic theory of atomic spectra which is in agreement with experiment [11]. This field does not violate the vacuum stability, therefore, the Furry picture can be constructed, and there exists the relativistic quantum mechanics of the spinning particle in such a Coulomb field. As for the Dirac equation with the Coulomb field with $Z > 137$, it was considered inconsistent and physically meaningless [12]–[15]. One of the standard arguments is that the formula for the lower $1S_{1/2}$ energy level,

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

formally gives imaginary eigenvalues for the Dirac Hamiltonian with $Z > 137$. On the one hand, the question of the consistency of the Dirac equation with the Coulomb field with $Z > 137$ has a pure theoretical (mathematical) interest, on the other hand, it is concerned with the question of the electron structure of atoms of atomic numbers $Z > 1/\alpha$ and especially of atoms with nuclei of supercritical charge $Ze > 170e$. The latter question is of fundamental importance. The formulation of QED cannot be considered really completed until an exhaustive answer to this question is given. Although nuclei of so large electric charges can hardly be synthesized³, 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 reproduce effectively the experimental situation where the electron experiences the supercritical Coulomb field [15]. Several groups of researchers attacked the problem of the behavior of the electron in the supercritical Coulomb field, see [15], [16]. The difficulty of the imaginary spectrum in the case of $Z > 137$ was attributed to an inadmissible singularity of the supercritical Coulomb field for a relativistic electron⁴. 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 $Z < 170$ at a radius $R \sim 1,2 \times 10^{-12} \text{cm}$, the Dirac equation has physically meaningful solutions [17]. But even in the presence of the cut off, another difficulty arises at $Z \sim 170$. 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 in the framework of

¹ $e = 4,803 \times 10^{-10} \text{CGSE}$ is the magnitude of the electron charge.

² $\alpha = e^2/\hbar c$ is the fine structure constant.

³At present, the maximum $Z = 118$.

⁴An equation for the radial components of wave functions has the form of the nonrelativistic Schrödinger equation with an effective potential with the r^{-2} singularity at the origin, which is associated with "a fall to the center".

this conception [15]. Unfortunately, experimental conditions for verifying the corresponding predictions are unavailable at present.

In this paper, we turn back to the problem of the consistency of the Dirac equation with the Coulomb field with no cut off and with arbitrary nucleus charge values (with arbitrary Z). Our point of view is that the above-mentioned difficulties with the spectrum for $Z > 137$ do not arise if the Dirac Hamiltonian is correctly defined as a s.a. operator. We present a rigorous treatment of all the aspects of this problem including a complete spectral analysis of the model based on the theory of s.a. extensions of symmetric operators and the Krein method of guiding functionals. We show that from the mathematical standpoint, the definition of the Dirac Hamiltonian as a s.a. operator for arbitrary Z presents no problem. What's more, the transition from the noncritical charge region to the critical one does not lead to qualitative changes in the mathematical description of the system. A specific feature of the overcritical charges is a non uniqueness of the s.a. Dirac Hamiltonian, but this non uniqueness is characteristic even for charge values less than the critical one (and larger than the subcritical value with $Z = (\sqrt{3}/2)\alpha^{-1} = 118$). Presenting a rigorous treatment of the problem, we also compare it with the conventional physical approach to constructing a quantum-mechanical description of the relativistic Coulomb system. It turns out that many of mathematical results can be obtained from physical considerations except the important property of completeness for the eigenfunctions of the Hamiltonian. The obtained complete sets of solutions can be used to construct the Furry picture in QED. However, it is unclear whether the neglect of the radiative interaction in such a Furry picture is a good zero approximation to describing quantum effects in QED with the Coulomb field with no cut off and with arbitrary nucleus charge values. In other words, a relevance of the constructed quantum-mechanics with an energy spectrum unbounded from below to the real physics of an electron in supercritical Coulomb fields where multiparticle effects may be of crucial importance is an open question.

The paper is organized as follows. In Sec. 2, we present basic facts and formulas clarifying the formulation of the problem and reduce the problem of constructing a s.a. Dirac Hamiltonian with an external Coulomb field in the whole Hilbert space to the problem of constructing s.a. one-dimensional radial Hamiltonians. In Sec. 3, we cite expressions for the general solution of the radial equations and some particular solutions of these equations used in the following. In Subsec. 4.1 and Appendix 4.5.2, we outline procedures for constructing s.a. extensions of symmetric differential operators and their spectral analysis. In Subsecs. 4.2–4.5, we construct s.a. Dirac Hamiltonians in all four possible charge regions and find their spectra and the corresponding complete sets of eigenfunctions.

2 Setting the problem

We consider the Dirac equation for a particle of charge q_1 moving in the external Coulomb field of a point-like charge q_2 ; for an electron in a hydrogen-like atom, we have $q_1 = -e$, $q_2 = Ze$. We choose the electromagnetic potentials for such a field in the form

$$A_0 = \frac{q_2}{r}, \quad A_k = 0.$$

The Dirac equation with this field, being written in the form of the Schrödinger equation, is⁵:

$$i\frac{\partial\Psi(x)}{\partial t} = \check{H}\Psi(x), \quad x = (x^0, x^k) = (t, \mathbf{r}),$$

where $\Psi(x) = \{\psi_\alpha(x)\}$ is a bispinor and the Dirac Hamiltonian \check{H} is given by

$$\check{H} = \boldsymbol{\alpha}\check{\mathbf{p}} + m\beta - \frac{q}{r} = \begin{pmatrix} m - q/r & \boldsymbol{\sigma}\check{\mathbf{p}} \\ \boldsymbol{\sigma}\check{\mathbf{p}} & -m - q/r \end{pmatrix}, \quad (1)$$

m is the fermion mass, $\check{\mathbf{p}} = (\check{p}^k = -i\partial_k)$, and $q = -q_1q_2$; for an electron in a hydrogen-like atom, we have $q = Z\alpha$. For brevity, we call the coupling constant q the charge. We restrict ourselves to the case of $q > 0$, because the results for the case of $q < 0$ can be obtained by the charge conjugation transformation.

At this initial stage of setting the problem, the Hamiltonian \check{H} and other operators are considered as formally s.a. differential operators, or s.a. differential expressions⁶, as we will say [18], which is denoted by the turned hat $\hat{\vee}$ above the corresponding letter. They become quantum-mechanical operators after a specification of their domains in the Hilbert space \mathcal{H} of bispinors $\Psi(\mathbf{r})$,

$$\mathcal{H} = \sum_{\alpha=1}^4 \oplus \mathcal{H}_\alpha, \quad \mathcal{H}_\alpha = L^2(R^3)$$

then the symbol \vee is replaced by the conventional symbol \wedge over the same letter. In what follows, we distinguish differential expressions \check{f} and operators \hat{f} and call \hat{f} the operator associated with the differential expression \check{f} .

The purposes of this paper are constructing a s.a. Hamiltonian \hat{H} associated with \check{H} , which primarily means indicating a domain of \hat{H} , and then finding its spectrum and eigenfunctions.

We note that in the physical literature, the eigenvalue problem is conventionally considered directly in terms of the s.a. differential expression \check{H} as the eigenvalue problem for the differential equation $\check{H}\Psi_E(\mathbf{r}) = E\Psi_E(\mathbf{r})$, the stationary Dirac equation, without any reference to the domain of the Hamiltonian⁷. It is solved by separating variables based on the rotation symmetry of the problem. The rotation symmetry is conventionally treated in terms of s.a. differential expressions as follows.

The Dirac Hamiltonian \check{H} formally commutes with the total angular momentum $\check{\mathbf{J}} = \check{\mathbf{L}} + \frac{1}{2}\boldsymbol{\Sigma}$, where $\check{\mathbf{L}} = [\mathbf{r} \times \check{\mathbf{p}}]$ is the orbital angular momentum operator and $\frac{1}{2}\boldsymbol{\Sigma}$ is the spin angular momentum operator, and the so-called spin operator \check{K} ,

$$\check{K} = \beta [1 + (\boldsymbol{\Sigma}\check{\mathbf{L}})] = \begin{pmatrix} \check{\varkappa} & 0 \\ 0 & -\check{\varkappa} \end{pmatrix}, \quad \check{\varkappa} = 1 + (\boldsymbol{\sigma}\check{\mathbf{L}}).$$

⁵We use the bold letters for three-vectors and the standard representation for γ -matrices where

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix},$$

and $\boldsymbol{\sigma} = (\sigma^1, \sigma^2, \sigma^3)$ are the Pauli matrices. We use the notation $\boldsymbol{\sigma}\mathbf{p} = \sigma^k p^k$, $\boldsymbol{\sigma}\mathbf{r} = \sigma^k x^k$, and so on. We set $\hbar = c = 1$ in what follows.

⁶S.a. by Lagrange in the mathematical terminology, or formally s.a. in the physical terminology.

⁷In fact, some natural domain is implicitly implied.

The differential expressions \check{H} , $\check{\mathbf{J}}^2$, \check{J}_3 , and \check{K} are considered a complete set of commuting operators, which allows separating the angular and radial variables and reducing the total stationary Dirac equation to the radial stationary Dirac equation with a fixed angular momentum, its z -axis projection, and a spin operator eigenvalue.

We here present a treatment of the problem which is proper from the functional analysis standpoint. We construct a s.a. Hamiltonian \hat{H} based on the theory of s.a. extensions of symmetric operators and on the rotation symmetry of the problem. This means that we first define a rotationally invariant symmetric operator $\hat{H}^{(0)}$ associated with s.a. differential expression \check{H} (1), which is rather simple, and then find its rotationally invariant s.a. extensions. Because the coefficient functions of \check{H} are smooth out of the origin, we choose the space of smooth bispinors with a compact support⁸ for the domain $D_{\hat{H}^{(0)}}$ of $\hat{H}^{(0)}$. To avoid troubles with the $1/r$ singularity of the potential at the origin, we additionally require that all bispinors in $D_{\hat{H}^{(0)}}$ vanish near the origin⁹. The operator $\hat{H}^{(0)}$ is thus defined by

$$\hat{H}^{(0)} : \begin{cases} D_{\hat{H}^{(0)}} = \{\Psi(\mathbf{r}) : \psi_\alpha(\mathbf{r}) \in D(R^3); \psi_\alpha(\mathbf{r}) = 0, \mathbf{r} \in U_\varepsilon\}, \\ \hat{H}^{(0)}\Psi(\mathbf{r}) = \check{H}\Psi(\mathbf{r}), \end{cases}$$

where $D(R^3)$ is the space of smooth functions in R^3 with a compact support and U_ε is some vicinity of the origin which is generally different for different bispinors. The domain $D_{\hat{H}^{(0)}}$ is dense in \mathcal{H} , $\overline{D_{\hat{H}^{(0)}}} = \mathcal{H}$, and the symmetricity of $\hat{H}^{(0)}$ is easily verified by integrating by parts.

We now take the rotational invariance into account. The operator $\hat{H}^{(0)}$ evidently commutes with the s.a. angular momentum operator $\hat{\mathbf{J}} = \{\hat{J}_k\}$ and the s.a. operator \hat{K} associated with the respective differential expressions $\check{\mathbf{J}}$ and \check{K} . The operators \hat{J}_k are defined as generators of the unitary representation of the rotation group Spin(3) in the Hilbert space \mathcal{H} . The Hilbert space \mathcal{H} is represented as a direct orthogonal sum,

$$\mathcal{H} = \sum_{j,\zeta}^{\oplus} \mathcal{H}_{j,\zeta}, \quad j = 1/2, 3/2, \dots, \quad \zeta = \pm 1, \quad (2)$$

of subspaces $\mathcal{H}_{j,\zeta}$. The subspaces $\mathcal{H}_{j,\zeta}$ reduce the operators $\hat{\mathbf{J}}^2$, J_k , and \hat{K} ,¹⁰

$$\hat{\mathbf{J}}^2 = \sum_{j,\zeta}^{\oplus} \hat{\mathbf{J}}_{j,\zeta}^2, \quad \hat{J}_k = \sum_{j,\zeta}^{\oplus} \hat{J}_{kj,\zeta}, \quad \hat{K} = \sum_{j,\zeta}^{\oplus} \hat{K}_{j,\zeta}.$$

In its turn, the subspaces $\mathcal{H}_{j,\zeta}$ are finite direct sums of the subspaces

$$\mathcal{H}_{j,\zeta} = \sum_M^{\oplus} \mathcal{H}_{j,M,\zeta}, \quad M = -j, -j+1, \dots, j. \quad (3)$$

The subspace $\mathcal{H}_{j,M,\zeta}$ is the subspace of bispinors $\Psi_{j,M,\zeta}(\mathbf{r})$ of the form

$$\Psi_{j,M,\zeta}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} \Omega_{j,M,\zeta}(\theta, \varphi) f(r) \\ i\Omega_{j,M,-\zeta}(\theta, \varphi) g(r) \end{pmatrix}, \quad (4)$$

⁸We thus avoid troubles associated with a behavior of wave functions at infinity.

⁹Strictly speaking, we thus leave room for δ -like terms in the potential.

¹⁰This means that the operators $\hat{\mathbf{J}}^2$, \hat{J}_3 , and \hat{K} commute with the projectors to the subspaces $\mathcal{H}_{j,\zeta}$, see [18].

where $\Omega_{j,M,\zeta}(\theta, \varphi)$ are spherical spinors and $f(r)$ and $g(r)$ are radial functions (the factors $1/r$ and i are introduced for convenience). The subspaces $\mathcal{H}_{j,M,\zeta}$ are the eigenspaces of the operators $\hat{\mathbf{J}}^2$, \hat{J}_3 , and \hat{K} :

$$\begin{aligned}\hat{\mathbf{J}}^2 \Psi_{j,M,\zeta}(\mathbf{r}) &= j(j+1) \Psi_{j,M,\zeta}(\mathbf{r}), \quad \hat{J}_3 \Psi_{j,M,\zeta}(\mathbf{r}) = M \Psi_{j,M,\zeta}, \\ \hat{K} \Psi_{j,M,\zeta}(\mathbf{r}) &= -\zeta(j+1/2) \Psi_{j,M,\zeta}(\mathbf{r}),\end{aligned}$$

and evidently reduce the operators $\hat{\mathbf{J}}^2$, \hat{J}_3 , and \hat{K} . In the physical language, decomposition (2), (3) corresponds to the expansion of bispinors $\Psi(\mathbf{r}) \in \mathcal{H}$ in terms of the eigenfunctions of the commuting operators $\hat{\mathbf{J}}^2$, \hat{J}_3 , and \hat{K} , which allows separating variables in the equations for eigenfunctions.

We note that the reductions $\hat{J}_{1,2j,\zeta}$ of the operators $\hat{J}_{1,2}$ to the subspaces $\mathcal{H}_{j,\zeta}$ are bounded operators.

The following fact is basic for us. Let $\mathcal{L}^2(0, \infty)$ be the Hilbert space of doublets $F(r)$,

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

with the scalar product

$$(F_1, F_2) = \int_0^\infty dr F_1^\dagger(r) F_2(r) = \int_0^\infty dr \left[\overline{f_1(r)} f_2(r) + \overline{g_1(r)} g_2(r) \right],$$

such that $\mathcal{L}^2(0, \infty) = L^2(0, \infty) \oplus L^2(0, \infty)$. Then formula (4) and the relation

$$\|\Psi_{j,M,\zeta}\|^2 = \int d\mathbf{r} \Psi_{j,M,\zeta}^\dagger(\mathbf{r}) \Psi_{j,M,\zeta}(\mathbf{r}) = \int dr [|f(r)|^2 + |g(r)|^2]$$

show that the Hilbert space $\mathcal{H}_{j,M,\zeta}$ is unitary equivalent to the Hilbert space $\mathcal{L}^2(0, \infty)$:

$$F = U_{j,M,\zeta} \Psi_{j,M,\zeta}, \quad \Psi_{j,M,\zeta} = U_{j,M,\zeta}^{-1} F,$$

the explicit form of the unitary operator U is defined by (4).

The rotational invariance of $\hat{H}^{(0)}$ is equivalent to the following statement.

1) The subspaces $\mathcal{H}_{j,M,\zeta}$ reduce this operator, such that $\hat{H}^{(0)}$ is represented as a direct orthogonal sum of its parts $\hat{H}_{j,\zeta}^{(0)}$ and $\hat{H}_{j,M,\zeta}^{(0)}$ that are the reductions of $\hat{H}^{(0)}$ to the respective $\mathcal{H}_{j,\zeta}$ and $\mathcal{H}_{j,M,\zeta}$,

$$\hat{H}^{(0)} = \sum_{j,\zeta} \hat{H}_{j,\zeta}^{(0)}, \quad \hat{H}_{j,\zeta}^{(0)} = \sum_M \hat{H}_{j,M,\zeta}^{(0)}. \quad (5)$$

Each part $\hat{H}_{j,M,\zeta}^{(0)}$ is a symmetric operator in the Hilbert space $\mathcal{H}_{j,M,\zeta}$. Each symmetric operator $\hat{H}_{j,M,\zeta}^{(0)}$ in the subspace $\mathcal{H}_{j,M,\zeta}$ evidently induces a symmetric operator $\hat{h}_{j,\zeta}^{(0)}$ in the Hilbert space $\mathcal{L}^2(0, \infty)$,

$$\hat{h}_{j,\zeta}^{(0)} F = U_{j,M,\zeta} \hat{H}_{j,M,\zeta}^{(0)} \Psi_{j,M,\zeta},$$

such that $\hat{h}_{j,\zeta}^{(0)} = U_{j,M,\zeta} \hat{H}_{j,M,\zeta}^{(0)} U_{j,M,\zeta}^{-1}$, and $\hat{h}_{j,\zeta}^{(0)}$ is given by

$$\hat{h}_{j,\zeta}^{(0)} : \begin{cases} D_{\hat{h}_{j,\zeta}^{(0)}} = \mathcal{D}(0, \infty), \\ \hat{h}_{j,\zeta}^{(0)} F(r) = \check{h}_{j,\zeta} F(r), \end{cases} \quad (6)$$

where $\mathcal{D}(0, \infty) = D(0, \infty) \oplus D(0, \infty)$, $D(0, \infty)$ is the standard space of smooth functions on $(0, \infty)$ with a compact support,

$$D(0, \infty) = \{f(r) : f(r) \in C^\infty, \text{supp } f \subset [a, b], 0 < a < b < \infty\},$$

the segment $[a, b]$ is generally different for different f , and the s.a. radial differential expression $\check{h}_{j,\zeta}$ is given by

$$\check{h}_{j,\zeta} = -i\sigma^2 \frac{d}{dr} + \frac{\varkappa}{r} \sigma^1 - \frac{q}{r} + m\sigma^3, \quad (7)$$

where $\varkappa = \zeta(j + 1/2)$.¹¹

2) The differential expression $\check{h}_{j,\zeta}$ and consequently, with taking (6) into account, the operator $\hat{h}_{j,\zeta}^{(0)}$ with fixed j and ζ is independent of M . This fact is equivalent to the commutativity of the operator $\hat{H}^{(0)}$ with the operators \hat{J}_1 and \hat{J}_2 , or more precisely, to the commutativity of the operator $\hat{H}_{j,\zeta}^{(0)}$ with the operators $\hat{J}_{1,2j,\zeta}$. In the physical terminology, $\check{h}_{j,\zeta}$ is called the radial Hamiltonian, but strictly speaking, the radial Hamiltonian is a s.a. operator $\hat{h}_{j,\zeta}$ associated with $\check{h}_{j,\zeta}$.

In what follows, by the rotational invariance of any operator \hat{f} , we mean the fulfilment of the following conditions:

1) the reducibility of this operator by the subspaces $\mathcal{H}_{j,M,\zeta}$ and therefore, by $\mathcal{H}_{j,\zeta}$, such that formula similar to (5) holds for the operator \hat{f} ;

2) the commutativity of its parts $\hat{f}_{j,\zeta}$ with the bounded operators $\hat{J}_{1,2j,\zeta}$ for fixed j, ζ .

Let $\hat{h}_{j,\zeta}$ be a s.a. extension of the symmetric operator $\hat{h}_{j,\zeta}^{(0)}$ in $\mathcal{L}^2(0, \infty)$. It evidently induces s.a. extensions $\hat{H}_{j,M,\zeta}$ of the symmetric operators $\hat{H}_{j,M,\zeta}^{(0)}$ in the subspaces $\mathcal{H}_{j,M,\zeta}$,

$$\hat{H}_{j,M,\zeta} = U_{j,M,\zeta}^{-1} \hat{h}_{j,\zeta} U_{j,M,\zeta}, \quad (8)$$

and the operator $\hat{H}_{j,\zeta} = \sum_M^\oplus \hat{H}_{j,M,\zeta}$ commutes with $\hat{J}_{1,2j,\zeta}$. Then the closure of the direct orthogonal sum

$$\hat{H} = \sum_{j,\zeta}^\oplus \hat{H}_{j,\zeta} = \sum_{j,M,\zeta}^\oplus \hat{H}_{j,M,\zeta} \quad (9)$$

is a s.a. operator in the whole Hilbert space \mathcal{H} [19], and \hat{H} is a rotationally invariant extension of the rotationally invariant symmetric operator $\hat{H}^{(0)}$.

Conversely, any rotationally invariant s.a. extension \hat{H} of the initial operator $\hat{H}^{(0)}$ has structure (9), and the operator $\hat{h}_{j,\zeta} = U_{j,M,\zeta} \hat{H}_{j,M,\zeta} U_{j,M,\zeta}^{-1}$ in $\mathcal{L}^2(0, \infty)$ is independent of M and is a s.a. extension of the symmetric operator $\hat{h}_{j,\zeta}^{(0)}$.¹²

The problem of constructing a rotationally invariant s.a. Hamiltonian \hat{H} is thus reduced to the problem of constructing s.a. radial Hamiltonians $\hat{h}_{j,\zeta}$.

In what follows, we operate with fixed j and ζ and therefore omit these indices for brevity. In fact, we consider the radial differential expressions $\check{h}_{j,\zeta}$ as a two-parameter

¹¹We note that $\mathcal{D}(0, \infty)$ is dense in $\mathcal{L}^2(0, \infty)$, because, as is known, $D(0, \infty)$ is dense in $L^2(0, \infty)$, and the symmetricity of $\hat{h}_{j,M,\zeta}^{(0)}$ is easily verified by integrating by parts, which confirms the above assertion.

¹²Roughly speaking, this means that s.a. extensions of the parts $\hat{H}_{j,M,\zeta}^{(0)}$ with fixed j and ζ and different M 's must be constructed "uniformly".

differential expression \check{h} with the parameters q and \varkappa (the parameters j and ζ enter through one parameter \varkappa , the parameter m is considered fixed) and similarly treat the associated radial operators $\check{h}^{(0)}$ and \check{h} defined in the same Hilbert space $\mathcal{L}^2(0, \infty)$.

3 General solution of radial equations

Later on, we need some special solutions of the differential equation

$$\check{h}F = WF,$$

or, which is the same, the system of equations

$$\begin{cases} \frac{df}{dr} + \frac{\varkappa}{r}f - (W + m + \frac{q}{r})g = 0, \\ \frac{dg}{dr} - \frac{\varkappa}{r}g + (W - m + \frac{q}{r})f = 0, \end{cases} \quad (10)$$

with an arbitrary complex W ; real W are denoted by E and have the conventional sense of energy. We call Eqs. (10) the radial equations. For completeness, we present the general solution of the radial equations following the standard procedure, see, e.g., [13, 14]. We first represent $f(r)$ and $g(r)$ as

$$f(r) = z^\Upsilon e^{-z/2} [P(z) + Q(z)], \quad g(r) = -i\Lambda z^\Upsilon e^{-z/2} [P(z) - Q(z)],$$

where $z = -2iKr$, Υ , Λ , and K are some complex numbers that are specified below. The radial equations then become the equations for the functions P and Q . Setting

$$\begin{aligned} \Upsilon^2 &= \varkappa^2 - q^2, \quad \alpha = \Upsilon - i\frac{qW}{K}, \quad \beta = 1 + 2\Upsilon, \\ W \pm m &= \rho_\pm e^{i\varphi_\pm}, \quad 0 \leq \varphi_\pm < 2\pi, \\ \Lambda &= \sqrt{\frac{W-m}{W+m}} = \sqrt{\frac{\rho_-}{\rho_+}} e^{\frac{i}{2}(\varphi_- - \varphi_+)}, \quad K = \sqrt{W^2 - m^2} = \sqrt{\rho_- \rho_+} e^{\frac{i}{2}(\varphi_- + \varphi_+)}, \end{aligned} \quad (11)$$

we reduce (10) to the system of equations

$$\begin{aligned} z \frac{d^2 Q}{dz^2} + (\beta - z) \frac{dQ}{dz} - \alpha Q &= 0, \\ P &= -\frac{1}{\varkappa - i(qm/K)} \left(z \frac{d}{dz} + \alpha \right) Q. \end{aligned} \quad (12)$$

The first equation in (12) is the confluent hypergeometric equation [20, 21] for Q .

Let¹³ $\Upsilon \neq -n/2$, $n = 1, 2, \dots$, then its general solution can be represented as

$$Q = A\Phi(\alpha, \beta; z) + B\Psi(\alpha, \beta; z), \quad (13)$$

¹³The parameter Υ is defined by (11) up to a sign. A specification of Υ is a matter of convenience. In particular, for specific values of charge, we also use a specification of Υ where $\Upsilon = -n/2$, this case is considered separately below.

where A and B are arbitrary constants, $\Phi(\alpha, \beta; z)$ and $\Psi(\alpha, \beta; z)$ are the known confluent hypergeometric functions, for their definition, see [20, 21] (the function $\Phi(\alpha, \beta; z)$ is not defined for $\beta = 0, -1, -2, \dots$). It follows from eqs. (12) and (13) that

$$P = -\frac{\alpha}{\varkappa - i(qm/K)} \left[A\Phi(\alpha + 1, \beta; z) - B(\Upsilon + i\frac{qW}{K})\Psi(\alpha + 1; \beta; z) \right].$$

The general solution of radial equations (10) for any complex W and real m , \varkappa , and q is finally given by

$$\begin{aligned} f(r) &= z^\Upsilon e^{-z/2} \{ A[\Phi(\alpha, \beta; z) - a_+ \Phi(\alpha + 1, \beta; z)] + B[\Psi(\alpha, \beta; z) + b\Psi(\alpha + 1; \beta; z)] \}, \\ g(r) &= i\Lambda z^\Upsilon e^{-z/2} \{ A[\Phi(\alpha, \beta; z) + a_+ \Phi(\alpha + 1, \beta; z)] + B[\Psi(\alpha, \beta; z) - b\Psi(\alpha + 1; \beta; z)] \}, \\ a_\pm &= \frac{\pm \Upsilon K - iqW}{\varkappa K - iqm}, \quad b = \frac{\varkappa K + iqm}{K}. \end{aligned}$$

Taking the relation

$$\Phi(\alpha + 1, \beta; -2iKr) = e^{-2iKr} \Phi(\beta - \alpha - 1, \beta; 2iKr)$$

into account, see [20, 21], it is convenient to represent the general solution of radial equations (10) in the form

$$F = \begin{pmatrix} f \\ g \end{pmatrix} = AX(r, \Upsilon, W) + Bz^\Upsilon e^{-z/2} [\Psi(\alpha, \beta; z)\vartheta_+ - b\Psi(\alpha + 1, \beta; z)\vartheta_-], \quad (14)$$

where the doublets ϑ_\pm are

$$\vartheta_\pm = \begin{pmatrix} \pm 1 \\ i\Lambda \end{pmatrix}$$

and the doublet X is

$$\begin{aligned} X &= \frac{(mr)^\Upsilon}{2} \left[\Phi_+(r, \Upsilon, W) + \Phi_-(r, \Upsilon, W) \begin{pmatrix} 0 & m+W \\ m-W & 0 \end{pmatrix} \right] u_+, \\ \Phi_+ &= e^{iKr} \Phi\left(\Upsilon + \frac{qW}{iK}, 1 + 2\Upsilon; -2iKr\right) + e^{-iKr} \Phi\left(\Upsilon - \frac{qW}{iK}, 1 + 2\Upsilon; 2iKr\right), \\ \Phi_- &= \frac{1}{iK} \left[e^{iKr} \Phi\left(\Upsilon + \frac{qW}{iK}, 1 + 2\Upsilon; -2iKr\right) - e^{-iKr} \Phi\left(\Upsilon - \frac{qW}{iK}, 1 + 2\Upsilon; 2iKr\right) \right], \end{aligned} \quad (15)$$

the doublet u_+ is one of doublets u_\pm which are used below,

$$u_\pm = \begin{pmatrix} 1 \\ \frac{\varkappa \pm \Upsilon}{q} \end{pmatrix}.$$

We now present some particular solutions of radial equations (10) which are used in the following.

One of the solutions given by (14) with $A = 1$, $B = 0$, and a specific choice for Υ is

$$U_{(1)}(r; W) = X(r, \Upsilon, W)|_{\Upsilon=\Upsilon_+}, \quad (16)$$

where

$$\Upsilon_+ = \begin{cases} \sqrt{\varkappa^2 - q^2}, & q \leq |\varkappa|, \\ \sqrt{q^2 - \varkappa^2}, & q > |\varkappa|, \end{cases}$$

in what follows, we set $\gamma = \sqrt{\varkappa^2 - q^2}$ and $\sigma = \sqrt{q^2 - \varkappa^2}$. The asymptotic behavior of the doublet $U_{(1)}(r; W)$ at the origin is given by

$$U_{(1)}(r; W) = (mr)^{\Upsilon_+ + u_+} + O(r^{\Upsilon_+ + 1}), \quad r \rightarrow 0. \quad (17)$$

In the case where $\Upsilon_+ \neq n/2$, $n = 1, 2, \dots$, we also use another solution

$$U_{(2)}(r; W) = X(r, \Upsilon, W)|_{\Upsilon = -\Upsilon_+} \quad (18)$$

with the asymptotic behavior

$$U_{(2)}(r; W) = (mr)^{-\Upsilon_+ + u_-} + O(r^{-\Upsilon_+ + 1}), \quad r \rightarrow 0. \quad (19)$$

For $q \neq q_{ej} = |\varkappa| = j + \frac{1}{2}$, i.e. for $\Upsilon_+ \neq 0$, the solutions $U_{(1)}(r; W)$ and $U_{(2)}(r; W)$ are linearly independent,

$$\text{Wr}(U_{(1)}, U_{(2)}) = -\frac{2\Upsilon_+}{q}, \quad (20)$$

where $\text{Wr}(F_1, F_2) = F_1 i \sigma^2 F_2 = f_1 g_2 - g_1 f_2$ is the Wronskian of the doublets $F_1 = \begin{pmatrix} f_1 \\ g_1 \end{pmatrix}$ and $F_2 = \begin{pmatrix} f_2 \\ g_2 \end{pmatrix}$.

It follows from the standard representation for the function Φ that for real Υ ($\Upsilon \neq -n/2$), the functions Φ_+ and Φ_- in (15) are real-entire functions of W , i.e., they are entire in W and real for real $W = E$. It then follows from representations (16) and (18) that the respective doublets $U_{(1)}(r; W)$ and $U_{(2)}(r; W)$ are also real-entire functions of W for real $\Upsilon_+ = \gamma$. If Υ_+ is pure imaginary, $\Upsilon_+ = i\sigma$, then $U_{(1)}(r; W)$ and $U_{(2)}(r; W)$ are entire in W and complex conjugate for real $W = E$, $\overline{U_{(1)}(r; E)} = U_{(2)}(r; E)$.

Another useful solution nontrivial for $\Upsilon_+ \neq n/2$, $n = 1, 2, \dots$, is given by (14) with $A = 0$ and a special choice for B :

$$\begin{aligned} V_{(1)}(r; W) &= B(W)(mr)^{\Upsilon_+} e^{iKr} [\Psi(\alpha, \beta; z) \vartheta_+ - b \Psi(\alpha + 1; \beta; z) \vartheta_-], \\ B(W) &= \frac{\Gamma(-\Upsilon_+ + qW/iK)}{\Gamma(-2\Upsilon_+)(1 - a_+)} \equiv \frac{1}{\Gamma(-2\Upsilon_+) \tilde{B}(W)}. \end{aligned} \quad (21)$$

As any solution, $V_{(1)}$ is a special linear combination of $U_{(1)}$ and $U_{(2)}$,

$$V_{(1)}(r; W) = U_{(1)}(r; W) + \frac{q}{2\Upsilon_+} \omega(W) U_{(2)}(r; W), \quad (22)$$

where

$$\begin{aligned} \omega(W) &= -\text{Wr}(U_{(1)}, V_{(1)}) = \\ &= \frac{2\Upsilon_+ \Gamma(2\Upsilon_+) \Gamma(-\Upsilon_+ + qW/iK) (1 - a_-) (2e^{-i\pi/2} K/m)^{-2\Upsilon_+}}{q \Gamma(-2\Upsilon_+) \Gamma(\Upsilon_+ + qW/iK) (1 - a_+)} \equiv \frac{\tilde{\omega}(W)}{\Gamma(-2\Upsilon_+)}. \end{aligned} \quad (23)$$

We note that if $\Im W > 0$ and $r \rightarrow \infty$, the doublet $U_{(1)}(r; W)$ increases exponentially while $V_{(1)}(r; W)$ decreases exponentially (with a polynomial accuracy).

The doublets $U_{(2)}$ and $V_{(1)}$ are not solutions linearly independent of $U_{(1)}$ at the points $\Upsilon_+ = \gamma = n/2$ where $U_{(2)}$ is not defined while $V_{(1)}$ vanishes. We need their analogues defined at these points and having all the required properties, in particular, real-entirety in W . Unfortunately, we can construct such solutions only in some neighborhood of fixed n . The corresponding solutions are labelled by the index n .

According to (21), the doublet $V_{(1)}$ tends to zero like $1/\Gamma(-2\gamma)$ as $\gamma \rightarrow n/2$. It then follows from (22) that the doublet $U_{(2)}$ has a singularity of the form $\Gamma(-2\gamma)$ at the point $\gamma = n/2$ and can be represented in a neighborhood of this point as

$$U_{(2)}(r; W) = \Gamma(-2\gamma)A_n(W)U_{(1)}(r; W) + U_{n(2)}(r; W), \quad (24)$$

where

$$A_n(W) = \left(-\frac{2\gamma}{q} \frac{1}{\tilde{\omega}(W)} \right)_{\gamma=n/2} \quad (25)$$

and $U_{n(2)}(r; W)$ has a finite limit as $\gamma \rightarrow n/2$ and evidently satisfies radial equations (10). A direct calculation¹⁴ shows that $A_n(W)$ is a polynomial in W with real coefficients, and because $U_{(1)}(r, W)$ and $U_{(2)}(r, W)$ are real entire in W , the doublet $U_{n(2)}(r; W)$ is also real entire. We thus obtain that the doublet $U_{n(2)}$ defined by

$$U_{n(2)}(r; W) = U_{(2)}(r; W) - \Gamma(-2\gamma)A_n(W)U_{(1)}(r; W) \quad (26)$$

and satisfying the condition

$$U_{n(2)}(r; W) = (mr)^{-\gamma}u_- + O(r^{-\gamma+1}), \quad r \rightarrow 0,$$

is a solution of radial equations which is well-defined in some neighborhood of the point $\gamma = n/2$, the point itself included. This solution is linear-independent of $U_{(1)}$, $\text{Wr}(U_{(1)}, U_{n(2)}) = -2\gamma/q$, and is real entire in W . According to relations (22)-(24), the doublet $V_{(1)}$ is represented in a neighborhood of the point $\gamma = n/2$ in terms of the finite doublets $U_{(1)}$ and $U_{n(2)}$ as

$$V_{(1)}(r; W) = \left[1 + \frac{q}{2\gamma} \tilde{\omega}(W)A_n(W) \right] U_{(1)}(r; W) + \frac{q}{2\gamma} \omega(W)U_{n(2)}(r; W),$$

where according to (25) and (23), the factors $1 + \frac{q}{2\gamma} \tilde{\omega}(W)A_n(W)$ and $\omega(W)$ tend to zero like $1/\Gamma(-2\gamma)$ as $\gamma \rightarrow n/2$. This allows introducing the doublet

$$V_{n(1)}(r; W) = \frac{1}{1 + \frac{q}{2\gamma} \tilde{\omega}(W)A_n(W)} V_{(1)}(r; W) = U_{(1)}(r; W) + \frac{q}{2\gamma} \omega_n(W)U_{n(2)}(r; W), \quad (27)$$

where

$$\omega_n(W) = \frac{\omega(W)}{1 + \frac{q}{2\gamma} \tilde{\omega}(W)A_n(W)} = \frac{\tilde{\omega}(W)}{\Gamma(-2\gamma)[1 + \frac{q}{2\gamma} \tilde{\omega}(W)A_n(W)]}, \quad (28)$$

which is evidently a solution of the radial equations well-defined in some neighborhood of the point $\gamma = n/2$, the point itself included, and exponentially decreasing as $r \rightarrow \infty$. The

¹⁴With the use of the equality $\Gamma(w+1) = w\Gamma(w)$.

function $\omega_n(W)$ is also well defined in some neighborhood of the point $\gamma = n/2$ and at the point itself. We point out that the useful relations

$$\frac{1}{\omega_n(W)} V_{n(1)}(r; W) = \frac{1}{\omega(W)} V_{(1)}(r; W), \quad (29)$$

$$\frac{1}{\omega_n(W)} = \frac{q}{2\gamma} \Gamma(-2\gamma) A_n(W) + \frac{1}{\omega(W)} \quad (30)$$

hold; strictly speaking, they are meaningful for $\gamma \neq n/2$ and show that the r.h.s.'s are continuous in γ at the points $\gamma = n/2$.

The doublets $U_{n(2)}(r; W)$ and $V_{n(1)}(r; W)$ are the required analogues of the doublets $U_{(2)}(r; W)$ and $V_{(1)}(r; W)$ defined in the neighborhood of the point $\gamma = n/2$ and at the point itself.

It remains to consider the special case of $q = q_{cj} = j + 1/2$, or $\Upsilon = 0$, where the doublets $U_{(1)}$ and $U_{(2)}$ coincide while $V_{(1)}$ vanishes. Let $U_{(1)}(r; W|\gamma)$, $U_{(2)}(r; W|\gamma)$, and $V_{(1)}(r; W|\gamma)$ denote $U_{(1)}$, $U_{(2)}$, and $V_{(1)}$ with $\gamma \neq 0$. Differentiating radial equations (10) for $U_{(1)}$ with respect to γ at $\gamma = 0$, we can easily verify that the doublet

$$\left. \frac{\partial U_{(1)}(r; W)}{\partial \gamma} \right|_{\gamma=0} = \lim_{\gamma \rightarrow 0} \frac{U_{(1)}(r; W|\gamma) - U_{(2)}(r; W|\gamma)}{2\gamma}$$

is a solution of these equations with $\gamma = 0$. For two linearly independent solutions of radial equations (10) with $\gamma = 0$, we choose

$$\begin{aligned} U_{(1)}(r; W) &= U_{(1)}(r; W|0), \\ U_{(1)}(r; W) &= u_+ + O(r), \quad r \rightarrow 0, \end{aligned} \quad (31)$$

and

$$\begin{aligned} U_{(2)}^{(0)}(r; W) &= \frac{\partial U_{(1)}(r; W|0)}{\partial \gamma} - \frac{\zeta}{q_{cj}} U_{(1)}(r; W|0), \\ U_{(2)}^{(0)}(r; W) &= u_-^{(0)}(r) + O(r \ln r), \quad r \rightarrow 0, \end{aligned} \quad (32)$$

where u_+ and $u_-^{(0)}(r)$ are

$$u_+ = \begin{pmatrix} 1 \\ \zeta \end{pmatrix}, \quad u_-^{(0)}(r) = \begin{pmatrix} \ln(mr) - \frac{\zeta}{q_{cj}} \\ \zeta \ln(mr) \end{pmatrix}. \quad (33)$$

The Wronskian of these solutions is

$$\text{Wr}(U_{(1)}, U_{(2)}^{(0)}) = \frac{1}{q_{cj}}. \quad (34)$$

The both doublets $U_{(1)}$ and $U_{(2)}^{(0)}$ are real entire in W .

As an analogue of $V_{(1)}$ in the case of $\gamma = 0$, we take the doublet

$$\begin{aligned} V_{(1)}^{(0)}(r; W) &= \lim_{\gamma \rightarrow 0} [-\Gamma(-2\gamma) V_{(1)}(r; W|\gamma)] = \\ &= -\frac{\Gamma(\alpha)}{1-a} e^{iKr} [\Psi(\alpha, 1; -2iKr) + b\Psi(\alpha + 1, 1; -2iKr) \sigma^3] \begin{pmatrix} 1 \\ i\Lambda \end{pmatrix}, \end{aligned} \quad (35)$$

where

$$\alpha = \frac{q_{cj}W}{iK}, \quad a = \frac{W}{m + i\zeta K}, \quad b = q_{cj} \frac{\zeta K + im}{K}.$$

Its representation in terms of $U_{(1)}$ and $U_{(2)}^{(0)}$ is given by

$$\begin{aligned} V_{(1)}^{(0)}(r; W) &= U_{(2)}^{(0)}(r; W) + q_{cj}\omega^{(0)}(W)U_{(1)}(r; W), \\ \omega^{(0)}(W) &= -\text{Wr}(U_{(2)}^{(0)}(r; W), V_{(1)}^{(0)}(r; W)) = \\ &= \frac{1}{q_{cj}} \left[\ln(2e^{-i\pi/2}K/m) + \psi(-iq_{cj}W/K) + \frac{\zeta(W-m) + iK}{2q_{cj}W} - 2\psi(1) \right], \end{aligned} \quad (36)$$

where ψ is a symbol of the logarithmic derivative of the Γ -function. We note that if $\Im W > 0$, the doublet $V_{(1)}^{(0)}(r; W)$ is square integrable, $V_{(1)}^{(0)}(r; W) \in \mathcal{L}^2(0, \infty)$, and exponentially decreases as $r \rightarrow \infty$.

4 Self-adjoint radial Hamiltonians for different regions of charge q

4.1 Generalities

In this section, we construct a s.a. radial Hamiltonian¹⁵ \hat{h} in the Hilbert space $\mathcal{L}^2(0, \infty)$ of doublets as a s.a. extension of symmetric radial operator $\hat{h}^{(0)}$ (6) associated with the radial differential expression \check{h} (7) and analyze its spectral properties.

The extension procedure includes the following steps [22]:

1) evaluating the adjoint operator $\hat{h}^* = (\hat{h}^{(0)})^+$ and estimating its asymmetry in terms of (asymptotic) boundary values of doublets belonging to the domain D_* of \hat{h}^* .

2) constructing s.a. extensions \hat{h} of $\hat{h}^{(0)}$ as s.a. restrictions of the adjoint \hat{h}^* specified by some (asymptotic) s.a. boundary conditions at the origin¹⁶.

It turns out¹⁷ that the result crucially depends on the value of the charge q : different regions of the charge are assigned different s.a. radial Hamiltonians in the sense that they are specified by completely different types of (asymptotic) s.a. boundary conditions. What is more, for sufficiently large charges, a s.a. radial Hamiltonian is defined non-uniquely, such that there is a one-parameter family of s.a. Hamiltonians for fixed \varkappa and q . Therefore, our exposition is naturally divided into subsections related to the corresponding regions of the charge; actually, there are four of them.

For each region, we perform a full spectral analysis of the obtained s.a. Hamiltonians, in particular, we find their spectra and (generalized) eigenfunctions. The analysis is based on the Krein method of guiding functionals and includes the following steps:

i) constructing the guiding functional,

¹⁵We omit indices in the notation of \hat{h} , $\hat{h}^{(0)}$, and \check{h} , see the end of Sec. 2.

¹⁶We note that this method of constructing \hat{h} allows avoiding an evaluation of the deficient subspaces and deficiency indices of $\hat{h}^{(0)}$, the latter are determined by passing.

¹⁷Actually, this becomes clear at the first step.

- ii) evaluating the resolvent,
- iii) evaluating the spectral function,
- iv) constructing the so-called inversion formulas that are mathematically rigorous formulas for the Fourier expansion of wave functions with respect to the (generalized) eigenfunctions of the s.a. Hamiltonian.

We compare this analysis with heuristic physical considerations based, in particular, on the rule of “normalization to δ -function” for eigenfunctions of the continuous spectrum.

Our first task is constructing a s.a. radial operator \hat{h} in accordance with the above scheme, which mainly reduces to indicating its domain $D_h, D_{h^{(0)}} \subset D_h \subseteq D_*$. It can happen that such a domain is non-unique, and it really is for some values of number parameters in \check{h} .

The domain for a s.a. differential operator on an interval of the real axis is conventionally specified by the so-called s.a. boundary conditions at the ends of the interval for the functions belonging to the domain. Our task is to indicate these conditions for the doublets $F \in D_h$ at the boundaries $r = 0$ and $r = \infty$ which are the so-called singular ends of the differential expression \check{h} (7), see [18]. The singularity of the left end $r = 0$ is due to the nonintegrability of the free terms (the coefficient functions without derivatives) in \check{h} . In the case of singular ends, there is no universal explicit method for formulating s.a. boundary conditions. In our case where the coefficient function in front of the derivative d/dr is independent of r , while the free terms are bounded as $r \rightarrow \infty$, the problem of s.a. boundary conditions is related only to the left end $r = 0$.

We begin with the adjoint \hat{h}^* of the initial symmetric operator $\hat{h}^{(0)}$. Using the known distribution theory arguments (or extending the known results for scalar differential operators [18] to the matrix differential operators), we can easily verify that the adjoint operator \hat{h}^* is given by

$$\hat{h}^* : \left\{ \begin{array}{l} D_{h^*} = D_* = \left\{ \begin{array}{l} F : F \text{ are absolutely continuous in } (0, \infty), \\ F, \check{h}F = G \in \mathcal{L}^2(0, \infty), \end{array} \right\}, \\ \hat{h}^*F(r) = \check{h}F(r), \end{array} \right\}, \quad (37)$$

i.e., the adjoint \hat{h}^* is associated with the same differential expression \check{h} , but defined on a more wide domain $D_*, D_{h^{(0)}} \subset D_*$, which is the so-called natural domain for the differential expression \check{h} . Because the coefficient functions of the differential expression \check{h} are real, it follows that the deficiency indices of the initial symmetric operator $\hat{h}^{(0)}$ are equal and therefore s.a. extensions of $\hat{h}^{(0)}$ do exist for any values of parameters \varkappa and q .

It is convenient to introduce a quadratic asymmetry form Δ_* for \hat{h}^* by

$$\begin{aligned} \Delta_*(F) &= (F, \hat{h}^*F) - (\hat{h}^*F, F) = 2i\Im (F, \hat{h}^*F) = \\ &= \int_0^\infty dr F^+(r) (\check{h}F)(r) - \int_0^\infty dr (\check{h}F)^+(r) F(r). \end{aligned} \quad (38)$$

The quantity $\Delta_*(F)$ is evidently pure imaginary¹⁸. The form Δ_* yields a measure of the asymmetry of the operator \hat{h}^* , it shows to what extent the operator \hat{h}^* is nonsymmetric. If $\Delta_* \equiv 0$, the operator \hat{h}^* is symmetric and therefore s.a.. This also means that $\hat{h}^{(0)}$ is

¹⁸The quadratic asymmetry form Δ_* is a restriction to the diagonal of the sesquilinear anti-Hermitian

essentially s.a. and its unique s.a. extension is its closure, $\hat{h} = \overline{\hat{h}^{(0)}}$, which coincides with the adjoint, $\hat{h} = \hat{h}^* = (\hat{h})^+$. If $\Delta_* \neq 0$, a s.a. operator $\hat{h} = (\hat{h})^+$ is constructed as a restriction of the operator \hat{h}^* to the domain $D_h \subset D_*$ such that the restriction of Δ_* to D_h vanishes and D_h is a maximum domain¹⁹ [22].

Using integrating by parts in r.h.s. in (38), it is easy to verify that Δ_* is represented as

$$\Delta_*(F) = [F](\infty) - [F](0), \quad (39)$$

where

$$[F](\infty) = \lim_{r \rightarrow \infty} [F](r) \quad \text{and} \quad [F](0) = \lim_{r \rightarrow 0} [F](r)$$

are the corresponding boundary values of the quadratic local form $[F](r)$ defined by²⁰

$$[F](r) = -iF^+(r)\sigma^2 F(r) = -[\overline{f(r)}g(r) - \overline{g(r)}f(r)] = -2i\Im \overline{f(r)}g(r).$$

These boundary values certainly exist because of the existence of the integrals in r.h.s. in (38); for brevity, we call them the boundary forms at infinity and at the origin respectively. The asymmetry form Δ_* is thus simply determined by the boundary forms²¹ $[F](\infty)$ and $[F](0)$.

We prove that for any $F \in D_*$, we have

$$\lim_{r \rightarrow \infty} F(r) = 0.$$

We first note that $F \in D_*$ implies that $\check{h}F = G$ is square integrable together with F . It in turn follows that

$$\frac{dF(r)}{dr} = \left(-\frac{\kappa}{r}\sigma^3 + i\frac{q}{r}\sigma^2 + m\sigma^1 \right) F(r) + i\sigma^2 G(r)$$

is square integrable at infinity²². It now remains to refer to the assertion that if an absolutely continuous $F(r)$ is square integrable at infinity together with its derivative $dF(r)/dr$, then $F(r) \rightarrow 0$ as $r \rightarrow \infty$; this assertion is an evident generalization of a similar assertion for scalar functions. Therefore, the boundary form at infinity is identically zero: for any $F \in D_*$, we have

$$[F](\infty) = 0,$$

asymmetry form ω_* defined by

$$\begin{aligned} \omega_*(F_1, F_2) &= (F_1, \hat{h}_2^* F_2) - (\hat{h}_1^* F_1, F_2) = \\ &= \int_0^\infty dr F_1^+(r) (\check{h} F_2)(r) - \int_0^\infty dr (\check{h} F_1)^+(r) F_2(r), \end{aligned}$$

the forms Δ_* and ω_* define each other [22].

¹⁹I.e., a domain that does not allow further extending with the condition $\Delta_* \equiv 0$ conserved.

²⁰The quadratic local form $[F](r)$ is a restriction to the diagonal of the sesquilinear anti-Hermitian local form

$[F_1, F_2](r) = -iF\sigma^2 F_2(r) = -[\overline{f_1(r)}g_2(r) - \overline{g_1(r)}f_2(r)]$. These two forms define each other.

²¹The representation (39) is a particular case of the so-called Lagrange identity in the integral form.

²²A doublet $F(r)$ is square integrable at infinity if $\int_R^\infty dr F^+(r)F(r) < \infty$ for sufficiently large R .

and the asymmetry form Δ_* is determined by the boundary form at the origin: for any $F \in D_*$, we have

$$\Delta_*(F) = -[F](0) = (\bar{f}g - \bar{g}f)|_{r=0}. \quad (40)$$

For evaluating this boundary form, we have to find the asymptotic behavior of the doublets $F \in D_*$ at the origin. It turns out that the doublets F can tend to zero, be finite, or infinite, or even have no limit as $r \rightarrow 0$ depending on the values of the parameters \varkappa and q : at fixed j , we must distinguish four regions of the charge q that are defined by the two characteristic values q_{uj} and q_{cj} ($q_{uj} < q_{cj}$) of the charge,

$$\begin{aligned} q_{uj} &= \sqrt{\varkappa^2 - \frac{1}{4}} = \sqrt{j(j+1)} \iff \\ \Upsilon &= \gamma = \frac{1}{2} \iff Z_{uj} = 137\sqrt{j(j+1)}, \\ q_{cj} &= |\varkappa| = j + \frac{1}{2} \iff \Upsilon = 0 \iff Z_{cj} = 137(j + 1/2). \end{aligned}$$

The evaluation of the asymptotic behavior of $F \in D_*$ at the origin is based on the following observation. According to definition (37), the doublets $F \in D_*$ can be considered as square-integrable solutions of the inhomogeneous differential equation

$$\check{h}F(r) = \left(-i\sigma^2 \frac{d}{dr} + \frac{\varkappa}{r} \sigma^1 - \frac{q}{r} + m\sigma^3 \right) F(r) = G(r), \quad (41)$$

with the r.h.s. G belonging to $\mathcal{L}^2(0, \infty)$ and therefore locally integrable, which allows applying the general theory of differential equations (see e.g. [18]) to equation (41). For estimating the asymptotic behavior of $F(r)$ at the origin, it is convenient to represent (41) as

$$\check{h}_- F(r) = G_-(r), \quad (42)$$

where

$$\check{h}_- = -i\sigma^2 \partial_r + \frac{\varkappa}{r} \sigma^1 - \frac{q}{r}, \quad G_-(r) = G(r) - m\sigma^3 F(r) \in \mathcal{L}^2(0, \infty).$$

Let U_1 and U_2 be linearly independent solutions of the homogeneous differential equation $\check{h}_- U = 0$,

$$\begin{aligned} U_1(r) &= (mr)^{\Upsilon+u_+}, \quad q > 0, \\ U_2(r) &= \begin{cases} (mr)^{-\Upsilon+u_-}, & q > 0, \quad q \neq q_{cj} \quad (\Upsilon_+ \neq 0), \\ u_-^{(0)}(r) = \begin{pmatrix} \ln(mr) - \zeta/q_{cj} \\ \zeta \ln(mr) \end{pmatrix}, & q = q_{cj} \quad (\Upsilon_+ = 0). \end{cases} \end{aligned} \quad (43)$$

Any solution $F(r)$ of inhomogeneous differential equation (42) can be represented as

$$F(r) = c_1 U_1(r) + c_2 U_2(r) + I_1(r) + I_2(r), \quad (44)$$

where c_1 and c_2 are some constants and

$$\begin{aligned} I_1(r) &= \begin{cases} \frac{q}{2\Upsilon_+} \int_r^{r_0} [U_1(r) \otimes U_2(y)] G_-(y) dy, & 0 < q \leq q_{uj}, \\ -\frac{q}{2\Upsilon_+} \int_0^r [U_1(r) \otimes U_2(y)] G_-(y) dy, & q > q_{uj}, \quad q \neq q_{cj}, \\ q_{cj} \int_0^r [U_1(r) \otimes U_2(y)] G_-(y) dy, & q = q_{cj}, \end{cases} \\ I_2(r) &= \begin{cases} \frac{q}{2\Upsilon_+} \int_0^r [U_2(r) \otimes U_1(y)] G_-(y) dy, & q > 0, \quad q \neq q_{cj}, \\ -q_{cj} \int_0^r [U_2(r) \otimes U_1(y)] G_-(y) dy, & q = q_{cj}, \end{cases} \end{aligned} \quad (45)$$

where \otimes is the symbol of tensor product, such that $[U_1(r) \otimes U_2(y)]$ is a 2×2 matrix, and $r_0 > 0$ is a constant. It turns out that the boundary form $[F](0)$ is determined by the two first terms in r.h.s. in representation (44) and essentially depends on the parameter Υ .

4.2 First noncritical region

The first noncritical region of the charge is defined by the condition

$$0 < q \leq q_{uj} \iff \Upsilon_+ = \gamma \geq \frac{1}{2}.$$

4.2.1 Self-adjoint radial Hamiltonians

The representation given by formulas (43) – (45) allows evaluating the asymptotic behavior of $F \in D_*$ at the origin. According to (43), the doublet $U_1(r) \sim r^\gamma$ is square integrable at the origin, whereas the doublet $U_2(r) \sim r^{-\gamma}$ is not. Using the Cauchy-Bounjakowsky inequality for estimating the integrals $I_1(r)$ and $I_2(r)$ (45), we find

$$I_1(r) = O(r^{1/2}), \quad I_2(r) = O(r^{1/2}), \quad r \rightarrow 0. \quad (46)$$

It follows that for $F(r)$ to belong to the space $\mathcal{L}^2(0, \infty)$, it is necessary that the coefficient c_2 in front of $U_2(r)$ in (44) be zero, $c_2 = 0$, which yields

$$F(r) = c_1 U_1(r) + I_1(r) + I_2(r) = O(r^{1/2}) \rightarrow 0, \quad r \rightarrow 0, \quad (47)$$

whence it follows that for any $F \in D_*$, we have

$$[F](0) = 0.$$

This means that in the first noncritical charge region, $0 < q \leq q_{uj}$, or $\gamma \geq 1/2$, the operator $\hat{h}^* = \hat{h}$ is s.a. and it is a unique s.a. operator associated with s.a. differential expression \check{h} (7)²³, such that

$$\hat{h} : \left\{ \begin{array}{l} D_{\hat{h}} = \left\{ \begin{array}{l} F : F \text{ are absolutely continuous in } (0, \infty), \\ F, \check{h}F \in \mathcal{L}^2(0, \infty), \end{array} \right\} \\ \hat{h}F(r) = \check{h}F(r). \end{array} \right\} \quad (48)$$

We note that this result actually justifies the standard treatment of the Dirac Hamiltonian with $q \leq \sqrt{3}/2$, or $Z \leq 118$, in the physical literature where the natural domain for \check{h} is implicitly assumed²⁴.

We now proceed to the spectral analysis of the obtained Hamiltonian in accordance with the scheme described in Subsec 4.1. A necessary short information on each item of this scheme is given in Appendix 4.5.2.

²³We point out a particular corollary: the deficiency indices of the initial symmetric operator $\check{h}^{(0)}$ are $(0, 0)$ in the charge region $0 < q \leq q_{uj}$ ($\gamma \geq 1/2$).

²⁴The uniqueness of the Hamiltonian also implies that the notion of δ potential for a relativistic Dirac particle cannot be introduced, which maybe manifests the nonrenormalizability of the four-fermion interaction.

4.2.2 Spectral analysis

Guiding functional In accordance with the requirements in Appendix 4.5.2, for the doublet U defining guiding functional $\Phi(F; W)$ (1), we choose the doublet $U_{(1)}(r; W)$ given by (16) – (17),

$$U(r; W) = U_{(1)}(r; W),$$

the doublet $U(r; W)$ is real-entire, see Sec. 3.

For \mathcal{D} , we choose the set of doublets $F(r) \in D_h = D_*$ with a compact support. It is evident that \mathcal{D} is dense in $\mathcal{L}^2(0, \infty)$.

The guiding functional Φ with these U and \mathcal{D} is simple, i.e., satisfies the properties 1)–3) presented in Appendix 4.5.2. The property 1) is evident, the property 3) is easily verified by integrating by parts, and it remains to verify the property 2): the equation

$$(\check{h} - E_0)\Psi(r) = F_0(r),$$

where $F_0 \in \mathcal{D}$ and satisfies the condition

$$\Phi(F_0; E_0) = \int_0^\infty U(r; E_0)F_0(r)dr = 0,$$

has a solution belonging to \mathcal{D} .

At this point, our exposition is divided into two parts because it is convenient to consider the cases of $\gamma \neq n/2$ and $\gamma = n/2$, $n = 1, 2, \dots$, separately. We first consider the case of $\gamma \neq n/2$, after which the extension of the obtained results to the case of $\gamma = n/2$ becomes evident.

In the case of $\gamma \neq n/2$, any solution of the inhomogeneous equation allows the representation

$$\begin{aligned} \Psi(r) = & c_1 U(r; E_0) + c_2 U_{(2)}(r; E_0) + \frac{q}{2\gamma} \int_r^\infty [U(r; E_0) \otimes U_{(2)}(y; E_0)] F_0(y) dy + \\ & + \frac{q}{2\gamma} \int_0^r [U_{(2)}(r; E_0) \otimes U(y; E_0)] F_0(y) dy, \end{aligned} \quad (49)$$

where $U_{(2)}(r; W)$ is given by (18) – (20). This representation is a copy of representation (43) – (45) for a solution of Eq. (42), where we can take $r_0 = \infty$ because of the compactness of the support of F_0 . The integral terms in this representation have a compact support: if $\text{supp} F_0 \subset [a, b]$, $0 \leq a < b < \infty$, they vanish for $r > b$. Choosing $c_1 = c_2 = 0$, we obtain a particular solution Ψ with a compact support that has the form

$$\begin{aligned} \Psi(r) = & \frac{q}{2\gamma} \int_r^\infty [U(r; E_0) \otimes U_{(2)}(y; E_0)] F_0(y) dy + \\ & + \frac{q}{2\gamma} \int_0^r [U_{(2)}(r; E_0) \otimes U(y; E_0)] F_0(y) dy. \end{aligned} \quad (50)$$

Taking the asymptotic behavior of the doublets $U = U_{(1)}$ and $U_{(2)}$ at the origin (see (17), (19)), and estimate (47) for F_0 into account, we find that the asymptotic behavior of this solution as $r \rightarrow 0$ is of the form $\Psi(r) = O(r^\delta)$, $\delta = \min(\gamma, 3/2)$, whence it follows that $\Psi \in \mathcal{D}$.

Green's function To find Green's function $G(r, r'; W)$, $\Im W \neq 0$, of the s.a. operator \hat{h} associated with the s.a. differential expression \check{h} is to represent a unique solution $\Psi(r) \in D_h$ of the differential equation

$$(\check{h} - W)\Psi(r) = F(r) \quad (51)$$

with any $F(r) \in \mathcal{L}^2(0, \infty)$ in the integral form

$$\Psi(r) = \int_0^\infty G(r, r'; W)F(r')dr'. \quad (52)$$

For our purposes, it is sufficient to consider the case of $\Im W > 0$. As any solution, Ψ allows the representation

$$\begin{aligned} \Psi(r) = & c_1 U(r; W) + c_2 V(r; W) + \frac{1}{\omega(W)} \int_r^\infty [U(r; W) \otimes V(y; W)]F(y)dy + \\ & + \frac{1}{\omega(W)} \int_0^r V(r; W) \otimes U(y; W)F(y)dy, \end{aligned}$$

where $V(r; W) = V_{(1)}(r; W)$ and $\omega(W)$ are given by the respective formulas (21), (22), and (23). This representation is a copy of representation (49) with the change of $U_{(2)}$ to $V_{(1)}$. It is correct because $V_{(1)}(r; W)$ with $\Im W > 0$ decreases exponentially as $r \rightarrow \infty$. The condition $\Psi \in \mathcal{L}^2(0, \infty)$, which is sufficient for Ψ to belong to D_h (because then automatically $\check{h}\Psi = W\Psi + F \in \mathcal{L}^2(0, \infty)$) implies that $c_1 = c_2 = 0$: otherwise, Ψ is non-square-integrable at infinity (if $c_1 \neq 0$) or at the origin (if $c_2 \neq 0$) because $U(r; W)$ with $\Im W > 0$ exponentially grows as $r \rightarrow \infty$ and $V(r; W)$ is non-square-integrable at the origin. We thus obtain that the solution $\Psi \in D_h$ of Eq. (51) with any $F \in D_h$ is represented as

$$\begin{aligned} \Psi(r) = & \frac{1}{\omega(W)} \int_r^\infty [U(r; W) \otimes V(y; W)]F(y)dy + \\ & + \frac{1}{\omega(W)} \int_0^r [V(r; W) \otimes U(y; W)]F(y)dy, \end{aligned}$$

which is the required representation (52) with

$$G(r, r'; W) = \begin{cases} \frac{1}{\omega(W)} V(r; W) \otimes U(r'; W), & r > r' \\ \frac{1}{\omega(W)} U(r; W) \otimes V(r'; W), & r < r' \end{cases} \quad (53)$$

This expression for Green's function allows evaluating the spectral function $\sigma(E)$ of the radial Hamiltonian \hat{h} and writing the inversion formulas in accordance with the instructions in Appendix 4.5.2 (see formulas (2) – (7)).

Spectral function and inversion formulas According to (7), (53), and (22) we obtain that

$$\begin{aligned} M(c; W) &= \frac{1}{\omega(W)} U(c; W) \otimes V(c; W) = \\ &= \frac{1}{\omega(W)} U(c; W) \otimes U(c; W) + \frac{q}{2\gamma} U(c; W) \otimes U_{(2)}(c; W), \end{aligned}$$

and because $U(c; E) = U_{(1)}(c; E)$ and $U_{(2)}(c; E)$ are real, formulas (5) and (6) then yield

$$\frac{d\sigma(E)}{dE} = \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \Im \frac{1}{\omega(E + i\varepsilon)} \quad (54)$$

for the spectral function $\sigma(E)$ of the radial Hamiltonian \hat{h} , where \lim in (54) is understood in a distribution theoretic sense as well as $d\sigma(E)/dE$.

The spectral function is thus determined by the (generalized) function $\Im\omega^{-1}(E)$,

$$\omega^{-1}(E) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\omega(E + i\varepsilon)}.$$

At the points where the function $\omega(E)$,

$$\omega(E) = \lim_{\varepsilon \rightarrow 0} \omega(E + i\varepsilon),$$

is different from zero, we have $\omega^{-1}(E) = 1/\omega(E)$.

The explicit form of $\omega(W)$ (23) shows that $\omega(E)$ exists and is qualitatively different in the two energy regions $|E| \geq m$ and $|E| < m$. Therefore, we naturally distinguish these two energy regions in the subsequent analysis.

We first consider the region $|E| \geq m$.

A direct verification shows that in this energy region, $\omega(E)$ is continuous, different from zero, and takes complex values. It follows that for $|E| \geq m$, the spectral function $\sigma(E)$ is absolutely continuous and

$$\begin{aligned} \frac{d\sigma(E)}{dE} &= \frac{1}{\pi} \Im \frac{1}{\omega(E)} \equiv Q^2(E), \quad |E| \geq m, \\ \omega(E) &= \frac{2\gamma\Gamma(2\gamma)e^{i\pi\gamma}\Gamma(-\gamma + q|E|/ik)[(\varkappa + \gamma)\varepsilon k + iq(E - m)](2k/m)^{-2\gamma}}{q\Gamma(-2\gamma)\Gamma(\gamma + q|E|/ik)[(\varkappa - \gamma)\varepsilon k + iq(E - m)]}, \\ \varepsilon &= E/|E|, \quad k = \sqrt{E^2 - m^2}. \end{aligned} \quad (55)$$

We now consider the case of $|E| < m$.

In this energy region, we have

$$\begin{aligned} \omega(E) &= \frac{2\gamma\Gamma(2\gamma)\Gamma(-\gamma - qE/\tau)[q(m - E) - (\varkappa + \gamma)\tau](2\tau/m)^{-2\gamma}}{q\Gamma(-2\gamma)\Gamma(\gamma - qE/\tau)[q(m - E) - (\varkappa - \gamma)\tau]}, \\ \tau &= \sqrt{m^2 - E^2}, \end{aligned} \quad (56)$$

$\omega(E)$ is real, and $\lim_{\varepsilon \rightarrow 0} [1/\omega(E + i\varepsilon)]$ can be complex only at the points where $\omega(E) = 0$. Because $\Gamma(x)$ does not vanish for real x , $\omega(E)$ can vanish only at the points satisfying one of the two conditions:

i) $q(m - E) - (\varkappa + \gamma)\tau = 0$ or ii) $\gamma - qE/\tau = -n$, $n = 0, 1, \dots$, these are the points where $|\Gamma(\gamma - qE/\tau)| = \infty$.

The case i) yields $E = -\gamma m/\varkappa$ for $\zeta = 1$, but at this point, we also have $-\gamma - qE/\tau = 0$, such that the product $\Gamma(-\gamma - qE/\tau)[q(m - E) - (\varkappa + \gamma)\tau] \neq 0$ and $\omega(E) \neq 0$.

The case ii) yields $E = E_n = m/\sqrt{1 + q^2/(n + \gamma)^2}$, $n = 0, 1, \dots$, but for $\zeta = 1$ at the point $E = E_0$, we also have $q(m - E) - (\varkappa - \gamma)\tau = 0$, and consequently, $|\Gamma(\gamma - qE/\tau)[q(m - E) - (\varkappa - \gamma)\tau]| < \infty$.

We thus obtain that $\omega(E)$ vanishes at the discrete points

$$E = E_n = \frac{m}{\sqrt{1 + \frac{q^2}{(n+\gamma)^2}}}, \quad n = \begin{cases} 1, 2, \dots, \zeta = 1, \\ 0, 1, 2, \dots, \zeta = -1, \end{cases} \quad (57)$$

which form the well-known discrete spectrum of bound states. We note that the discrete spectrum accumulates at the point $E = m$, and its asymptotic form as $n \rightarrow \infty$ is

$$\epsilon_n \equiv m - E_n = \frac{mq^2}{2n^2},$$

which is the well-known nonrelativistic formula for bound state energies.

In the vicinity of these points, we have

$$\frac{1}{\omega(E + i\epsilon)} = -\frac{Q_n^2}{E - E_n + i\epsilon} + O(1), \quad Q_n^2 = \lim_{E \rightarrow E_n} \frac{E_n - E}{\omega(E)}.$$

It follows that for $|E| < m$, the spectral function $\sigma(E)$ is a jump function with the jumps Q_n^2 located at the points $E = E_n$ (the discrete energy eigenvalues(57)) and

$$\frac{d\sigma(E)}{dE} = \sum_n Q_n^2 \delta(E - E_n), \quad n = \begin{cases} 1, 2, \dots, \zeta = 1 \\ 0, 1, 2, \dots, \zeta = -1 \end{cases}, \quad |E| < m. \quad (58)$$

We finally obtain that the spectrum $\text{Spec} \hat{h}$ of the operator \hat{h} is the union of the discrete spectrum $U_n\{E_n\} \subset (-m, m)$ and the continuous spectrum containing the positive part $[m, \infty)$ and the negative part $(-\infty, m]$,

$$\text{Spec} \hat{h} = (-\infty, -m] \cup (U_n\{E_n\}) \cup [m, \infty). \quad (59)$$

We introduce a notation

$$U_{\text{norm}}(r; E) = \begin{cases} Q(E)U(r; E), & |E| \geq m, \\ Q_n U(r; E_n), & E = E_n, |E| < m, \end{cases} \quad (60)$$

$$\varphi(E) = \begin{cases} Q(E)\Phi(E), & |E| \geq m, \\ Q_n \Phi(E_n), & E = E_n, |E| < m. \end{cases} \quad (61)$$

The inversion formulas (2), (3) and Parseval equality (4) then become

$$\varphi(E) = \int_0^\infty U_{\text{norm}}(r; E) F(r) dr, \quad E \in (-\infty, -m] \cup (U_n\{E_n\}) \cup [m, \infty), \quad (62)$$

$$F(r) = \int_{-\infty}^{-m} dE U_{\text{norm}}(r; E) \varphi(E) + \sum_n U_{\text{norm}}(r; E_n) \varphi(E_n) + \int_m^\infty dE U_{\text{norm}}(r; E) \varphi(E), \quad (63)$$

$$\int_0^\infty |F(r)|^2 dr = \int_{-\infty}^{-m} |\varphi(E)|^2 dE + \sum_n |\varphi(E_n)|^2 + \int_m^\infty |\varphi(E)|^2 dE. \quad (64)$$

$$n = \begin{cases} 1, 2, \dots, \zeta = 1 \\ 0, 1, 2, \dots, \zeta = -1 \end{cases},$$

Inversion formulas and Parseval equality (62) – (64) are conventionally treated as the formulas for the generalized Fourier expansion of doublets $F \in \mathcal{L}^2(0, \infty)$ with respect to the complete orthonormalized set of the eigenfunctions $U_{\text{norm}}(r; E)$ of s.a. radial Hamiltonian \hat{h} (48) associated with s.a. differential expression \check{h} (7).

The obtained results for the energy spectrum and (generalized) eigenfunctions coincide with the results obtained by the standard method based on the physical arguments: the energy eigenstates must be locally square integrable solutions of the differential equation $\check{h}F = EF$, their moduli must be bounded at infinity, the eigenvalues E corresponding to the square-integrable bound eigenstates form the discrete energy spectrum, and the non-square-integrable eigenstates corresponding to the continuous energy spectrum must allow a “normalization to δ -function”.

As the first example, we apply these considerations to the energy region $|E| < m$. In this energy region, the solutions of the differential equation $\check{h}F = EF$ either exponentially grow or exponentially decrease (in addition, they can be non-square-integrable at the origin). Because the required solutions must be locally square integrable, the energy eigenstates must belong to $\mathcal{L}^2(0, \infty)$. It is convenient to first find the solutions square integrable at infinity. They are given by (21)-(23),

$$F(r) = cV_{(1)}(r; E) = c \left[U_{(1)}(r; E) + \frac{q}{2\gamma} \omega(E) U_{(2)}(r; E) \right],$$

c is a constant. These functions are square integrable at the origin and therefore on the whole semiaxis only under the condition $\omega(E) = 0$, which reproduces the above results concerning the discrete spectrum and the corresponding eigenfunctions.

As another example of an illustration of the standard method, we show that by a direct calculation of the corresponding integrals, we can establish the orthonormality relations for the eigenfunctions that are conventionally represented in the physical literature as

$$\begin{aligned} \int_0^{\infty} U_{\text{norm}}(r; E_n) U_{\text{norm}}(r; E_{n'}) dr &= \delta_{nn'}, \\ \int_0^{\infty} U_{\text{norm}}(r; E_n) U_{\text{norm}}(r; E') dr &= 0, \\ \int_0^{\infty} U_{\text{norm}}(r; E) U_{\text{norm}}(r; E') dr &= \delta(E - E'), \quad |E|, |E'| \geq m. \end{aligned} \quad (65)$$

The method for calculating is presented in Appendix 4.5.2 where it is demonstrated by the example of the second noncritical charge region. Unfortunately, we are unable to establish the completeness relation for the eigenfunctions that is conventionally written as

$$\begin{aligned} \int_{-\infty}^{-m} U_{\text{norm}}(r; E) \otimes U_{\text{norm}}(r'; E) dE + \sum_n \sum_n U_{\text{norm}}(r; E_n) \otimes U_{\text{norm}}(r'; E_n) + \\ + \int_m^{\infty} U_{\text{norm}}(r; E) \otimes U_{\text{norm}}(r'; E) dE = \delta(r - r') I, \end{aligned}$$

I is the identity 2×2 matrix, by a direct calculation of the corresponding integrals, and we know no heuristic physical arguments in support of the validity of this relation.

It now remains to consider the exceptional cases of $\gamma = n/2$, $n = 1, 2, \dots$. As follows from Sec. 3, in a neighborhood of each point $\gamma = n/2$ and at the point itself, we can equivalently use the doublets $U_{n(2)}$ and $V_{n(1)}$ (28) with the change of $\omega(W)$ to $\omega_n(W)$ (see formulas (26) and (28)) and obtain exactly the same conclusions about the guiding functional and the same results for the Green's function, spectral function and eigenfunctions as those for the case of $\gamma \neq n/2$. This evidently follows from relations (29), (27), and (30), where, in particular, the term $\frac{q}{2\gamma}\Gamma(-2\gamma)A_n(W)$ in the r.h.s. in (30) is real for real $W = E$. It also follows from these formulas that Green's function and the spectral function are continuous in γ at each point $\gamma = n/2$.

4.3 Second noncritical region

This domain is characterized by the condition

$$q_{uj} < q < q_{cj} \iff 0 < \Upsilon_+ = \gamma < \frac{1}{2}.$$

4.3.1 Self-adjoint radial Hamiltonians

As in the previous section, we first evaluate asymmetry form $\Delta_*(F)$ (40) evaluating the asymptotic behavior of the doublets $F \in D_{h^*}$ at the origin with the use of representation (43) – (45). In the case of $0 < \gamma < 1/2$ under consideration, the both $U_1(r) \sim r^\gamma$ and $U_2(r) \sim r^{-\gamma}$ are square integrable at the origin and estimates (46) hold true, such that for any $F \in D_{h^*}$, we have

$$F(r) = c_1(mr)^\gamma u_+ + c_2(mr)^{-\gamma} u_- + O(r^{1/2}), \quad r \rightarrow 0,$$

$$u_\pm = \begin{pmatrix} 1 \\ \kappa \pm \gamma \\ q \end{pmatrix},$$

which in turn yields

$$\Delta_*(F) = \frac{2\gamma}{q}(\bar{c}_2 c_1 - \bar{c}_1 c_2). \quad (66)$$

The asymmetry form $\Delta_*(F)$ thus turns out to be a nontrivial anti-Hermitian quadratic form in the asymptotic coefficients c_1 and c_2 , which means that operator \hat{h}^* (37) is not symmetric and the problem of constructing nontrivial s.a. extensions of the initial symmetric operator $\hat{h}^{(0)}$ (6) arises.

In solving this problem, we follow a method in [22] that comprises two steps.

1. Reducing the quadratic anti-Hermitian form Δ_* as a form in boundary values or asymptotic coefficients c_a , $a = 1, 2, \dots$, to a canonical diagonal form by a linear transformation of the coefficients c_a to coefficients c_{+k} , $k = 1, \dots, m_+$, and c_{-l} , $l = 1, \dots, m_-$, such that Δ_* becomes

$$\Delta_* = i\kappa \left(\sum_1^{m_+} |c_{+k}|^2 - \sum_1^{m_-} |c_{-l}|^2 \right),$$

where κ is some real coefficient.

2. Relating c_{+k} and c_{-l} by a unitary $m \times m$ matrix U ,

$$c_{-l} = \sum_1^m U_{kl} c_{+k}, \quad l = 1, \dots, m,$$

if the inertia indices m_+ and m_- of the form²⁵ are equal, $m_+ = m_- = m$. Each such a relation with a fixed U convert the form Δ_* to zero and yields s.a. (asymptotic) boundary conditions specifying a s.a. extension of the initial symmetric operator, different U define different s.a. extensions. Conversely, any s.a. extension is specified by some U , and when U runs over the group $U(m)$, we obtain the whole m^2 -parameter $U(m)$ -family of all possible s.a. extensions.

We apply this method to our case.

By a linear transformation

$$c_{1,2} \rightarrow c_{\pm} = c_1 \pm ic_2,$$

the asymmetry form Δ_* is reduced to a canonical diagonal form:

$$\Delta_*(F) = i \frac{\gamma}{q} (|c_+|^2 - |c_-|^2).$$

Its inertia indices are $(1, 1)$, which in particular means that the deficiency indices of $\hat{h}^{(0)}$ with $0 < \gamma < 1/2$ are $(1, 1)$.

The relation

$$c_- = e^{i\theta} c_+, \quad 0 \leq \theta \leq 2\pi, \quad 0 \sim 2\pi, \quad (67)$$

with any fixed θ yields boundary conditions specifying a s.a. extension \hat{h}_θ of the operator $\hat{h}^{(0)}$. Different θ 's are assigned different s.a. extensions, except equivalent cases of $\theta = 0$ and $\theta = 2\pi$. When θ runs over a circle, we obtain the whole one-parameter $U(1)$ -family of all s.a. extensions of the operator $\hat{h}^{(0)}$.

Relation (67) is equivalent to the relation

$$c_2 = \xi c_1, \quad -\infty \leq \xi = -\tan \frac{\theta}{2} \leq +\infty, \quad -\infty \sim +\infty,$$

the values $\xi = \pm\infty$ are equivalent and mean that $c_1 = 0$; we will say that $\xi = \infty$ in these cases.

We let \hat{h}_ξ redenote the corresponding s.a. operator, $\hat{h}_\xi \equiv \hat{h}_\theta$, and let D_ξ denote its domain. The final result in a more extended form is formulated as follows. In the second noncritical region $0 < \gamma < 1/2$, we have a one-parameter $U(1)$ -family $\{\hat{h}_\xi\}$ of s.a. operators associated with s.a. differential expression \check{h} (7). They are specified by s.a. boundary conditions and are given by

$$\hat{h}_\xi : \left\{ \begin{array}{l} D_\xi = \left\{ \begin{array}{l} F(r) : F(r) \text{ is absolutely continuous in } (0, \infty), F, \check{h}F \in \mathcal{L}^2(0, \infty), \\ F(r) = c[(mr)^\gamma u_+ + \xi(mr)^{-\gamma} u_-] + O(r^{1/2}), \quad r \rightarrow 0, \quad -\infty < \xi < +\infty, \\ F(r) = c(mr)^{-\gamma} u_- + O(r^{1/2}), \quad r \rightarrow 0, \quad \xi = \infty, \end{array} \right\} \\ \hat{h}_\xi F = \check{h}F, \end{array} \right. \quad (68)$$

²⁵The inertia indices coincide with the deficiency indices of an initial symmetric operator.

where c is an arbitrary complex number.

In other words, the only s.a. differential expression \check{h} does not uniquely define a s.a. operator in the charge region $0 < \gamma < 1/2$, and an additional specification of the domain in terms of s.a asymptotic boundary conditions involving one real parameter ξ is required.

4.3.2 Spectral analysis

The spectral analysis in this charge region is quite similar to the analysis performed in Subsec. 4.2 related to the first noncritical region²⁶. We therefore only point out necessary modifications and formulate the final results.

In the case of $\xi = 0$, the the corresponding analysis is identical to that in the previous Subsec. 4.2 and the results obtained there are directly extended to the region $0 < \gamma < 1/2$ and are given by the same formulas.

Until said otherwise, we assume that $0 < |\xi| < \infty$, ξ is arbitrary, but fixed. The case of $\xi = \infty$ is considered separately below.

For the doublet $U(r; W)$ defining guiding functional (1), we choose the doublet

$$U_\xi(r; W) = U_{(1)}(r; W) + \xi U_{(2)}(r; W) \quad (69)$$

satisfying the condition

$$U_\xi(r; W) = (mr)^\gamma u_+ + \xi (mr)^{-\gamma} u_- + O(r^{-\gamma+1}), \quad r \rightarrow 0,$$

where $U_{(1)}$ and $U_{(2)}$ are given by formulas (16) – (20). As before, $U_\xi(r; W)$ is real-entire in W . The corresponding guiding functional is denoted by $\Phi_\xi(F, W)$.

For \mathcal{D} , we choose the set \mathcal{D}_ξ of doublets belonging to D_ξ and having a compact support.

The guiding functional Φ_ξ with the chosen U_ξ and \mathcal{D}_ξ is simple. Indeed, the properties 1) and 3) are evident; as to the property 2), the solution Ψ of the inhomogeneous equation $(\hat{h} - E_0)\Psi = F_0$, $F_0 \in \mathcal{D}_\xi$, with the property $\Psi \in \mathcal{D}_\xi$ is given by a copy of (50), where the solutions $U = U_{(1)}$ and $U_{(2)}$ of the homogeneous equation are replaced by the respective solutions U_ξ and $U_{(1)}$ with the Wronskian $\text{Wr}(U_\xi, U_{(1)}) = 2\gamma\xi/q$,

$$\begin{aligned} \Psi(r) = & -\frac{q}{2\gamma\xi} \int_r^\infty [U_\xi(r; E_0) \otimes U_{(1)}(y; E_0)] F_0(y) dy + \\ & -\frac{q}{2\gamma\xi} \int_0^r U_{(1)}(r; E_0) \otimes U_\xi(y; E_0)] F_0(y) dy. \end{aligned}$$

Green's function $G_\xi(r, r'; W)$, $\Im W > 0$, of the operator \hat{h}_ξ is defined as the kernel of the integral representation for any $\Psi \in \mathcal{D}_\xi$ in terms of the doublet $F = (\hat{h}_\xi - W)\Psi \in \mathcal{L}^2(0, \infty)$:

$$\Psi(r) = \int_0^\infty G_\xi(r, r'; W) F(r') dr'.$$

This representation is a copy of formula (52). The natural difference is the change of $U = U_{(1)}$ to $U = U_\xi$ because the condition $\Psi \in \mathcal{D}_\xi$ implies that Ψ satisfies s.a. asymptotic boundary

²⁶A simplifying thing is that the particular cases of $\gamma = 0$ and $\gamma = 1/2$ are excluded.

conditions (68). The final result is

$$G_{\xi}(r, r'; W) = \begin{cases} \frac{1}{\omega_{\xi}(W)} V(r; W) \otimes U_{\xi}(r'; W), & r > r', \\ \frac{1}{\omega_{\xi}(W)} U_{\xi}(r; W) \otimes V(r'; W), & r < r', \end{cases}$$

where

$$\begin{aligned} V(r; W) &= V_{(1)}(r; W) = U_{\xi}(r; W) + \frac{q}{2\gamma} \omega_{\xi}(W) U_{(2)}(r; W), \\ \omega_{\xi}(W) &= -\text{Wr}(U, V) = \omega(W) - \frac{2\gamma\xi}{q}, \end{aligned} \quad (70)$$

$V_{(1)}(r; W)$ and $\omega(W)$ are given by (21) – (23), which is a copy of representation (53) with the natural change of $U = U_{(1)}$ and ω to the respective $U = U_{\xi}$ and ω_{ξ} .

It follows, see (5) – (7), that

$$\begin{aligned} M(c; W) &= \frac{1}{\omega_{\xi}(W)} U_{\xi}(c; W) \otimes V(c; W) = \\ &= \frac{1}{\omega_{\xi}(W)} U_{\xi}(c; W) \otimes U_{\xi}(c; W) + \frac{q}{2\gamma} U_{(2)}(c; W) \otimes U_{\xi}(c; W), \end{aligned}$$

and, because the both $U_{\xi}(c; E)$ and $U_{(2)}(c; E)$ are real, that the spectral function $\sigma_{\xi}(E)$ of the radial Hamiltonian \hat{h}_{ξ} , $0 < |\xi| < \infty$, is given by

$$\frac{d\sigma_{\xi}(E)}{dE} = \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \Im \frac{1}{\omega_{\xi}(E + i\varepsilon)},$$

a copy of expression (54) with the change of ω to ω_{ξ} . The spectral function is determined by the (generalized) function $\Im \omega_{\xi}^{-1}(E)$,

$$\omega_{\xi}^{-1}(E) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\omega_{\xi}(E + i\varepsilon)} = \lim_{\varepsilon \rightarrow 0} \frac{1}{\omega(E + i\varepsilon) - 2\gamma\xi/q}.$$

At the points where the function

$$\omega_{\xi}(E) = \lim_{\varepsilon \rightarrow 0} \omega_{\xi}(E + i\varepsilon) = \lim_{\varepsilon \rightarrow 0} [\omega(E + i\varepsilon) - 2\gamma\xi/q]$$

is different from zero, we have $\omega_{\xi}^{-1}(E) = 1/\omega_{\xi}(E)$. Because $\omega_{\xi}(E)$ differs from $\omega(E)$ by a real constant $-2\gamma\xi/q$, the two energy regions $|E| \geq m$ and $|E| < m$ are naturally distinguished as before, and the corresponding analysis in each region is similar to the analysis in the previous subsection. In the energy region $|E| \geq m$, the function $\omega_{\xi}(E)$ is continuous, different from zero, and complex as well as $\omega(E)$ (55). The spectral function $\sigma_{\xi}(E)$ for $|E| \geq m$ is therefore absolutely continuous, and

$$\frac{d\sigma_{\xi}(E)}{dE} = \frac{1}{\pi} \Im \frac{1}{\omega(E) - \frac{2\gamma\xi}{q}} \equiv Q_{\xi}^2(E),$$

which is an analogue of (55) with the change of $\omega(E)$ and $Q(E)$ to the respective $\omega_{\xi}(E)$ and $Q_{\xi}(E)$.

In the energy region $|E| < m$, function $\omega(E)$ (56) is real, and therefore, the function $\omega_\xi(E)$ is also real. As in the case of the first noncritical charge region, it follows that for $|E| < m$, the spectral function $\sigma_\xi(E)$ is a jump function with the jumps $Q_{\xi,n}^2$ located at the points $E = E_{\xi,n}$, the discrete energy eigenvalues, where $\omega_\xi(E_{\xi,n}) = 0$, and

$$Q_{\xi,n}^2 = \lim_{E \rightarrow E_{\xi,n}} \frac{E_{\xi,n} - E}{\omega_\xi(E)}.$$

As a result, we obtain that

$$\frac{d\sigma_\xi(E)}{dE} = \sum_n Q_{\xi,n}^2 \delta(E - E_{\xi,n}), \quad |E| < m,$$

which is an analogue of (58) with the change of E_n and Q_n to the respective $E_{\xi,n}$ and $Q_{\xi,n}$.

Unfortunately, we are unable to find an explicit formula for the discrete energy eigenvalues $E_{\xi,n}$ with $\xi \neq 0$, we only note that, as in the first noncritical charge region, there are infinitely many of such levels accumulating at the point $E = m$, and their asymptotic form as $n \rightarrow \infty$ is given by the previous nonrelativistic expression independent of ξ :

$$\epsilon_{\xi,n} \equiv m - E_{\xi,n} = \frac{mq^2}{2n^2}.$$

The lower bound state energy essentially depends on ξ , and there exists a value of ξ for which the lower bound state energy coincides with the boundary $E = -m$ of the lower (positron) continuous spectrum.

The whole spectrum $\text{Spec} \hat{h}_\xi$ of the radial Hamiltonian \hat{h}_ξ is given by a copy of (59) with the change of E_n to $E_{\xi,n}$.

The inversion formulas and the Parseval equality

$$\begin{aligned} \varphi_\xi(E) &= \int_0^\infty U_{\xi,\text{norm}}(r; E) F(r) dr, \quad E \in (-\infty, -m] \cup (\cup_n \{E_{\xi,n}\}) \cup [m, \infty), \\ F(r) &= \int_{-\infty}^{-m} dE U_{\xi,\text{norm}}(r; E) \varphi_\xi(E) + \sum_n U_{\xi,\text{norm}}(r; E_{\xi,n}) \varphi_\xi(E_{\xi,n}) + \\ &+ \int_m^\infty dE U_{\xi,\text{norm}}(r; E) \varphi_\xi(E), \\ \int_0^\infty |F(r)|^2 dr &= \int_{-\infty}^{-m} |\varphi_\xi(E)|^2 dE + \sum_n |\varphi_\xi(E_{\xi,n})|^2 + \int_m^\infty |\varphi_\xi(E)|^2 dE, \end{aligned}$$

are written in terms of the normalized eigenfunctions $U_{\xi,\text{norm}}(r; E)$ and the Fourier coefficients $\varphi_\xi(E)$ that are defined by copies of formulas (60) and (61) with the addition of the subscript ξ to all the symbols Q , U , Q_n , E_n , and Φ . These relations are copies of formulas (62)-(64).

As before, the energy spectrum and (generalized) eigenfunctions of the radial Hamiltonian \hat{h}_ξ can be obtained by the standard method using the physical arguments.

As an example, we consider the energy region $|E| < m$ where the solutions F of the differential equation $\hat{h}F = EF$ either exponentially grow or exponentially decrease as $r \rightarrow \infty$, all solutions being square integrable at the origin. Only exponentially decreasing solutions

$$\begin{aligned}
F(r) &= cV_{(1)}(r; E) = c[U_{(1)}(r; E) + \frac{q}{2\gamma}\omega(E)U_{(2)}(r; E)] = \\
&= c[U_{\xi}(r; E) + \frac{q}{2\gamma}\omega_{\xi}(E)U_{(2)}(r; E)],
\end{aligned}$$

c is a constant, are proper. It is remarkable that such solutions are square-integrable on the whole semiaxis for any energy values $E \in (-m, m)$. But they satisfy s.a. asymptotic boundary conditions (68) only if $\omega_{\xi}(E) = 0$, which reproduces the results for the eigenvalues and eigenfunctions of the discrete spectrum of the operator \hat{h}_{ξ} . We note that the s.a. boundary conditions have a physical meaning of the condition that probability flux density vanish at the boundary, the origin in our case. We did not refer to this requirement in the first noncritical charge region because it is automatically satisfied in this region.

We can also establish the orthonormality relations for the eigenfunctions $U_{\xi, \text{norm}}(r; E)$, which are copies of relations (65), by a direct calculation of the corresponding integrals. This calculation illustrating the general method applicable to all the charge regions is presented in Appendix 4.5.2.

As before, we are unable to establish the completeness relation for the eigenfunctions by a direct calculation or based on heuristic physical arguments.

We now touch briefly on the case of $\xi = \infty$ where the s.a. asymptotic boundary conditions for any $F \in D_{\infty}$ are

$$F(r) = c(mr)^{-\gamma}u_{-} + O(r^{1/2}), \quad r \rightarrow 0.$$

For the doublets U and V , we choose the respective

$$\begin{aligned}
U(r; W) &= U_{\infty}(r; W) = U_{(2)}(r; W), \\
U_{\infty}(r; W) &= (mr)^{-\gamma}u_{-} + O(r^{1-\gamma}), \quad r \rightarrow 0,
\end{aligned}$$

and

$$\begin{aligned}
V(r; W) &= \frac{2\gamma}{q\omega(W)}V_{(1)}(r; W) = U_{(2)}(r; W) - \frac{q}{2\gamma}\omega_{\infty}(W)U_{(1)}(r; W), \\
\omega_{\infty}(W) &= -\text{Wr}(U, V) = -\frac{4\gamma^2}{q^2\omega(W)}.
\end{aligned}$$

Performing calculations completely similarly to those in the case of $|\xi| < \infty$, we find the spectral function $\sigma_{\infty}(E)$,

$$\frac{d\sigma_{\infty}(E)}{dE} = \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \Im \frac{1}{\omega_{\infty}(E + i\varepsilon)} = -\frac{1}{\pi} \frac{q^2}{4\gamma^2} \lim_{\varepsilon \rightarrow 0} \Im \omega(E + i\varepsilon).$$

All other results concerning the structure of the spectrum and inversion formulas are also completely similar to the results in the case of $|\xi| < \infty$. In particular, the bound state spectrum is determined by the poles of the function $\omega(E)$ in the energy region $|E| < m$; it can be evaluated explicitly.

In conclusion, we note that the spectrum and the normalized eigenfunctions $U_{\xi, \text{norm}}(r; E)$ are continuous in ξ , the points $\xi = 0$ and $\xi = \infty$ included.

4.4 Critical charges

This region is defined by the charge values

$$q = q_{cj} = |\varkappa| = j + 1/2 \iff \Upsilon_+ = \gamma = 0.$$

The charge values $q = q_{cj}$ stand out because for $q > q_{cj}$, the standard formula (57) for the bound state spectrum ceased to be true yielding complex energy values. But we will see that from the mathematical standpoint, no extraordinary happens with the system for the charge values $q \geq q_{cj}$, at least, in comparison with the previous case of $q_{uj} < q < q_{cj}$.

4.4.1 Self-adjoint radial Hamiltonians

In constructing the s.a. Hamiltonians with critical charges, we literally follow the method presented in the previous Subsec. 4.3 where the second noncritical charge region was considered and therefore restrict ourselves to only key remarks.

It follows from representation (43) – (45) that the asymptotic behavior of the doublets $F \in D_*$ in the case of $q = q_{cj}$ is given by

$$F(r) = c_1 u_+ + c_2 u_-^{(0)}(r) + O(r^{1/2} \ln r), \quad r \rightarrow 0, \quad \forall F \in D_{h^*},$$

which yields the expression

$$\Delta_*(F) = \frac{1}{q_{cj}} (\overline{c_1} c_2 - \overline{c_2} c_1)$$

for $\Delta_*(F)$, this expression is completely similar to the previous case, see (66) with the changes $2\gamma/q \rightarrow 1/q_{cj}$ and $c_1 \leftrightarrow c_2$.

Therefore, in the case of critical charges, i.e., for $\gamma = 0$, we also have the one-parameter $U(1)$ -family $\{\hat{h}_{(0)\xi}\}$, $-\infty \leq \xi \leq +\infty$, of s.a. operators associated with s.a. differential expression \check{h} (7) and specified by s.a. asymptotic boundary conditions,

$$\hat{h}_{(0)\xi} : \left\{ \begin{array}{l} D_\xi^{(0)} = \left\{ \begin{array}{l} F(r) : F(r) \text{ is absolutely continuous in } (0, \infty), F, \check{h}F \in \mathcal{L}^2(0, \infty), \\ F(r) = c(u_-^{(0)}(r) + \xi u_+) + O(r^{1/2} \ln r), \quad r \rightarrow 0, \quad -\infty < \xi < +\infty, \\ F(r) = c u_+ + O(r^{1/2} \ln r), \quad r \rightarrow 0, \quad \xi = \infty, \end{array} \right\} \\ \hat{h}_{(0)\xi} F = \check{h}F, \end{array} \right. \quad (71)$$

$D_\xi^{(0)}$ denotes the domain of the operator $\hat{h}_{(0)\xi}$, and $\xi = \infty$ corresponds to the equivalent cases of $\xi = +\infty$ and $\xi = -\infty$.

4.4.2 Spectral analysis

The spectral analysis follows the standard way presented in the previous subsections, and therefore, we only cite the final results.

We first consider the case of $\xi \neq \infty$. For the doublet $U(r; W)$ defining the guiding functional (1), we choose the doublet

$$U_\xi^{(0)}(r; W) = U_{(2)}^{(0)}(r; W) + \xi U_{(1)}(r; W)$$

with the asymptotic behavior

$$U_\xi^{(0)}(r; W) = u_-^{(0)}(r) + \xi u_+ + O(r \ln r), \quad r \rightarrow 0,$$

where the doublets $U_{(1)}$ and $U_{(2)}^{(0)}$ are given by formulas (31) – (34); $U_\xi^{(0)}(r; W)$ is real-entire in W .

For \mathcal{D} , we choose the set $\mathcal{D}_\xi^{(0)}$ of doublets belonging to $D_\xi^{(0)}$ and having a compact support.

The guiding functional $\Phi_\xi^{(0)}$ with these $U_\xi^{(0)}$ and $\mathcal{D}_\xi^{(0)}$ is simple. In particular, the solution $\Psi \mathcal{D}_\xi^{(0)}$ of the inhomogeneous equation $(\hat{h} - E_0)\Psi = F_0$, $F_0 \in \mathcal{D}_\xi^{(0)}$, is given by a copy of (50) with the change of $U_{(1)}$, $U_{(2)}$, and $\frac{q}{2\gamma} = -(\text{Wr}(U_{(1)}, U_{(2)}))^{-1}$ to the respective $U_\xi^{(0)}$, $U_{(1)}$, and $-q_{cj} = -(\text{Wr}(U_\xi^{(0)}, U_{(1)}))^{-1}$.

Green's function $G_\xi^{(0)}(r, r'; W)$, $\Im W > 0$, of the Hamiltonian $\hat{h}_{(0)\xi}$ is defined by a copy of (53) with the change of $U = U_{(1)}$, $V = V_{(1)}$, and $\omega = -\text{Wr}(U_{(1)}, V_{(1)})$ to the respective $U = U_\xi^{(0)}$, $V = V_{(1)}^{(0)}$, and $\omega_\xi^{(0)} = -\text{Wr}(U_\xi^{(0)}, V_{(1)}^{(0)})$,

$$G_\xi^{(0)}(r, r'; W) = \begin{cases} \frac{1}{\omega_\xi^{(0)}(W)} V_{(1)}^{(0)}(r; W) \otimes U_\xi^{(0)}(r'; W), & r > r', \\ \frac{1}{\omega_\xi^{(0)}(W)} U_\xi^{(0)}(r; W) \otimes V_{(1)}^{(0)}(r'; W), & r < r', \end{cases}$$

see formulas (35) and (36); $V_{(1)}^{(0)}$ is conveniently represented as

$$V_{(1)}^{(0)}(r; W) = U_\xi^{(0)}(r; W) + q_{cj} \omega_\xi^{(0)}(W) U_{(1)}(r; W), \quad (72)$$

where

$$\omega_\xi^{(0)}(W) = -\text{Wr}(U_\xi^{(0)}, V_{(1)}^{(0)}) = \omega^{(0)}(W) - \frac{\xi}{q_{cj}},$$

$\omega^{(0)}(W)$ is given in (36).

The spectral function $\sigma_\xi^{(0)}(E)$ of the radial Hamiltonian $\hat{h}_{(0)\xi}$ is defined by

$$\frac{d\sigma_\xi^{(0)}(E)}{dE} = \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \Im \frac{1}{\omega_\xi^{(0)}(E + i\varepsilon)}$$

and is determined by the (generalized) function $\Im \omega_\xi^{(0)-1}(E)$,

$$\omega_\xi^{(0)-1}(E) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\omega_\xi^{(0)}(E + i\varepsilon)} = \lim_{\varepsilon \rightarrow 0} \frac{1}{\omega^{(0)}(E + i\varepsilon) - \xi/q_{cj}}.$$

At the points where the function

$$\omega_\xi^{(0)}(E) = \lim_{\varepsilon \rightarrow 0} \omega_\xi^{(0)}(E + i\varepsilon) = \omega^{(0)}(E) - \xi/q_{cj}$$

with

$$\omega^{(0)}(E) = \lim_{\varepsilon \rightarrow 0} \omega^{(0)}(E + i\varepsilon),$$

is different from zero, we have $\omega_\xi^{(0)-1}(E) = 1/\omega_\xi^{(0)}(E)$.

The two energy regions $|E| \geq m$ and $|E| < m$ are naturally distinguished as before.

In the region $|E| \geq m$, the function $\omega^{(0)}(E)$ is given by

$$\omega^{(0)}(E) = \frac{1}{q_{cj}} \left\{ \ln[2e^{-i\epsilon\pi/2}k/m] + \psi(-iq_{cj}|E|/k) + \frac{i\epsilon k - \zeta m}{2q_{cj}E} - 2\psi(1) + \zeta/(2q_{cj}) \right\},$$

$$\epsilon = E/|E|, \quad k = \sqrt{E^2 - m^2}.$$

It is continuous, different from zero, and complex, therefore, the spectral function $\sigma_\xi^{(0)}(E)$ for $|E| \geq m$ is absolutely continuous, and

$$\frac{d\sigma_\xi^{(0)}(E)}{dE} = \frac{1}{\pi} \Im \frac{1}{\omega^{(0)}(E) - \frac{\xi}{q_{cj}}} \equiv [Q_\xi^{(0)}(E)]^2.$$

In the region $|E| < m$, the function $\omega^{(0)}(E)$ is given by

$$\omega^{(0)}(E) = \frac{1}{q_{cj}} \left\{ \ln(2\tau/m) + \psi(-q_{cj}E/\tau) - \frac{\tau + \zeta m}{2q_{cj}E} - 2\psi(1) + \zeta/(2q_{cj}) \right\},$$

$$\tau = \sqrt{m^2 - E},$$

it is real, and therefore, the function $\omega_\xi^{(0)}(E)$ is also real. As in the previous cases, the spectral function $\sigma_\xi^{(0)}(E)$ for $|E| < m$ is a jump function with the jumps

$$[Q_{\xi,n}^{(0)}]^2 = \lim_{E \rightarrow E_{\xi,n}^{(0)}} \frac{E_{\xi,n}^{(0)} - E}{\omega_\xi^{(0)}(E)}$$

located at the discrete energy eigenvalues $E_{\xi,n}^{(0)}$ where $\omega_\xi^{(0)}(E_{\xi,n}^{(0)}) = 0$, such that

$$\frac{d\sigma_\xi^{(0)}(E)}{dE} = \sum_n [Q_{\xi,n}^{(0)}]^2 \delta(E - E_{\xi,n}^{(0)}).$$

As in the previous case, we are unable to find an explicit formula for $E_{\xi,n}^{(0)}$ (except the case of $\xi = \infty$, see below), we only note that there exists an infinite number of discrete levels which accumulate at the point $E = m$, and their asymptotic behavior as $n \rightarrow \infty$ is described by the same nonrelativistic formula:

$$\epsilon_{\xi,n}^{(0)} \equiv m - E_{\xi,n}^{(0)} = \frac{mq^2}{2n^2}.$$

The lower bound state energy essentially depends on ξ , and there exists a value of ξ for which the lower bound state energy coincides with the boundary $E = -m$ of the lower (positron) continuous spectrum.

All other results concerning the inversion formulas and Parseval equality are written in terms of the normalized (generalized) eigenfunctions $U_{\xi,\text{norm}}^{(0)}(r; E)$ and the Fourier coefficients

$\varphi_\xi^{(0)}(E)$ as copies of relations (60)-(64) with the addition of the subscript ξ and superscript (0) to all the symbols Q , U , Q_n , E_n , and Φ .

As before, the energy spectrum and eigenfunctions of the radial Hamiltonian $\hat{h}_{(0)\xi}$ can be obtained by the standard method using the physical arguments. As an example, we again consider the energy region $|E| < m$ where the solutions F of the differential equation $\hat{h}F = EF$ either exponentially grow or exponentially decrease and are square integrable at the origin. The exponentially decreasing solutions are described by the doublets

$$F(r) = cV_{(1)}^{(0)}(r; E) = c[U_\xi^{(0)}(r; E) + q_{cj}\omega_\xi^{(0)}(E)U_{(1)}(r; E)],$$

where c is a constant. They are square integrable, $F \in \mathcal{L}^2(0, \infty)$, for any E in the interval $E \in (-m, m)$, but satisfy s.a. asymptotic boundary conditions (71) only if $\omega_\xi^{(0)}(E) = 0$, which reproduces the results for the eigenvalues and eigenfunctions of the discrete spectrum. We can also verify the orthonormality relations for the eigenfunctions $U_{\xi, \text{norm}}^{(0)}(r; E)$ that are analogues of relations (65) by a direct calculation of the corresponding integrals with the method described in Appendix 4.5.2.

We touch briefly on the case of $\xi = \infty$ where the s.a asymptotic boundary conditions for any $\forall F \in D_\infty$ are

$$F(r) = cu_+ + O(r^{1/2} \ln r), \quad r \rightarrow 0.$$

For the doublets U and V , we choose the respective

$$\begin{aligned} U(r; W) &= U_\infty^{(0)}(r; W) = U_{(1)}(r; W), \\ U_\infty^{(0)}(r; W) &= cu_+ + O(r), \quad r \rightarrow 0, \end{aligned}$$

and

$$\begin{aligned} V(r; W) &= \frac{1}{q_{cj}\omega_\infty^{(0)}(W)} V_{(1)}^{(0)}(r; W) = U_{(2)}^{(0)}(r; W) - q_{cj}\omega_\infty^{(0)}(W)U_{(1)}(r; W), \\ \omega_\infty^{(0)}(W) &= -\text{Wr}(U_{(1)}, V) = -\frac{1}{q_{cj}^2\omega_\infty^{(0)}(W)}. \end{aligned}$$

Proceeding completely similarly to the case of $|\xi| < \infty$, we find the spectral function $\sigma_\infty^{(0)}(E)$:

$$\frac{d\sigma_\infty^{(0)}(E)}{dE} = \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \Im \frac{1}{\omega_\infty^{(0)}(E + i\varepsilon)} = -\frac{1}{\pi} q_{cj}^2 \lim_{\varepsilon \rightarrow 0} \Im \omega_\infty^{(0)}(E + i\varepsilon).$$

The structure of the spectrum, the inversion formulas, and the orthonormality relations are also completely similar to the corresponding results in the case of $|\xi| < \infty$. In particular, the bound state spectrum is determined by the poles of the function $\omega_\infty^{(0)}(E)$ in the interval $|E| < m$. It can be evaluated explicitly and is given by formula (57) with $\gamma = 0$, the energy of the lower level with $\zeta = -1$ is equal to zero, $E_{\infty, 0}^{(0)} = 0$.

In conclusion, we note that the spectrum and the normalized eigenfunctions $U_{\xi, \text{norm}}^{(0)}(r; E)$ are continuous in ξ , the point $\xi = \infty$ included.

4.5 Overcritical charges

This region is defined by the charge values

$$q > q_{cj} = |\varkappa| = j + 1/2 \iff \Upsilon_+ = i\sigma, \sigma = \sqrt{q^2 - \varkappa^2} > 0.$$

In constructing s.a. Hamiltonians and analyzing their spectral properties in this charge region, we canonically follow the methods used in the previous cases and therefore only cite the main results.

4.5.1 Self-adjoint radial Hamiltonians

According to representation (43) – (45), the asymptotic behavior of the doublets $F \in D_*$ in the case of $q > q_{cj}$ is given by

$$F(r) = c_1(mr)^{i\sigma}u_+ + c_2(mr)^{-i\sigma}u_- + O(r^{1/2}), \quad r \rightarrow 0, \quad \forall F \in D_{h^*},$$

$$u_{\pm} = \begin{pmatrix} 1 \\ \frac{\varkappa \pm i\sigma}{q} \end{pmatrix},$$

which yields

$$\Delta_*(F) = \frac{2i\sigma}{q}(|c_1|^2 - |c_2|^2).$$

It follows that in the case of overcritical charges, i.e., for $\Upsilon_+ = i\sigma$, we have the one-parameter $U(1)$ -family $\{\hat{h}_\theta\}$, $0 \leq \theta \leq \pi$, $0 \sim \pi$, of s.a. operators associated with s.a. differential expression \check{h} (7) and specified by s.a. asymptotic boundary conditions²⁷

$$\hat{h}_\theta : \left\{ \begin{array}{l} D_\theta = \left\{ \begin{array}{l} F(r) : F(r) \text{ is absolutely continuous in } (0, \infty), F, \check{h}F \in \mathcal{L}^2(0, \infty), \\ F(r) = c[e^{i\theta}(mr)^{i\sigma}u_+ + e^{-i\theta}(mr)^{-i\sigma}u_- + O(r^{1/2})], \quad r \rightarrow 0, \\ 0 \leq \theta \leq \pi, \quad 0 \sim \pi, \end{array} \right. \\ \hat{h}_\theta F = \check{h}F, \end{array} \right. \quad (73)$$

D_θ is the domain of \hat{h}_θ .

4.5.2 Spectral analysis

For the doublet $U(r; W)$ defining guiding functional (1), we choose the doublet

$$U_\theta(r; W) = e^{i\theta}U_{(1)}(r; W) + e^{-i\theta}U_{(2)}(r; W)$$

with the asymptotic behavior

$$U(r; W) = e^{i\theta}(mr)^{i\sigma}u_+ + e^{-i\theta}(mr)^{-i\sigma}u_- + O(r), \quad r \rightarrow 0,$$

where $U_{(1)}$ and $U_{(2)}$ are given by formulas (16) – (20) (with $\Upsilon_+ = i\sigma$); $U_\theta(r; W)$ is real-entire in W because $U_{(2)} = \overline{U_{(1)}}$ for $\Upsilon_+ = i\sigma$ and real $W = E$.

²⁷The relation $c_2 = e^{i\theta}c_1$, $0 \leq \theta \leq 2\pi$, defining s.a. boundary conditions (compare with (67)), is equivalent to the relations $c_1 = e^{i\theta}c$, $c_2 = e^{-i\theta}c$, $0 \leq \theta \leq \pi$, with the change $\theta \rightarrow 2\pi - 2\theta$.

For \mathcal{D} , we choose the set \mathcal{D}_θ of the doublets belonging to D_θ and having a compact support.

Using the doublets $U_\theta(r; E_0)$ and $U_{(1)}(r; E_0)$ for constructing the solution $\Psi \in \mathcal{D}_\theta$ of the inhomogeneous equation $(\hat{h} - E_0)\Psi = F_0$, $F_0 \in \mathcal{D}_\theta$, we verify that the guiding functional Φ_θ is simple.

Green's function $G_\theta(r, r'; W)$, $\Im W > 0$, of the Hamiltonian \hat{h}_θ is constructed in terms of the doublets $U = U_\theta$ and $V = V_\theta$, where

$$\begin{aligned} V_\theta(r; W) &= \frac{2}{e^{-i\theta} + e^{i\theta}\tilde{\omega}(W)} V_{(1)}(r; W) = U_\theta(r; W) - \frac{q}{4\sigma}\omega_\theta(W)\tilde{U}_\theta(r; W), \\ \tilde{U}_\theta(r; W) &= \frac{1}{i}[e^{i\theta}U_{(1)}(r; W) - e^{-i\theta}U_{(2)}(r; W)], \\ \tilde{\omega}(W) &= \frac{q}{2i\sigma}\omega(W), \quad \omega_\theta(W) = -\text{Wr}(U, V) = -\frac{4i\sigma}{q} \frac{1 - \tilde{\omega}(W)e^{2i\theta}}{1 + \tilde{\omega}(W)e^{2i\theta}}, \end{aligned}$$

$V_{(1)}(r; W)$ and $\omega(W)$ are given in (21) – (23) (with $\Upsilon_+ = i\sigma$); $\tilde{U}_\theta(r; W)$ is real-entire in W . As a result, we obtain that

$$G_\theta(r, r'; W) = \begin{cases} \frac{1}{\omega_\theta(W)} V_\theta(r; W) \otimes U_\theta(r'; W), & r > r', \\ \frac{1}{\omega_\theta(W)} U_\theta(r; W) \otimes V_\theta(r'; W), & r < r'. \end{cases}$$

The spectral function $\sigma_\theta(E)$ of the radial Hamiltonian \hat{h}_θ is defined by

$$\frac{d\sigma_\theta(E)}{dE} = \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \Im \frac{1}{\omega_\theta(E + i\varepsilon)}$$

and is determined by the (generalized) function $\Im\omega^{-1}(E)$,

$$\omega_\theta^{-1}(E) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\omega_\theta(E + i\varepsilon)}.$$

At the points where the function

$$\omega_\theta(E) = \lim_{\varepsilon \rightarrow 0} \omega_\theta(E + i\varepsilon)$$

is different from zero, we have $\omega_\theta^{-1}(E) = 1/\omega_\theta(E)$.

The two energy regions $|E| \geq m$ and $|E| < m$ are naturally distinguished as before.

In the region $|E| \geq m$, the function $\omega_\theta(E)$ is continuous, different from zero, and complex, therefore, the spectral function $\sigma_\theta(E)$ for $|E| \geq m$ is absolutely continuous, and

$$\frac{d\sigma_\theta(E)}{dE} = \frac{1}{\pi} \Im \frac{1}{\omega_\theta(E)} \equiv Q_\theta^2(E).$$

In the region $|E| < m$, we have

$$\tilde{\omega}(E) = \frac{\Gamma(2i\sigma)}{\Gamma(-2i\sigma)} \frac{\Gamma(-i\sigma - Eq/\tau)}{\Gamma(i\sigma - Eq/\tau)} \frac{\tau(\varkappa + i\sigma) - q(m - E)}{\tau(\varkappa - i\sigma) - q(m - E)} (2\tau/m)^{-2i\sigma} \equiv e^{-2i\Theta(E)},$$

therefore the function

$$\omega_\theta(E) = \frac{4\sigma}{q} \tan(\Theta(E) - \theta)$$

is real.

It follows that the spectral function $\sigma_\theta(E)$ for $|E| < m$ is a jump function with the jumps $Q_{\theta,n}^2$,

$$Q_{\theta,n}^2 = \lim_{E \rightarrow E_{\theta,n}} \frac{E_{\theta,n} - E}{\omega_\theta(E)},$$

located at the discrete points $E_{\theta,n}$ where $\omega_\theta(E_{\theta,n}) = 0$, such that

$$\frac{d\sigma_\theta(E)}{dE} = \sum_n Q_{\theta,n}^2 \delta(E - E_{\theta,n}).$$

We failed to find an explicit formula for the discrete energy eigenvalues $E_{\theta,n}$. We only note that there is an infinite number of the discrete levels which accumulate at the point $E = m$. Their asymptotic form as $n \rightarrow \infty$ is given by the previous nonrelativistic formula:

$$\epsilon_{\theta,n} \equiv m - E_{\theta,n} = \frac{mq^2}{2n^2}.$$

The lower bound state energy essentially depends on θ , and there exists a value of θ for which the lower bound state energy coincides with the boundary $E = -m$ of the lower (positron) continuous spectrum.

The inversion formulas and Parseval equality in terms of normalized (generalized) eigenfunctions $U_{\theta,\text{norm}}(r; E)$ and the Fourier coefficients $\varphi_\theta(E)$ are copies of formulas (60), (61), (62), (63), and (64).

As in the previous subsections, a comment on the applicability of the standard method for finding the energy spectrum and eigenfunctions based on the physical arguments holds. As an example, we consider the energy region $|E| < m$ where the solutions F of the differential equation $\hbar F = EF$ either exponentially grow or exponentially decrease as $r \rightarrow \infty$, any solution being square integrable at the origin. Only exponentially decreasing solutions

$$F = cV_\theta(r; W) = c[U_\theta(r; W) - \frac{q}{4\sigma}\omega_\theta(W)\tilde{U}_\theta(r; W)],$$

c is a constant, are proper. They are square integrable, $F \in \mathcal{L}^2(0, \infty)$, for any E in the interval $|E| < m$, but satisfy s.a. asymptotic boundary conditions (73) only if $\omega_\theta(E) = 0$, which reproduces the results for the eigenvalues and eigenfunctions of the discrete spectrum. We can also establish the orthonormality relations for the eigenfunctions $U_{\theta,\text{norm}}(r; E)$, which are analogues of relations (65), by a direct calculation of the corresponding integrals with the method described in Appendix 4.5.2.

In conclusion, we point out that the number of s.a. extensions of the total Dirac Hamiltonian (i.e., the number of independent parameters of s.a. extensions) depends on the charge values q (on the value of Z) as follows: it is easy to verify that in the interval $q_n < q \leq q_{n+1}$, where

$$q_n = \begin{cases} 0, & n = 0, \\ \sqrt{n^2 - 1/4}, & n = 1, 2, \dots, \end{cases}$$

the number of independent parameters of s.a. extensions is equal to $2n$. This follows from the fact that the total Dirac Hamiltonian is a direct sum of its parts unitary equivalent to the radial Hamiltonians, see (9), (8).

Appendix A

One of the methods for finding the spectrum of a s.a. differential operator and its complete system of (generalized) eigenfunctions and constructing the corresponding Fourier expansion with respect to these eigenfunctions (the so-called inversion formulas) is based on the Krein method of guiding functionals. For ordinary scalar differential operators, this method is described in [18], but it is directly extended to the case of ordinary matrix operators. We here present the key points of the method as applied to our case where it suffices to consider only one guiding functional. This implies that the operator spectrum is simple²⁸; we call such a functional a simple guiding functional.

By definition, a guiding functional $\Phi(F; W)$ for a s. a. operator \hat{h} associated with a differential expression \check{h} is a functional of the form

$$\Phi(F; W) = \int_0^\infty U(r; W)F(r)dr, \quad (1)$$

where $U(r; W)$ is a solution of the homogeneous equation

$$(\check{h} - W)U = 0$$

which is real-entire in W and $F(r)$ belongs to some subspace $\mathcal{D} \subset D \cap D_h$, where D is a space of doublets with a compact support such that \mathcal{D} is dense in $\mathcal{L}^2(0, \infty)$.

A guiding functional $\Phi(F; W)$ is called simple if it satisfies the following conditions:

- 1) for a fixed F , the functional $\Phi(F; W)$ is an entire function of W ;
- 2) if

$$\Phi(F_0; E_0) = 0, \quad \Im E_0 = 0, \quad F_0 \in \mathcal{D},$$

then the inhomogeneous equation

$$(\check{h} - E_0)\Psi = F_0$$

has a solution $\Psi \in \mathcal{D}$;

- 3) $\Phi(\hat{h}F; W) = W\Phi(F; W)$.

We note, that the existence of a simple guiding functional is conditioned by the existence of appropriate U and \mathcal{D} . A guiding principle for the choice of $U(r; W)$ is that its behavior as $r \rightarrow 0$ must conform to the asymptotic behavior admissible for the doublets belonging to D_h , or, roughly speaking, $U(r; W)$ at the origin must belong to D_h . This corresponds to the conventional physical requirement that the (generalized) eigenfunctions of the operator \hat{h} , being generally non-square-integrable, but "normalizable to δ -function", satisfy the s.a. boundary conditions specifying \hat{h} .

If a simple guiding functional exists, then the s. a. operator \hat{h} has the following spectral properties:

²⁸For a definition, see [18]. In the physical terminology, this means that the spectrum is nondegenerate.

1) the spectrum of \hat{h} is simple, and there exists a spectral function $\sigma(E)$, a nondecreasing real function continuous from the right and such that the set of spectrum points coincides with the set of growth points²⁹ of the function $\sigma(E)$;

2) the inversion formulas

$$\Phi(E) = \int_0^\infty U(r; E)F(r)dr, \quad (2)$$

$$F(r) = \int_{-\infty}^\infty U(r; E)\Phi(E)d\sigma(E), \quad (3)$$

and the Parseval equality

$$\int_0^\infty |F(r)|^2 dr = \int_{-\infty}^\infty |\Phi(E)|^2 d\sigma(E) \quad (4)$$

hold, where $\Phi(E) \in L^2_\sigma(-\infty, \infty)$, $F(r) \in \mathcal{L}^2(0, \infty)$, the function $U(r; E)$ in the integrands in (2) and (3) can be defined as zero outside of the spectrum points of the operator \hat{h} (outside of the growth points of $\sigma(E)$), and the convergence of the integrals in (2) and (3) in general must be understood in the sense of the convergence with respect to the metrics of the respective spaces $L^2_\sigma(-\infty, \infty)$ and $\mathcal{L}^2(0, \infty)$. This means that the set of the (generalized) eigenfunctions $\{U(r; E), E \in \text{Spec}\hat{h}\}$ of the operator \hat{h} forms a complete orthogonal system.

The spectral function $\sigma(E)$ can be expressed via the resolvent of the operator \hat{h} . As is known, see [18], the resolvent $\hat{R}(W) = (\hat{h} - W)^{-1}$ with $\Im W \neq 0$ is an integral operator with the kernel $G(r, r'; W)$ (Green's function). The spectral function $\sigma(E)$ is expressed in terms of Green's function as follows:

$$U(c; E) \otimes U(c; E)d\sigma(E) = d\mathcal{M}(c; E), \quad (5)$$

$$\mathcal{M}(c; E) = \lim_{\delta \rightarrow +0} \lim_{\varepsilon \rightarrow +0} \frac{1}{\pi} \int_\delta^{E+\delta} \Im M(c; E' + i\varepsilon) dE', \quad (6)$$

$$M(c; W) = G(c - 0, c + 0; W), \quad (7)$$

where c is an arbitrary internal point of the interval $(0, \infty)$. We note that for any E , one of the diagonal elements of the matrix $U(c; E) \otimes U(c; E)$ is different from zero. Of course, $\sigma(E)$ is independent of c .

Appendix B

In this Appendix, we describe a method for calculating the so-called overlap integrals for the solutions of the differential equation $\hat{h}F = EF$. It is based on the integral Lagrange identity and on evaluating the asymptotic behavior of the solutions at the boundaries, the origin and infinity. We apply this method to proving the orthonormality relations for the (generalized) eigenfunctions of the radial Hamiltonian and illustrate it by the example of the second noncritical charge region.

²⁹The set of growth points of the function $\sigma(E)$ is the complement of the open set of constancy points of the function $\sigma(E)$. A point E_0 is the constancy point of the function $\sigma(E)$ if there exists a vicinity of the point E_0 where $\sigma(E)$ is constant.

We call the integral³⁰

$$\int_0^\infty F(r; W)F'(r; W')dr = \lim_{R \rightarrow \infty, \epsilon \rightarrow 0} \int_\epsilon^R F(r; W)F'(r; W')dr$$

for two doublets F and F' the overlap integral for these doublets. Let F and F' satisfy the respective homogeneous equations

$$(\check{h} - W)F(r; W) = 0 \text{ and } (\check{h} - W')F'(r; W') = 0.$$

Then the equality for the overlap integral

$$\int_0^\infty F(r; W)F'(r; W')dr = I^\infty - I_0, \quad (1)$$

where

$$I^\infty = \lim_{r \rightarrow \infty} \frac{\text{Wr}(r; F, F')}{W - W'}, \quad (2)$$

$$I_0 = \lim_{r \rightarrow 0} \frac{\text{Wr}(r; F, F')}{W - W'} \quad (3)$$

holds. The equality (1) is a special case of the integral Lagrange identity. In what follows, we are interested in the case of real W and W' , $W = E$ and $W' = E'$. The overlap integral is understood as a generalized function of E and E' . Evaluating the overlap integrals is thus reduced to evaluating the asymptotics of the Wronskian of the corresponding doublets at the boundaries.

We begin with evaluating the asymptotics of some basic functions and doublets.

Let $|E| \geq m$, in which case we have $K = |E|k/E$, $k = \sqrt{E^2 - m^2}$, and let $r \rightarrow \infty$. Using the known asymptotics of the functions $\Phi(\alpha, \beta; x)$ (see, for example, [21]), we have

$$\Phi(\alpha, \beta; 2i\xi_1 kr) \rightarrow \frac{\Gamma(1 + 2\Upsilon)}{\Gamma(1 + \Upsilon - i\xi_2 qE/k)} e^{i\xi_1 \pi \Upsilon / 2} e^{-\xi_1 \xi_2 \pi E q / (2k)} (2kr)^{-\Upsilon - i\xi_2 E q / k},$$

$$\alpha = \Upsilon + i\xi_2 qE/k, \quad \xi_1 = \pm 1, \quad \xi_2 = \pm 1, \quad \beta = 1 + 2\Upsilon,$$

where Υ is any real or pure imaginary number, $\Upsilon \neq -n/2$, $n = 1, 2, \dots$. If Υ is real, $\Upsilon = \gamma \neq -n/2$, $n = 1, 2, \dots$, then

$$(mr)^\Upsilon \Phi_+(r, \Upsilon, E, k) \rightarrow 2\Delta(\Upsilon, E) \cos \psi(r; \Upsilon, E),$$

$$(mr)^\Upsilon \Phi_-(r, \Upsilon, E, k) \rightarrow \frac{2}{k} \Delta(\Upsilon, E) \sin \psi(r; \Upsilon, E),$$

where

$$\Delta(\Upsilon, E) = \frac{\Gamma(1 + 2\Upsilon)(2k/m)^{-\Upsilon} e^{-\pi qE/(2k)}}{|\Gamma(1 + \Upsilon + iqE/k)|},$$

$$\psi(r; \Upsilon, E) = kr + \frac{qE}{k} \ln(2kr) - \frac{\pi \Upsilon}{2} - \psi_\Gamma(\Upsilon, E),$$

$$\psi_\Gamma(\Upsilon, E) = \arg \Gamma(1 + \Upsilon + iqE/k),$$

³⁰In this Appendix, a notation like F' denotes another function, but not a derivative.

which yields

$$X(r, \Upsilon, E, k) \rightarrow \Delta(\Upsilon, E) \left[\cos \psi(r; \Upsilon, E) u_+ + \frac{\sin \psi(r; \Upsilon, E)}{k} \binom{(m+W)(\alpha+\gamma)}{m-E} \right].$$

Let $|E| < m$. For our purposes, it suffices to know that the doublets $U(r; E_n)$ and $V(r; E)$ decrease exponentially as $r \rightarrow \infty$.

We use the relation

$$\begin{aligned} \frac{E}{|E|} \frac{\sin[\psi_\Gamma(r; \Upsilon, E) \pm \psi_\Gamma(r; \Upsilon', E')]}{E - E'} &\rightarrow \frac{|E|}{k} \frac{\sin[(k - k')r]}{k - k'} \rightarrow \\ &\rightarrow \frac{|E|}{k} \pi \delta(k - k') = \pi \delta(E - E'), \quad r \rightarrow \infty, \end{aligned} \quad (4)$$

which holds in a distribution-theoretic sense. We call the expressions of the form

$$\begin{aligned} a_\pm(E, E') \sin[\psi_\Gamma(r; \Upsilon, E) \pm \psi_\Gamma(r; \Upsilon', E')], \\ b_\pm(E, E') \cos[\psi_\Gamma(r; \Upsilon, E) \pm \psi_\Gamma(r; \Upsilon', E')], \end{aligned}$$

where $a_\pm(E, E')$, $b_\pm(E, E')$ are finite at $E = E'$, the quickly oscillating expressions (QO); such expressions have the zero limit in a distribution-theoretic sense as $r \rightarrow \infty$.

This allows obtaining the limits I^∞ for the basic doublets. We have

$$\begin{aligned} U_{(1)} &= U_{(1)}(r; \gamma, E), \quad U'_{(1)} = U'_{(1)}(r; \gamma, E'), \quad \gamma > 0, \\ (E - E')^{-1} W(r; U_{(1)}, U'_{(1)}) &\rightarrow \\ &\rightarrow A(\gamma, E) \frac{E}{|E|} \frac{\sin[\psi_\Gamma(\gamma, E) - \psi_\Gamma(\gamma, E')]}{\pi(E - E')} + \text{QO} \rightarrow \\ &\rightarrow A(\gamma, E) \delta(E - E'), \quad r \rightarrow \infty \end{aligned} \quad (5)$$

$$\begin{aligned} U_{(1)} &= U_{(1)}(r; \gamma, E), \quad U'_{(2)} = U'_{(2)}(r; \gamma, E'), \quad 0 < \gamma < 1/2, \\ (E - E')^{-1} W(r; U_{(1)}, U'_{(2)}) &\rightarrow \\ &\rightarrow B(\gamma, E) \frac{E}{|E|} \frac{\sin[\psi_\Gamma(\gamma, E) - \psi_\Gamma(-\gamma, E')]}{\pi(E - E')} - \\ &- B(\gamma, E) \frac{\gamma k}{q|E|} \frac{\cos[\psi_\Gamma(\gamma, E) - \psi_\Gamma(-\gamma, E')]}{\pi(E - E')} + \text{QO} \rightarrow \\ &\rightarrow B(\gamma, E) \delta(E - E') - B(\gamma, E) \frac{\gamma k}{q|E|} \frac{\cos[\psi_\Gamma(\gamma, E) - \psi_\Gamma(-\gamma, E')]}{\pi(E - E')}, \quad r \rightarrow \infty, \end{aligned} \quad (6)$$

$$\begin{aligned} U_{(2)} &= U_{(2)}(r; \gamma, E), \quad U'_{(1)} = U'_{(1)}(r; \gamma, E'), \quad 0 < \gamma < 1/2, \\ (E - E')^{-1} W(r; U_{(2)}, U'_{(1)}) &\rightarrow \\ &\rightarrow B(\gamma, E) \delta(E' - E) - B(\gamma, E) \frac{\gamma k}{q|E|} \frac{\cos[\psi_\Gamma(\gamma, E') - \psi_\Gamma(-\gamma, E)]}{\pi(E' - E)} \rightarrow \\ &\rightarrow B(\gamma, E) \delta(E - E') + B(\gamma, E) \frac{\gamma k}{q|E|} \frac{\cos[\psi_\Gamma(\gamma, E) - \psi_\Gamma(-\gamma, E')]}{\pi(E - E')}, \quad r \rightarrow \infty, \end{aligned} \quad (7)$$

$$\begin{aligned}
U_{(2)} &= U_{(2)}(r; \gamma, E), \quad U'_{(2)} = U'_{(2)}(r; \gamma, E'), \quad 0 < \gamma < 1/2, \\
(E - E')^{-1}W(r; U_{(2)}, U'_{(2)}) &\rightarrow \\
&\rightarrow A(-\gamma, E) \frac{E \sin[\psi_{\Gamma}(-\gamma, E) - \psi_{\Gamma}(-\gamma, E')]}{|E| \pi(E - E')} + \text{QO} \rightarrow \\
&\rightarrow A(-\gamma, E) \delta(E - E'), \quad r \rightarrow \infty,
\end{aligned} \tag{8}$$

where

$$A(\Upsilon, E) = \Delta^2(\Upsilon, E) \frac{2\pi(q_{ej} + \zeta\Upsilon)(q_{ej}|E| + \zeta m\Upsilon)}{kq^2}, \tag{9}$$

$$B(\gamma, E) = \frac{|E|}{k} \Delta(\gamma, E) \Delta(-\gamma, E). \tag{10}$$

For the corresponding limits I_0 , we respectively find (the relations are valid for any E, E')

$$\begin{aligned}
U_{(1)} &= U_{(1)}(r; \gamma, E), \quad U'_{(1)} = U'_{(1)}(r; \gamma, E'), \quad \gamma > 0, \\
(E - E')^{-1}W(r; U_{(1)}, U'_{(1)}) &\rightarrow 0, \quad r \rightarrow 0,
\end{aligned} \tag{11}$$

$$\begin{aligned}
U_{(1)} &= U_{(1)}(r; \gamma, E), \quad U'_{(2)} = U'_{(2)}(r; \gamma, E'), \quad 0 < \gamma < 1/2, \\
(E - E')^{-1}W(r; U_{(1)}, U'_{(2)}) &\rightarrow -\frac{2\gamma}{q(E - E')}, \quad r \rightarrow 0,
\end{aligned} \tag{12}$$

$$\begin{aligned}
U_{(2)} &= U_{(2)}(r; \gamma, E), \quad U'_{(1)} = U'_{(1)}(r; \gamma, E'), \quad 0 < \gamma < 1/2, \\
(E - E')^{-1}W(r; U_{(2)}, U'_{(1)}) &\rightarrow \frac{2\gamma}{q(E - E')}, \quad r \rightarrow 0,
\end{aligned} \tag{13}$$

$$\begin{aligned}
U_{(2)} &= U_{(2)}(r; \gamma, E), \quad U'_{(2)} = U'_{(2)}(r; \gamma, E'), \quad 0 < \gamma < 1/2, \\
(E - E')^{-1}W(r; U_{(2)}, U'_{(2)}) &\rightarrow 0, \quad r \rightarrow 0.
\end{aligned} \tag{14}$$

The obtained relations allow calculating the overlap integrals and proving the orthonormality relations for the eigenfunctions of the radial Hamiltonians. As an example, we consider the second noncritical charge region, the other charge regions, including the critical and overcritical regions, are considered quite similarly.

We have to calculate the integral

$$\int_0^{\infty} U_{\xi}(r; E) U_{\xi}(r; E') dr,$$

where $U_{\xi}(r; E)$ is defined by Eq. (69). Using relations (1) – (3) and (5) – (14), we find

$$\begin{aligned}
\int_0^{\infty} U_{\xi}(r; E) U_{\xi}(r; E') dr &= C_{\xi}(E) \delta(E - E'), \quad |E|, |E'| \geq m, \\
C_{\xi}(E) &= A(\gamma, E) + 2\xi B(\gamma, E) + \xi^2 A(-\gamma, E),
\end{aligned}$$

$$\int_0^\infty U_\xi(r; E_{\xi,n})U_\xi(r; E')dr = 0, \quad |E'| \geq m,$$

$$\int_0^\infty U_\xi(r; E_{\xi,n})U_\xi(r; E_{\xi,n'})dr = 0, \quad n \neq n'.$$

The normalization factor A_n for the eigenfunctions of the discrete spectrum,

$$A_n^2 = \int_0^\infty U_\xi^2(r; E_{\xi,n})dr,$$

can also be calculated (see, for example, [14]). It is interesting to note that we can explicitly verify the fulfillment of the relation $A_n = Q_{\xi,n}^{-1}$. For this purpose, we consider the integral

$$\int_0^\infty U_\xi(r; E_{\xi,n})V(r; E')dr = \lim_{r \rightarrow 0} \frac{\text{Wr}(r; U_\xi, V')}{E' - E_{\xi,n}}, \quad V' = V(r; E'), \quad |E'| < m,$$

where $V(r; E)$ is defined by (70). Using relations (11) – (14), we find

$$\int_0^\infty U_\xi(r; E_{\xi,n})V(r; E')dr = \frac{\omega_\xi(E')}{E_{\xi,n} - E'}.$$

We now recall that $V(r; E_{\xi,n}) = U_\xi(r; E_{\xi,n})$ and finally obtain that

$$\int_0^\infty U_\xi^2(r; E_{\xi,n})dr = \lim_{E' \rightarrow E_{\xi,n}} \frac{\omega_\xi(E')}{E_{\xi,n} - E'} = Q_{\xi,n}^{-2}.$$

We also note that it follows from the inversion formulas that $C_\xi(E) = Q_\xi^{-2}(E)$.

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