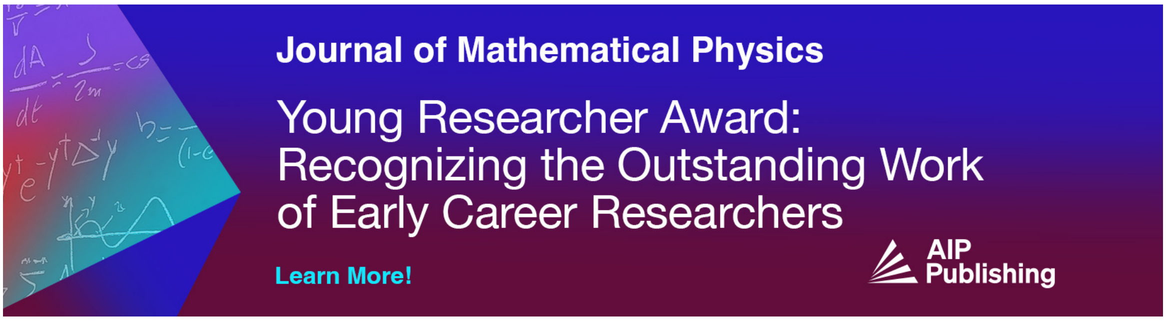
Journal of Mathematical Physics

RESEARCH ARTICLE | APRIL 12 2019

Boundary triples for the Dirac operator with Coulomb-type spherically symmetric perturbations

Biagio Cassano ; Fabio Pizzichillo

J. Math. Phys. 60, 041502 (2019)
https://doi.org/10.1063/1.5063986



Journal of
Mathematical Physics ARTICLE scitation.org/journal/jmp

Boundary triples for the Dirac operator with Coulomb-type spherically symmetric perturbations

Cite as: J. Math. Phys. 60, 041502 (2019); doi: 10.1063/1.5063986
Submitted: 3 October 2018 • Accepted: 23 March 2019 •
Published Online: 12 April 2019

Biagio Cassano[1,a] and Fabio Pizzichillo[2,b]

AFFILIATIONS

[1] The Czech Academy of Science, Nuclear Physics Institute, Rez/Prague, Czech
[2] CNRS and CEREMADE, Université Paris-Dauphine, PSL Research University, F-75016 Paris, France

[a] E-mail: cassano@ujf.cas.cz
[b] E-mail: pizzichillo@ceremade.dauphine.fr

ABSTRACT

We determine explicitly a boundary triple for the Dirac operator $H := -i\alpha\cdot\nabla + m\beta + \mathbb{V}(x)$ in $\mathbb{R}^3$, for $m \in \mathbb{R}$ and $\mathbb{V}(x) = |x|^{-1}(\nu\mathbb{I}_4 + \mu\beta - i\lambda\alpha\cdot x/|x|\beta)$, with $\nu,\mu,\lambda \in \mathbb{R}$. Consequently, we determine all the self-adjoint realizations of H in terms of the behavior of the functions of their domain in the origin. When $\sup_x |x||\mathbb{V}(x)| \le 1$, we discuss the problem of selecting the *distinguished* extension requiring that its domain is included in the domain of the appropriate quadratic form.

I. INTRODUCTION AND MAIN RESULTS

In this paper, we determine a boundary triple and describe all the self-adjoint realizations of the differential operator

$$H := H_0 + \mathbb{V}, \tag{1.1}$$

where H_0 is the free Dirac operator in $\mathbb{R}^3$ defined by

$$H_0 := -i\alpha\cdot\nabla + m\beta, \tag{1.2}$$

with $m \in \mathbb{R}$,

$$\beta := \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & -\mathbb{I}_2 \end{pmatrix}, \quad \alpha := (\alpha_1,\alpha_2,\alpha_3), \quad \alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \quad \text{for } j = 1,2,3,$$

and σ_j are the *Pauli matrices*

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and finally

$$\mathbb{V}(x) := \frac{1}{|x|}\left(\nu\mathbb{I}_4 + \mu\beta + \lambda\left(-i\alpha\cdot\frac{x}{|x|}\beta\right)\right) \quad \text{for } x \neq 0, \tag{1.3}$$

where ν, λ, and μ are real numbers, and $\mathbb{I}_4$ is the 4×4 identity matrix.

The operator $H_0 + \mathbb{V}$ describes the motion of relativistic $\frac{1}{2}$-spin particles in the external potential $\mathbb{V}$. In detail, setting

$$\mathbb{V} = \mathbb{V}_{el} + \mathbb{V}_{sc} + \mathbb{V}_{am} := v_{el}(x)\mathbb{I}_4 + v_{sc}(x)\beta + v_{am}(x)\left(-i\alpha\cdot\frac{x}{|x|}\beta\right)$$

for real valued v_{el}, v_{sc}, and v_{am}, the potentials $\mathbb{V}_{el}$, $\mathbb{V}_{sc}$, and $\mathbb{V}_{am}$ are called *electric*, *scalar*, and *anomalous magnetic* potential, respectively. This particular class of potentials has the property that, in the case that v_{el}, v_{sc}, and v_{am} only depend on the radial variable, the action of $H_0 + \mathbb{V}$ leaves the *partial wave subspaces* invariant (see below). Moreover, in the case that they have a singularity $\sim|x|^{-1}$ in the origin, the potential has the same scaling as the Dirac operator.

The dynamics of quantum systems is described in terms of self-adjoint operators, as shown by Stone's theorem, see, e.g., Ref. 27. For this reason, it is a primary task to describe all the self-adjoint extensions (if any exists) of a given symmetric operator associated with a physical system. Von Neumann gave the first complete solution to this problem: his theory is fully general and completely describes all the self-adjoint extensions of every densely defined and symmetric operator in an abstract Hilbert space in terms of unitary operators between its deficiency spaces, see, e.g., Ref. 26. Von Neumann's theory works at an abstract level: for specific classes of operators, it is desirable to have a more concrete characterization of the self-adjoint extensions. In many cases, self-adjoint operators arise when one introduces some boundary conditions for a differential expression: perturbing operators with potentials with a singularity in one point, one would like to establish a direct link between self-adjoint extensions and behavior in the point of the functions in their domain. Referring to Refs. 5 and 12 for a general overview on the theories of self-adjoint extensions, we cite here the theory of *boundary triples*, see Refs. 5, 9, 25, and 31 and references therein, that gives this desired description. The main result of this paper (Theorem 1.5) is the explicit determination of a boundary triple for the operator H: thanks to this, we are then able to describe all the self-adjoint realizations in terms of the behavior in the origin of the functions in the domain.

The vast literature has been dedicated to the problem of the self-adjointness of perturbed Dirac operators. Making reference to the Introduction of Ref. 7, to the survey,[13] and to the book[32] for more details, we list here some relevant studies. In Ref. 18, it was observed that thanks to the Hardy inequality,

$$\frac{1}{4}\int_{\mathbb{R}^3}\frac{|f|^2}{|x|^2}\,dx \le \int_{\mathbb{R}^3}|\nabla f|^2\,dx \quad \text{for } f\in C_c^\infty(\mathbb{R}^3), \tag{1.4}$$

and the Kato-Rellich theorem, it is possible to prove that, for $|\nu|\in\left[0,\frac{1}{2}\right)$, the operator $H_0+\nu/|x|$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)^4$ and self-adjoint on $\mathcal{D}(H_0)=H^1(\mathbb{R}^3)^4$. In fact, the optimal range for the self-adjointness is $|\nu|\in\left[0,\frac{\sqrt{3}}{2}\right)$, as shown in Refs. 16, 28, 30, and 34. For $|\nu|>\sqrt{3}/2$, $H_0+\nu/|x|$ is not essentially self-adjoint and infinite self-adjoint extensions can be constructed. Among these, for $|\nu|\in\left(\frac{\sqrt{3}}{2},1\right)$, there exists one *distinguished* extension H_S such that

$$\mathcal{D}(H_D)\subset\mathcal{D}(r^{-1/2})^4=\{\psi\in L^2(\mathbb{R}^3)^4 : |x|^{-1/2}\psi\in L^2(\mathbb{R}^3)^4\} \tag{1.5}$$

or equivalently $\mathcal{D}(H_D)\subset H^{1/2}(\mathbb{R}^3)^4$: in other words, one requires that all the functions in the domain of the extension are in the form domain of the potential and the momentum. For details, see Refs. 6, 14, 21, 23, 29, and 35. For $|\nu|\ge1$, many self-adjoint extensions can be built, and for $|\nu|>1$, none appears to be *distinguished* in some suitable sense, see Refs. 17, 33, and 36. The definition of a distinguished extension for the case $|\nu|=1$ has been given in Ref. 11, where it is considered a potential $V:\mathbb{R}^3\to\mathbb{R}$ such that for some constant $c(V)\in(-1,1)$, $\Gamma:=\sup(V)<1+c(V)$ and for every $\varphi\in C_c^\infty(\mathbb{R}^3)^2$,

$$\int_{\mathbb{R}^3}\left(\frac{|\sigma\cdot\nabla\varphi|^2}{1+c(V)-V}+(1+c(V)+V)|\varphi|^2\right)dx\ge0. \tag{1.6}$$

In particular, for an electrostatic potential $\mathbb{V}(x):=V(x)\mathbb{I}_4$, $-\nu|x|^{-1}\le V(x)<1+\sqrt{1-\nu^2}$, $0<\nu\le1$, the operator $H_0+\mathbb{V}$ is self-adjoint on a suitable domain. If $0<\nu<1$, the self-adjoint extension described is the distinguished one, as also shown in Ref. 22; for $\nu=1$, the self-adjoint extension described is the distinguished one, since continuous prolongation of the sub-critical case can cover it. Recently, in Ref. 10, it is shown that this extension can be obtained as the limit in the norm resolvent sense of potentials where the singularity has been removed with a cutoff around the singularity.

The approach of Ref. 18 could be used independently on the spherical symmetry of the potential: $H_0+\mathbb{V}$ is self-adjoint when $\mathbb{V}$ is a 4×4 Hermitian real-valued matrix potential $\mathbb{V}$ such that

$$|\mathbb{V}(x)|\le a\frac{1}{|x|}+b,\qquad x\in\mathbb{R}^3\backslash\{0\},$$

with $b\in\mathbb{R}$ and $a<1/2$, see Ref. 20, Theorem V 5.10. In Refs. 3, 4, and 19, more general 4×4 matrix-valued measured functions $\mathbb{V}$ are considered, in the assumption that $|x||\mathbb{V}(x)|\le\nu<1$, and a distinguished self-adjoint extension [in the sense of (1.5)] is constructed, exploiting the *Kato-Nenciu* inequality

$$\int_{\mathbb{R}^3}\frac{|\psi|^2}{|x|}\,dx\le\int_{\mathbb{R}^3}|(-i\alpha\cdot\nabla+m\beta+i\epsilon)\psi|^2|x|\,dx,\qquad \text{for }\psi\in C_c^\infty(\mathbb{R}^3)^4, m,\epsilon\in\mathbb{R}. \tag{1.7}$$

In our previous work,[7] we considered matrix-valued potentials as in (1.3) and we investigated the existence of self-adjoint extensions T such that

$$\mathring{H}_{min} \subseteq T = T^* \subseteq H_{max}, \tag{1.8}$$

where the *minimal operator* $\mathring{H}_{min}$ and the *maximal operator* H_{max} are defined as follows:

$$\mathcal{D}(\mathring{H}_{min}) := C_c^\infty(\mathbb{R}^3\backslash\{0\})^4, \qquad \mathring{H}_{min}\psi := H\psi \quad \text{for } \psi \in \mathcal{D}(\mathring{H}_{min}), \tag{1.9}$$

$$\mathcal{D}(H_{max}) := \{\psi \in L^2(\mathbb{R}^3)^4 : H\psi \in L^2(\mathbb{R}^3)^4\}, \qquad H_{max}\psi := H\psi \quad \text{for } \psi \in \mathcal{D}(H_{max}), \tag{1.10}$$

where $H\psi$ in (1.9) is computed in the classical sense and in (1.10), $H\psi \in L^2(\mathbb{R}^3)^4$ has to be read in the distributional sense. It is easy to see that $\mathring{H}_{min}$ is symmetric and $(\mathring{H}_{min})^* = H_{max}$. The strategy of Ref. 7 consists in considering the self-adjointness of $H_0 + \mathbb{V}$ on the *partial wave subspaces*: such spaces are left invariant by H_0 and potentials $\mathbb{V}$ as in (1.3). We sketch here this topic, referring to Ref. 7 and Ref. 32, Sec. 4.6 for further details.

Let Y_n^l be the spherical harmonics. They are defined for $n = 0, 1, 2, \ldots$, and $l = -n, -n+1, \ldots, n$, and they satisfy $\Delta_{\mathbb{S}^2} Y_n^l = n(n+1)Y_n^l$, where $\Delta_{\mathbb{S}^2}$ denotes the usual spherical Laplacian. Moreover, Y_n^l form a complete orthonormal set in $L^2(\mathbb{S}^2)$. For $j = 1/2, 3/2, 5/2, \ldots$, and $m_j = -j, -j+1, \ldots, j$, set

$$\psi_{j-1/2}^{m_j} := \frac{1}{\sqrt{2j}} \begin{pmatrix} \sqrt{j+m_j}\, Y_{j-1/2}^{m_j-1/2} \\ \sqrt{j-m_j}\, Y_{j-1/2}^{m_j+1/2} \end{pmatrix},$$

$$\psi_{j+1/2}^{m_j} := \frac{1}{\sqrt{2j+2}} \begin{pmatrix} \sqrt{j+1-m_j}\, Y_{j+1/2}^{m_j-1/2} \\ -\sqrt{j+1+m_j}\, Y_{j+1/2}^{m_j+1/2} \end{pmatrix},$$

then $\psi_{j\pm1/2}^{m_j}$ form a complete orthonormal set in $L^2(\mathbb{S}^2)^2$. Moreover, we set

$$r = |x|, \quad \hat{x} = x/|x|, \quad \text{and} \quad L = -ix \times \nabla \quad \text{for } x \in \mathbb{R}^3\backslash\{0\}.$$

Then,

$$(\sigma\cdot\hat{x})\psi_{j\pm1/2}^{m_j} = \psi_{j\mp1/2}^{m_j} \quad \text{and} \quad (1 + \sigma\cdot L)\psi_{j\pm1/2}^{m_j} = \pm(j+1/2)\psi_{j\pm1/2}^{m_j},$$

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of *Pauli's matrices*. For $k_j := \pm(j+1/2)$, we set

$$\Phi^+_{m_j,\pm(j+1/2)} := \begin{pmatrix} i\,\psi_{j\pm1/2}^{m_j} \\ 0 \end{pmatrix}, \quad \Phi^-_{m_j,\pm(j+1/2)} := \begin{pmatrix} 0 \\ \psi_{j\mp1/2}^{m_j} \end{pmatrix}.$$

Then, the set $\{\Phi^+_{m_j,k_j}, \Phi^-_{m_j,k_j}\}_{j,k_j,m_j}$ is a complete orthonormal basis of $L^2(\mathbb{S}^2)^4$. We prescribe the following ordering for the triples (j, m_j, k_j), for $j = \frac{1}{2}, \frac{3}{2}, \ldots$; $m_j = -j, \ldots, j$; $k_j = j + 1/2, -j - 1/2$:

$$\begin{gathered}
\left(\frac{1}{2}, -\frac{1}{2}, 1\right), \left(\frac{1}{2}, \frac{1}{2}, 1\right), \left(\frac{1}{2}, -\frac{1}{2}, -1\right), \left(\frac{1}{2}, \frac{1}{2}, -1\right), \\
\left(\frac{3}{2}, -\frac{3}{2}, 2\right), \left(\frac{3}{2}, -\frac{1}{2}, 2\right), \left(\frac{3}{2}, \frac{1}{2}, 2\right), \left(\frac{3}{2}, \frac{3}{2}, 2\right), \\
\left(\frac{3}{2}, -\frac{3}{2}, -2\right), \left(\frac{3}{2}, -\frac{1}{2}, -2\right), \left(\frac{3}{2}, \frac{1}{2}, -2\right), \left(\frac{3}{2}, \frac{3}{2}, -2\right), \ldots, \\
\left(j, -j, j + \frac{1}{2}\right), \ldots, \left(j, j, j + \frac{1}{2}\right), \left(j, -j, -j - \frac{1}{2}\right), \ldots, \left(j, j, -j - \frac{1}{2}\right), \ldots.
\end{gathered} \tag{1.11}$$

We define the following space:

$$\mathcal{H}_{m_j,k_j} := \left\{ \frac{1}{r}\left(f^+_{m_j,k_j}(r)\Phi^+_{m_j,k_j}(\hat{x}) + f^-_{m_j,k_j}(r)\Phi^-_{m_j,k_j}(\hat{x})\right) \in L^2(\mathbb{R}^3) \mid f^\pm_{m_j,k_j} \in L^2(0, +\infty) \right\}.$$

From Ref. 32, Theorem 4.14, we know that the operators $\mathring{H}_{min}$ and H_{max} leave the partial wave subspace $\mathcal{H}_{m_j,k_j}$ invariant and their action can be decomposed in terms of the basis $\{\Phi^+_{m_j,k_j}, \Phi^-_{m_j,k_j}\}$ as follows:

$$\mathring{H}_{min} \cong \bigoplus_{j=\frac{1}{2},\frac{3}{2},\ldots}^{\infty} \bigoplus_{m_j=-j}^{j} \bigoplus_{k_j=\pm(j+1/2)} h_{m_j,k_j},$$
$$H_{max} \cong \bigoplus_{j=\frac{1}{2},\frac{3}{2},\ldots}^{\infty} \bigoplus_{m_j=-j}^{j} \bigoplus_{k_j=\pm(j+1/2)} h^*_{m_j,k_j}, \tag{1.12}$$

where "≅" means that the operators are unitarily equivalent, with

$$D(h_{m_j,k_j}) = C_c^\infty(0,+\infty)^2,$$
$$h_{m_j,k_j}(f^+,f^-) := \begin{pmatrix} m + \frac{\nu+\mu}{r} & -\partial_r + \frac{k_j+\lambda}{r} \\ \partial_r + \frac{k_j+\lambda}{r} & -m + \frac{\nu-\mu}{r} \end{pmatrix}\begin{pmatrix} f^+ \\ f^- \end{pmatrix} \tag{1.13}$$

and

$$D(h^*_{m_j,k_j}) = \{(f^+,f^-) \in L^2(0,+\infty) : h^*_{m_j,k_j}(f^+,f^-) \in L^2(0,+\infty)^2\},$$
$$h^*_{m_j,k_j}(f^+,f^-) := \begin{pmatrix} m + \frac{\nu+\mu}{r} & -\partial_r + \frac{k_j+\lambda}{r} \\ \partial_r + \frac{k_j+\lambda}{r} & -m + \frac{\nu-\mu}{r} \end{pmatrix}\begin{pmatrix} f^+ \\ f^- \end{pmatrix}, \tag{1.14}$$

where $h^*_{m_j,k_j}(f^+,f^-)$ has to be read in the distributional sense as done in (1.10). It is easy to see that $h^*_{m_j,k_j}$ is the adjoint of h_{m_j,k_j}.

The main result of Ref. 7 is the classification of all the self-adjoint extensions t_{m_j,k_j} such that $h_{m_j,k_j} \subseteq t_{m_j,k_j} = t^*_{m_j,k_j} \subseteq h^*_{m_j,k_j}$; as an immediate consequence, we can build up self-adjoint operators T as in (1.8) setting

$$T \cong \bigoplus_{j=\frac{1}{2},\frac{3}{2},\ldots}^{\infty} \bigoplus_{m_j=-j}^{j} \bigoplus_{k_j=\pm(j+1/2)} t_{m_j,k_j}.$$

The self-adjointness of t_{m_j,k_j} is related to the quantity

$$\delta_{k_j} = \delta_{k_j}(\lambda,\mu,\nu) := (k_j+\lambda)^2 + \mu^2 - \nu^2. \tag{1.15}$$

In Ref. 7, Theorems 1.1, 1.2, and 1.3, we show that if $\delta_{k_j} \geq 1/4$, then t_{m_j,k_j} is essentially self-adjoint and if $\delta_{k_j} < 1/4$, then there exists a one (real) parameter family $\big(t(\theta)_{m_j,k_j}\big)_{\theta\in[0,\pi)}$ of self-adjoint extensions such that $h_{m_j,k_j} \subset t(\theta)_{m_j,k_j} = t(\theta)^*_{m_j,k_j} \subset h^*_{m_j,k_j}$. In conclusion, we can define a family of self-adjoint extensions parameterized by d real parameters, with

$$d := \sum_{\substack{j,m_j,k_j \\ (k_j+\lambda)^2+\mu^2-\nu^2<1/4}} 1 = \sum_{\substack{k\in\mathbb{Z}\setminus\{0\} \\ (k+\lambda)^2+\mu^2-\nu^2<1/4}} 2|k|. \tag{1.16}$$

In this paper, we show that the totality of the self-adjoint extensions is a much richer set. Indeed, they are in one-to-one correspondence with the unitary matrices

$$\mathcal{U}(d) := \{U \in \mathbb{C}^{d\times d} : U^*U = UU^* = \mathbb{I}_d\},$$

that is, they are a family of d^2 real parameters. This correspondence relates the self-adjoint extensions to the behavior in the origin of the functions in their domain. In order to do so, we exploit the theory of the boundary triples: we remind here its definition, following the notations from Ref. 5, Definition 1.7.

Definition 1.1. Let $E : \mathcal{D}(E) \subseteq \mathcal{H} \to \mathcal{H}$ be a closed linear operator in a Hilbert space $\mathcal{H}$, and let $\mathcal{G}$ be another Hilbert space. Let $\Gamma_1,\Gamma_2 : \mathcal{D}(E) \to \mathcal{G}$ be linear maps, and finally define $(\Gamma_1,\Gamma_2) : \mathcal{D}(E) \to \mathcal{G}\oplus\mathcal{G}$ as $(\Gamma_1,\Gamma_2)\psi := (\Gamma_1\psi, \Gamma_2\psi)$ for any $\psi \in \mathcal{D}(E)$. We say that the triple $(\mathcal{G},\Gamma_1,\Gamma_2)$ is a *boundary triple* for E if and only if

$$\langle\psi, E\widetilde{\psi}\rangle_{\mathcal{H}} - \langle E\psi,\widetilde{\psi}\rangle_{\mathcal{H}} = \langle\Gamma_1\psi,\Gamma_2\widetilde{\psi}\rangle_{\mathcal{G}} - \langle\Gamma_1\psi,\Gamma_2\widetilde{\psi}\rangle_{\mathcal{G}} \quad \text{for all } \psi,\widetilde{\psi} \in \mathcal{D}(E); \tag{1.17}$$

$$\text{the map } (\Gamma_1,\Gamma_2) : \mathcal{D}(E) \to \mathcal{G}\oplus\mathcal{G} \text{ is surjective;} \tag{1.18}$$

$$\text{the set } \ker(\Gamma_1,\Gamma_2) \text{ is dense in } \mathcal{H}. \tag{1.19}$$

The theory of the boundary triples is well developed and powerful; the explicit knowledge of a boundary triple for a symmetric and closed operator can be used to obtain many important results. In this paper, we exploit it to describe all the self-adjoint extensions: the following proposition is a consequence of Theorem 1.2, Proposition 1.5, and Theorem 1.12 in Ref. 5 or equivalently of Proposition 14.4 and Theorem 14.10 in Ref. 31; hence, the proof is omitted.

Proposition 1.2. Let E_0 be a symmetric operator on a Hilbert space $\mathcal{H}$, and let $(\mathcal{G}, \Gamma_1, \Gamma_2)$ be a boundary triple for $E^* := (E_0)^*$. Then, the following hold:

(i) *if $\mathcal{G} = \{0\}$, E_0 is essentially self-adjoint;*
(ii) *if $\mathcal{G} \neq \{0\}$, E_0 has many self-adjoint extensions. They can be classified in the following equivalent ways:*

- *For any A, B bounded linear operators on $\mathcal{G}$, the extension $E_{A,B}$ with domain*

$$\mathcal{D}(E_{A,B}) = \{\psi \in \mathcal{D}(E^*) : A\Gamma_1(\psi) = B\Gamma_2(\psi)\} \tag{1.20}$$

is self-adjoint if and only if

$$AB^* = BA^*, \tag{1.21}$$

$$ker\begin{pmatrix} A & -B \\ B & A \end{pmatrix} = 0. \tag{1.22}$$

- *There exists a one-to-one correspondence between the self-adjoint extensions of E_0 and the unitary operators $\mathcal{U}(\mathcal{G})$. For $U \in \mathcal{U}(\mathcal{G})$, the corresponding self-adjoint extension E_U has domain*

$$\mathcal{D}(E_U) = \{\psi \in \mathcal{D}(E^*) : i(\mathbb{I}_{\mathcal{G}} + U)\Gamma_1(\psi) = (\mathbb{I}_{\mathcal{G}} - U)\Gamma_2(\psi)\}. \tag{1.23}$$

Remark 1.3. The descriptions of the self-adjoint extensions in (1.20) and (1.23) are equivalent and both useful and interesting. Indeed, (1.20) is useful for the applications: for example, we will exploit it in Theorem 1.12 to determine the distinguished extension for the Dirac-Coulomb operator. The description in (1.23) is interesting from a more theoretical point of view, since it gives a one-to-one correspondence between the self-adjoint extensions and the elements of the unitary operators on $\mathcal{G}$, allowing us to label these extensions with a unique choice of parameters.

We introduce some notations.

Definition 1.4 Let

$$\psi(x) = \sum_{j,m_j,k_j} \frac{1}{r}\left(f^+_{m_j,k_j}(r)\Phi^+_{m_j,k_j}(\hat{x}) + f^-_{m_j,k_j}(r)\Phi^-_{m_j,k_j}(\hat{x})\right) \in \mathcal{D}(H_{max})$$

and set $f_{m_j,k_j} := \left(f^+_{m_j,k_j}, f^-_{m_j,k_j}\right) \in \mathcal{D}(h^*_{m_j,k_j})$. Following the order given by (1.11), we array the triples (j, m_j, k_j) such that $\delta_{k_j} := (k_j+\lambda)^2 + \mu^2 - \nu^2 < 1/4$ and we denote this ordered set I; we have that I has exactly d elements. Moreover, we set

$$\gamma_{k_j} := \sqrt{|\delta_{k_j}|} \quad \text{for all } j = \frac{1}{2}, \frac{3}{2}, \ldots. \tag{1.24}$$

Then, for any $(j, m_j, k_j) \in I$,

(i) if $0 < \delta_{k_j} < 1/4$ from Ref. 7, Proposition 3.1 (iii), we know that

$$\lim_{r\to 0}\left|\begin{pmatrix} f^+_{m_j,k_j}(r) \\ f^-_{m_j,k_j}(r) \end{pmatrix} - D_{k_j}\begin{pmatrix} A^+ r^{\gamma_{k_j}} \\ A^- r^{-\gamma_{k_j}} \end{pmatrix}\right| r^{-1/2} = 0, \tag{1.25}$$

with $D_{k_j} \in \mathbb{R}^{2\times 2}$ being the invertible matrix

$$D_{k_j} := \begin{cases} \frac{1}{2\gamma(\lambda+k_j-\gamma_{k_j})}\begin{pmatrix} \lambda + k_j - \gamma_{k_j} & \nu - \mu \\ -(\nu+\mu) & -(\lambda + k_j - \gamma_{k_j}) \end{pmatrix} & \text{if } \lambda + k_j - \gamma_{k_j} \neq 0, \\ \frac{1}{-4\gamma^2_{k_j}}\begin{pmatrix} \mu - \nu & 2\gamma_{k_j} \\ 2\gamma_{k_j} & -(\nu+\mu) \end{pmatrix} & \text{if } \lambda + k_j - \gamma_{k_j} = 0, \end{cases} \tag{1.26}$$

we set

$$\begin{pmatrix} \Gamma^+_{m_j,k_j}(f_{m_j,k_j}) \\ \Gamma^-_{m_j,k_j}(f_{m_j,k_j}) \end{pmatrix} := D_{k_j}\begin{pmatrix} A^+ \\ A^- \end{pmatrix}; \tag{1.27}$$

(ii) if $\delta_{k_j} = 0$, from Ref. 7, Proposition 3.1 (iv), we know that

$$\lim_{r\to 0}\left|\begin{pmatrix} f^+_{m_j,k_j}(r) \\ f^-_{m_j,k_j}(r)\end{pmatrix} - (M_{k_j}\log r + \mathbb{I}_2)\begin{pmatrix} A^+ \\ A^-\end{pmatrix}\right| r^{-1/2} = 0, \tag{1.28}$$

being $M_{k_j} \in \mathbb{R}^{2\times 2}$, $M^2_{k_j} = 0$ defined as follows:

$$M_{k_j} := \begin{pmatrix} -(k_j+\lambda) & -\nu+\mu \\ \nu+\mu & k_j+\lambda\end{pmatrix}; \tag{1.29}$$

we set

$$\begin{pmatrix} \Gamma^+_{m_j,k_j}(f_{m_j,k_j}) \\ \Gamma^-_{m_j,k_j}(f_{m_j,k_j})\end{pmatrix} := \begin{pmatrix} A^+ \\ A^-\end{pmatrix}; \tag{1.30}$$

(iii) if $\delta_{k_j} < 0$, from Ref. 7, Proposition 3.1 (v), we know that

$$\lim_{r\to 0}\left|\begin{pmatrix} f^+_{m_j,k_j}(r) \\ f^-_{m_j,k_j}(r)\end{pmatrix} - E_{k_j}\begin{pmatrix} A^+ r^{i\gamma_{k_j}} \\ A^- r^{-i\gamma_{k_j}}\end{pmatrix}\right| r^{-1/2} = 0, \tag{1.31}$$

being $E_{k_j} \in \mathbb{C}^{2\times 2}$ the invertible matrix

$$E_{k_j} := \frac{1}{2i\gamma_{k_j}(\lambda+k-i\gamma_{k_j})}\begin{pmatrix} \lambda+k-i\gamma_{k_j} & \nu-\mu \\ -(\nu+\mu) & -(\lambda+k-i\gamma_{k_j})\end{pmatrix}, \tag{1.32}$$

we set

$$\begin{pmatrix} \Gamma^+_{m_j,k_j}(f_{m_j,k_j}) \\ \Gamma^-_{m_j,k_j}(f_{m_j,k_j})\end{pmatrix} := E_{k_j}\begin{pmatrix} A^+ \\ A^-\end{pmatrix}. \tag{1.33}$$

Finally, set $\Gamma^+, \Gamma^- : \mathcal{D}(H_{max}) \to \mathbb{C}^d$ as follows:

$$\Gamma^\pm(\psi) = \left(\Gamma^\pm_{m_j,k_j}(f_{m_j,k_j})\right)_{(j,m_j,k_j)\in I} \in \mathbb{C}^d. \tag{1.34}$$

Then, by definition, for any $(j, m_j, k_j) \in I$,

$$\left(\Gamma^\pm(\psi)\right)_{m_j,k_j} = \Gamma^\pm_{m_j,k_j}(f_{m_j,k_j}) \in \mathbb{C}. \tag{1.35}$$

We are now in position to state the main result of this paper.

Theorem 1.5 (Boundary triples for H_{max}). *Let H_{max} be defined as in (1.10), let $d \in \mathbb{N}$ be as in (1.16) and assume that $d > 0$. Let Γ^+, Γ^- be defined as in (1.34). Then, $(\mathbb{C}^d, \Gamma^+, \Gamma^-)$ is a boundary triple for H_{max}.*

Remark 1.6. In general, boundary triples are not unique (see Ref. 5, Propositions 1.14 and 1.15). For example, a different boundary triple is determined already by choosing an ordering of the triples different from the one in (1.11).

Thanks to the theory of the boundary triples, we can now describe all the self-adjoint extensions of $\mathring{H}_{min}$: the following theorem is a consequence of Theorem 1.5 and Proposition 1.2:

Theorem 1.7. *Let $\mathring{H}_{min}$ be defined as in (1.9) and $d \in \mathbb{N}$ as in (1.16). The following holds:*

(i) *if $d = 0$, $\mathring{H}_{min}$ is essentially self-adjoint;*
(ii) *if $d > 0$, $\mathring{H}_{min}$ has many self-adjoint extensions. They can be classified in the following equivalent ways:*

- *For any $A, B \in \mathbb{C}^{d\times d}$, the extension $T_{A,B}$ with domain*

$$\mathcal{D}(T_{A,B}) = \{\psi \in \mathcal{D}(H_{max}) : A\Gamma^+(\psi) = B\Gamma^-(\psi)\} \tag{1.36}$$

is self-adjoint if and only if

$$AB^* = BA^*,$$

$$ker\begin{pmatrix} A & -B \\ B & A \end{pmatrix} = 0.$$

- *There exists a one-to-one correspondence between the self-adjoint extensions of $\mathring{H}_{min}$ and the unitary matrices $\mathcal{U}(d)$. For $U \in \mathcal{U}(d)$, the corresponding self-adjoint extension T_U has domain*

$$\mathcal{D}(T_U) = \{\psi \in \mathcal{D}(H_{max}) :\ i(\mathbb{I}_d + U)\Gamma^+(\psi) = (\mathbb{I}_d - U)\Gamma^-(\psi)\}. \tag{1.37}$$

Remark 1.8. It is difficult to obtain the results of Theorem 1.7 using Von Neumann's theory. Indeed, to exploit it, one has to find all the solutions to $(H_{max} \pm i)\psi = 0$ that is hard to do for the general class of potentials considered in (1.3). By the way, Theorems 1.1, 1.2, and 1.3 in Ref. 7 tell us that h_{m_j,k_j} has deficiency indices (1, 1) if $\delta_{k_j} < 1/4$ and (0, 0) if $\delta_{k_j} \geq 1/4$ on $C_c^\infty(0, +\infty)^2$. Consequently, $\mathring{H}_{min}$ has deficiency indices *(d, d),* with d defined as in (1.16). We can now use Von Neumann's theory, getting that all the self-adjoint extensions of $\mathring{H}_{min}$ are in one-to-one correspondence with the unitary matrices $\mathcal{U}(d)$, but we cannot provide an explicit bijection. Moreover, such correspondence does not describe the self-adjoint extensions: in Theorem 1.7, we provide a much clearer characterization of them in terms of the boundary behavior in the origin of the functions in their domain.

In the spirit of Refs. 4, 11, and 22 in Theorem 1.9, we select a *distinguished* self-adjoint extension among the ones defined in Theorem 1.7, requiring that its domain is included in the domain of an appropriate quadratic form. Let $q : C_c^\infty(\mathbb{R}^3; \mathbb{C}^4) \to \mathbb{R}$ be defined as

$$q(\psi) := \int_{\mathbb{R}^3} \left[|x||-i\alpha\cdot\nabla\psi|^2 - |x||\mathbb{V}\psi|^2\right] dx.$$

If $\sup_{x\in\mathbb{R}^3}|x||\mathbb{V}(x)| \leq 1$, this form is symmetric and non-negative as a consequence of (1.7), and hence closable: we denote its closure q (with abuse of notation) and its maximal domain $\mathcal{Q}$. In Theorem 1.9, we consider $\mathbb{V}$ as in the class in (1.3), to exploit the complete description of all the self-adjoint extensions in Theorem 1.7. We show that the condition $\mathcal{D}(T) \subset \mathcal{Q}$ selects a self-adjoint extension T in the case that $\mathbb{V}$ is not a critical anomalous magnetic potential, i.e., $\mathbb{V}(x) \neq \pm i\alpha\cdot\hat{x}\beta|x|^{-1}$. Indeed, in this case, this approach does not select any extension, suggesting that it is not possible to use this criterion for the general case.

Theorem 1.9. *Let $\mathring{H}_{min}$ be defined as in (1.9), γ_{k_j} as in (1.24); let $d \in \mathbb{N}$ be defined as in (1.16) and assume that $d > 0$. Assume moreover that*

$$\sup_{x\in\mathbb{R}^3}|x||\mathbb{V}(x)| \leq 1, \quad \mathbb{V}(x) \neq \pm\frac{i\alpha\cdot\hat{x}\beta}{|x|}. \tag{1.38}$$

Then, there exists only one self-adjoint extension $\mathring{H}_{min} \subseteq T_{A,B} \subseteq H_{max}$ such that $\mathcal{D}(T_{A,B}) \subseteq \mathcal{Q}$, with $A, B \in \mathbb{C}^{d\times d}$ determined by the following conditions for all $\psi \in \mathcal{D}(H_{max})$:

(i) *for all (j, m_j, k_j) such that $0 \neq \gamma_{k_j} = k_j + \lambda$,*

$$(k_j + \lambda + \gamma_{k_j})\big(\Gamma^+(\psi)\big)_{m_j,k_j} = (\mu - \nu)\big(\Gamma^-(\psi)\big)_{m_j,k_j}; \tag{1.39}$$

(ii) *for all (j, m_j, k_j) such that $0 \neq \gamma_{k_j} \neq k_j + \lambda$,*

$$(\mu + \nu)\big(\Gamma^+(\psi)\big)_{m_j,k_j} = -(k_j + \lambda - \gamma_{k_j})\big(\Gamma^-(\psi)\big)_{m_j,k_j}; \tag{1.40}$$

(iii) *for all (j, m_j, k_j) such that $\gamma_{k_j} = 0$;*

$$(k_j + \lambda)\big(\Gamma^+(\psi)\big)_{m_j,k_j} = (\mu - \nu)\big(\Gamma^-(\psi)\big)_{m_j,k_j}, \tag{1.41}$$

or equivalently

$$(\mu + \nu)\big(\Gamma^+(\psi)\big)_{m_j,k_j} = -(k_j + \lambda)\big(\Gamma^-(\psi)\big)_{m_j,k_j}. \tag{1.42}$$

Remark 1.10. In the case that $\mathbb{V}$ is a general Hermitian matrix-valued potential such that $v := \sup_{x\in\mathbb{R}^3}|x||\mathbb{V}(x)| < 1$, a classification of all the self-adjoint extensions in the spirit of Theorem 1.7 is not available. However, it is still true that there exists only one self-adjoint extension whose domain is included in $\mathcal{Q}$. Indeed, thanks to (1.7), for all $\psi \in C_c^\infty(\mathbb{R}^3)^4$,

$$q(\psi) \geq \int_{\mathbb{R}^3}\left[|x||-i\alpha\cdot\nabla\psi|^2 - v^2\frac{|\psi|^2}{|x|}\right] dx \geq (1 - v^2)\int_{\mathbb{R}^3}\frac{|\psi|^2}{|x|}\, dx \tag{1.43}$$

that immediately implies $\mathcal{Q} \subset \mathcal{D}(r^{-1/2})$. If there exists a self-adjoint extension T such that $\mathcal{D}(T) \subset \mathcal{Q}$, then it must be the distinguished one, the only one whose domain is contained in $\mathcal{D}(r^{-1/2})$, see Ref. 21. Vice versa, constructing a self-adjoint extension with the property that $\mathcal{D}(T) \subseteq \mathcal{Q}$ is not trivial, and it is the subject of Ref. 4.

Remark 1.11. In the case that $\sup_{x\in\mathbb{R}^3}|x||\mathbb{V}(x)| = 1$, the condition $\mathcal{D}(T) \subset \mathcal{Q}$ appears not to be enough to select a self-adjoint extension T. Indeed, for $\mathbb{V}(x) = \pm i\alpha \cdot \hat{x}\beta/|x|$, condition (3.2) is true for all the functions in all the domains of self-adjointness. A similar phenomenon was observed in Ref. 7, Remark 1.10.

Remark 1.12. As an application of Theorems 1.7 and 1.9, we describe the distinguished self-adjoint extension of the Dirac-Coulomb operator $H := H_0 - \frac{\nu}{|x|}\mathbb{I}_4$, for $|\nu| \le 1$,

- for $0 \le |\nu| \le \sqrt{3}/2$, H is essentially self-adjoint;
- for $\sqrt{3}/2 < |\nu| < 1$, we have that $d = 4$, $\delta_1 = \delta_{-1} = 1 - \nu^2 \in (0, 1/4)$, and $\Gamma^\pm = \left(\Gamma^\pm_{-\frac{1}{2},1}, \Gamma^\pm_{\frac{1}{2},1}, \Gamma^\pm_{-\frac{1}{2},-1}, \Gamma^\pm_{\frac{1}{2},-1}\right)$. Then the distinguished extension has domain
$$\mathcal{D}(T_{A_\nu,\mathbb{I}_4}) = \{\psi \in \mathcal{D}(H_{max}) : A_\nu\Gamma^+(\psi) = \Gamma^-(\psi)\}, \tag{1.44}$$
with
$$A_\nu := \begin{pmatrix} \frac{\nu}{1+\sqrt{1-\nu^2}} & 0 & 0 & 0 \\ 0 & \frac{\nu}{1+\sqrt{1-\nu^2}} & 0 & 0 \\ 0 & 0 & -\frac{\nu}{1-\sqrt{1-\nu^2}} & 0 \\ 0 & 0 & 0 & -\frac{\nu}{1-\sqrt{1-\nu^2}} \end{pmatrix};$$
- for $|\nu| = 1$, we have that $d = 4$, $\delta_1 = \delta_{-1} = 0$, $\Gamma^\pm = \left(\Gamma^\pm_{-\frac{1}{2},1}, \Gamma^\pm_{\frac{1}{2},1}, \Gamma^\pm_{-\frac{1}{2},-1}, \Gamma^\pm_{\frac{1}{2},-1}\right)$, and the distinguished extension has domain $\mathcal{D}(T_{\nu\beta,\mathbb{I}_4})$.

In the case that $\mathbb{V} = -1/|x|$, Theorem 1.9 selects the distinguished self-adjoint extension, as defined in Ref. 11. In general, in the case that $\mathbb{V}$ is the same as in (1.3), Theorem 1.9 selects the distinguished extension, as in Ref. 7, Propositions 1.7 and 1.8.

A fundamental tool in the Proof of Theorem 1.9 is the following improved version of (1.7) that we state independently.

Lemma 1.13. Let $\psi \in C_c^\infty(\mathbb{R}^3)^4$. Then for all $R > 0$,
$$\int_{\mathbb{R}^3} |x||-i\alpha\cdot\nabla\psi(x)|^2\,dx \ge \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|}\,dx + \frac{1}{4}\int_{\mathbb{R}^3} \frac{\left|\psi(x) - \frac{R}{|x|}\psi\left(R\frac{x}{|x|}\right)\right|^2}{|x|\log^2(|x|/R)}\,dx. \tag{1.45}$$
Moreover, the inequality is sharp.

Remark 1.14. Theorem 1.13 can be considered the analogous of Ref. 10, Lemma 18 in the general case (1.38). Indeed, it allows us to exclude a logarithmic decay in the origin for the functions in the domain of the self-adjoint extension.

This paper is organized as follows: in Sec. II, we prove Theorem 1.5 and in Sec. III, we prove Theorems 1.13 and 1.9.

II. PROOF OF THEOREM 1.5

We first prove the following lemma:

Lemma 2.1. Let $j \in \{1/2, 3/2, \ldots\}$, $m_j \in \{-j, \ldots, j\}$, $k_j \in \{j + 1/2, -j - 1/2\}$ such that $(j, m_j, k_j) \in I$, and let $h^*_{m_j,k_j}$ be defined as in (1.14). Let $\Gamma^+_{m_j,k_j}, \Gamma^-_{m_j,k_j}$ be defined as in Theorem 1.4. Then, $\left(\mathbb{C}, \Gamma^+_{m_j,k_j}, \Gamma^-_{m_j,k_j}\right)$ is a boundary triple for $h^*_{m_j,k_j}$.

Proof. In this proof, we will suppress the subscripts, since $j \in \{1/2, 3/2, \ldots\}$, $m_j \in \{-j, \ldots, j\}$, $k_j \in \{j + 1/2, -j - 1/2\}$ are fixed. We distinguish various cases.

In the case $0 < \delta < \frac{1}{4}$, thanks to Ref. 7, Proposition 3.1 (iii), we have that $f = (f^+, f^-) \in \mathcal{D}(h^*_{m_j,k_j})$ if and only if $f \in H^1(\epsilon, +\infty)^2$ for any $\epsilon > 0$, and there exists $(A^+, A^-) \in \mathbb{C}^2$ such that (1.25) holds true, for $D \in \mathbb{R}^{2\times 2}$ defined in (1.26). Moreover, for any $\widetilde{f} = (\widetilde{f}^+, \widetilde{f}^-) \in \mathcal{D}(h^*_{m_j,k_j})$, we have

$$\lim_{r\to 0}\begin{vmatrix} f^+(r) & \overline{\widetilde{f}^+(r)} \\ f^-(r) & \overline{\widetilde{f}^-(r)} \end{vmatrix} = \left| D\begin{pmatrix} A^+ \\ A^- \end{pmatrix} \overline{D\begin{pmatrix} \widetilde{A}^+ \\ \widetilde{A}^- \end{pmatrix}} \right|, \tag{2.1}$$

where, with abuse of notation, we denoted

$$\left| \begin{pmatrix} a \\ c \end{pmatrix} \begin{pmatrix} b \\ d \end{pmatrix} \right| := \begin{vmatrix} a & b \\ c & d \end{vmatrix}. \tag{2.2}$$

Then for $f, \widetilde{f} \in \mathcal{D}(h^*_{m_j,k_j})$, by the dominated convergence theorem, we have that

$$\begin{aligned} &\int_0^{+\infty} f \cdot \overline{h^*_{m_j,k_j}(\widetilde{f})}\, dr - \int_0^{+\infty} h^*_{m_j,k_j}(f) \cdot \overline{\widetilde{f}}\, dr \\ &= \lim_{\epsilon\to 0} \int_\epsilon^{+\infty} f \cdot \overline{h^*_{m_j,k_j}(\widetilde{f})}\, dr - \int_\epsilon^{+\infty} h^*_{m_j,k_j}(f) \cdot \overline{\widetilde{f}}\, dr = \lim_{\epsilon\to 0}\begin{vmatrix} f^+(\epsilon) & \overline{\widetilde{f}^+(\epsilon)} \\ f^-(\epsilon) & \overline{\widetilde{f}^-(\epsilon)} \end{vmatrix}, \end{aligned} \tag{2.3}$$

where in the last equality, we used the fact that $f, \widetilde{f} \in H^1(\epsilon, +\infty)^2$. We get (1.17) combining in (1.27), (2.1), and (2.3). The surjectivity of the maps $\Gamma^+_{m_j,k_j}, \Gamma^-_{m_j,k_j}$ is easy to show: indeed let $(A^+, A^-) \in \mathbb{C}^2$ and let $f \in C^\infty(0, +\infty)^2$ such that

$$f(r) = \begin{cases} D\begin{pmatrix} A^+ r^\gamma \\ A^- r^{-\gamma} \end{pmatrix} & \text{for } r < 1, \\ 0 & \text{for } r > 2. \end{cases}$$

Then $f \in \mathcal{D}(h^*_{m_j,k_j})$ and $\Gamma^\pm_{m_j,k_j}(f)$ are defined as in (1.27). Finally, (1.19) descends from the fact that $C_c^\infty(0, +\infty)^2 \subset \ker(\Gamma^+_{m_j,k_j}, \Gamma^-_{m_j,k_j})$.

Let us now consider the case that $\delta = 0$. Thanks to Ref. 7, Proposition 3.1 (iv), $f = (f^+, f^-) \in \mathcal{D}(h^*_{m_j,k_j})$ if and only if $f \in H^1(\epsilon, +\infty)^2$ for any $\epsilon > 0$, and there exists $(\Gamma^+_{m_j,k_j}(f), \Gamma^-_{m_j,k_j}(f)) := (A^+, A^-) \in \mathbb{C}^2$ such that (1.28) holds true, with $M \in \mathbb{R}^{2\times 2}$, $M^2 = 0$ defined as in (1.29). Moreover, for any $\widetilde{f} = (\widetilde{f}^+, \widetilde{f}^-) \in \mathcal{D}(h^*_{m_j,k_j})$, we have

$$\lim_{r\to 0}\begin{vmatrix} f^+(r) & \overline{\widetilde{f}^+(r)} \\ f^-(r) & \overline{\widetilde{f}^-(r)} \end{vmatrix} = \begin{vmatrix} \Gamma^+(f) & \overline{\Gamma^+(\widetilde{f})} \\ \Gamma^-(f) & \overline{\Gamma^-(\widetilde{f})} \end{vmatrix}. \tag{2.4}$$

Reasoning as in the previous case, we get (1.17). Finally, (1.18) and (1.19) are proved as in the previous case.

Let us finally assume that $\delta < 0$. In this case, thanks to Ref. 7, Proposition 3.1 (v), we have that $f = (f^+, f^-) \in \mathcal{D}(h^*_{m_j,k_j})$ if and only if $f \in H^1(\epsilon, +\infty)^2$ for any $\epsilon > 0$, and there exists $(A^+, A^-) \in \mathbb{C}^2$ such that (1.31) holds true, with $E \in \mathbb{C}^{2\times 2}$ defined as in (1.32). Moreover, for any $\widetilde{f} = (\widetilde{f}^+, \widetilde{f}^-) \in \mathcal{D}(h^*_{m_j,k_j})$, with the same notation of (2.2), we get

$$\lim_{r\to 0}\begin{vmatrix} f^+(r) & \overline{\widetilde{f}^+(r)} \\ f^-(r) & \overline{\widetilde{f}^-(r)} \end{vmatrix} = \left| E\begin{pmatrix} A^+ \\ A^- \end{pmatrix} \overline{E\begin{pmatrix} \widetilde{A}^+ \\ \widetilde{A}^- \end{pmatrix}} \right|. \tag{2.5}$$

Due to (1.33), one gets (1.17), (1.18), and (1.19) reasoning as before. □

We are now ready to prove Theorem 1.5.

Proof of Theorem 1.5. Let us start proving the condition (1.17) in Theorem 1.1. Let for any $\psi, \widetilde{\psi} \in \mathcal{D}(H_{max})$ such that

$$H_{max}\psi = \sum_{j,m_j,k_j} h^*_{m_j,k_j} f_{m_j,k_j}, \quad H_{max}\widetilde{\psi} = \sum_{j,m_j,k_j} h^*_{m_j,k_j} \widetilde{f}_{m_j,k_j} \tag{2.6}$$

for appropriate f_{m_j,k_j} and $\widetilde{f}_{m_j,k_j}$ in $\mathcal{D}(h^*_{m_j,k_j})$. Then,

$$\begin{aligned} &\langle \psi, H_{max}\widetilde{\psi}\rangle_{L^2(\mathbb{R}^3)^4} - \langle H_{max}\psi, \widetilde{\psi}\rangle_{L^2(\mathbb{R}^3)^4} \\ &= \sum_{j,m_j,k_j} \langle f_{m_j,k_j}, h^*_{m_j,k_j}\widetilde{f}_{m_j,k_j}\rangle_{L^2(0,\infty)^2} - \langle h^*_{m_j,k_j} f_{m_j,k_j}, \widetilde{f}_{m_j,k_j}\rangle_{L^2(0,\infty)^2} \\ &= \sum_{\substack{j,m_j,k_j \\ (k_j+\lambda)^2+\mu^2-\nu^2<1/4}} \langle f_{m_j,k_j}, h^*_{m_j,k_j}\widetilde{f}_{m_j,k_j}\rangle_{L^2(0,\infty)^2} - \langle h^*_{m_j,k_j} f_{m_j,k_j}, \widetilde{f}_{m_j,k_j}\rangle_{L^2(0,\infty)^2}, \end{aligned}$$

where in the last equality, we used the fact that $h^*_{m_j,k_j}$ is self-adjoint when $(k_j+\lambda)^2 + \mu^2 - \nu^2 \geq 1/4$, as proved in Ref. 7, Theorem 1.1. Thanks to Theorem 2.1, we conclude that

$$\langle \psi, H_{max}\widetilde{\psi}\rangle_{L^2(\mathbb{R}^3)^4} - \langle H_{max}\psi, \widetilde{\psi}\rangle_{L^2(\mathbb{R}^3)^4} = \sum_{(j,m_j,k_j)\in I} \Gamma^+_{m_j,k_j}(f)\cdot\overline{\Gamma^-_{m_j,k_j}(\tilde{f})} - \Gamma^-_{m_j,k_j}(f)\cdot\overline{\Gamma^+_{m_j,k_j}(\tilde{f})} \tag{2.7}$$

that gives immediately (1.17).

The surjectivity of Γ^+ and Γ^- descends immediately from the surjectivity of any $\Gamma^+_{m_j,k_j}$ and $\Gamma^-_{m_j,k_j}$ that has been showed in Theorem 2.1. Finally, since $C_c^\infty(\mathbb{R}^3\backslash\{0\})^4 \subseteq \ker(\Gamma^+,\Gamma^-)$, we deduce the condition (1.18). □

III. PROOF OF THEOREM 1.9

In this section, we provide Proof of Theorem 1.13 and Theorems 3.1 and 1.9.

Proof of Theorem 1.13. By direct computation [see, for example, Ref. 32, Eq. (4.102)]

$$-i\alpha\cdot\nabla = -i\alpha\cdot\hat{x}\left(\partial_r + \frac{1}{|x|} - \frac{1+2\mathbf{S}\cdot L}{|x|}\right),$$

where $\boldsymbol{S}$ is the *spin angular momentum operator*

$$\mathbf{S} = \frac{1}{2}\begin{pmatrix}\sigma & 0\\ 0 & \sigma\end{pmatrix}. \tag{3.1}$$

Consider $\psi\in C_c^\infty(\mathbb{R}^3;\mathbb{C}^4)$. Since $i\alpha\cdot\hat{x}$ is a unitary matrix, we have

$$\begin{aligned}\int_{\mathbb{R}^3}|x|| - i\alpha\cdot\nabla\psi| - i\alpha\cdot\nabla\psi 2\,dx &= \int_{\mathbb{R}^3}|x|\left|\left(\partial_r + \frac{1}{|x|} - \frac{1+2\mathbf{S}\cdot L}{|x|}\right)\psi\right|^2 dx\\ &= \int_{\mathbb{R}^3}|x|\left|\left(\partial_r + \frac{1}{|x|}\right)\psi\right|^2 dx + \int_{\mathbb{R}^3}\left|\frac{1+2\mathbf{S}\cdot L}{|x|}\psi\right|^2 dx\\ &\quad - 2\,\mathrm{Re}\int_{\mathbb{R}^3}\left(\partial_r + \frac{1}{|x|}\right)\psi\,\overline{(1+2\mathbf{S}\cdot L)\psi}\,dx.\end{aligned}$$

It is standard (see, for example, Ref. 8, Lemma 2.1) to show that the last term in the previous equation vanishes, indeed $1+2\mathbf{S}\cdot L$ and $\partial_r + \frac{1}{|x|}$ are symmetric and skew-symmetric, respectively, on $C_c^\infty(\mathbb{R}^3)^4$, and the two operators commute with each other.

Let $\phi := |x|\psi$. We have that $\partial_r\phi = |x|(\partial_r + |x|^{-1})\psi$ and consequently

$$\int_{\mathbb{R}^3}|x|\left|\left(\partial_r + \frac{1}{|x|}\right)\psi\right|^2 dx = \int_0^{+\infty}\int_{\mathbb{S}^2} r|\partial_r\phi(r\omega)|^2\,d\omega dr.$$

Thanks to Proposition 2.4 (iii) in Ref. 7,

$$\int_{\mathbb{S}^2}\int_0^{+\infty} r|\partial_r\phi(r\omega)|^2\,drd\omega \geq \frac{1}{4}\int_{\mathbb{S}^2}\int_0^{+\infty}\frac{|\phi(r\omega)-\phi(R\omega)|^2}{r\log^2(r/R)}\,drd\omega.$$

This inequality is sharp, as underlined in Ref. 7, Remark 2.5. Observing that $|1+2\mathbf{S}\cdot L|\geq 1$, we finally get the thesis. □

Proposition 3.1 For all $\psi\in\mathcal{Q}$,

$$\int_{\{|x|<1\}}\frac{|\psi(x)|^2}{|x|\log^2|x|}\,dx < +\infty. \tag{3.2}$$

Proof. We show that for all $\psi\in\mathcal{Q}$,

$$q(\psi) \geq \frac{1}{4}\int_{\mathbb{R}^3}\frac{\left|\psi(x) - \frac{R}{|x|}\psi\left(R\frac{x}{|x|}\right)\right|^2}{|x|\log^2(|x|/R)}\,dx. \tag{3.3}$$

Since $Q = \overline{C_c^\infty(\mathbb{R}^3)}^{\|\cdot\|_q}$, with $\|\cdot\|_q^2 := q(\cdot) + \|\cdot\|_2^2$, there exists a sequence $(\psi_j)_j \subset C_c^\infty(\mathbb{R}^3)$ such that $\|\psi - \psi_j\|_q \to 0$ and $\psi - \psi_j \to 0$ almost everywhere as $j \to +\infty$. Since (1.45) holds for $\psi_j - \psi_m \in C_c^\infty(\mathbb{R}^3)$, $(\chi_j)_j$ is a Cauchy sequence in $L^2(\mathbb{R}^3, |x|^{-1}dx)$, for

$$\chi_j(x) := \frac{\psi_j(x) - \psi_j(Rx/|x|)}{\log(|x|/R)}.$$

Consequently, $\chi_j \to \chi \in L^2(\mathbb{R}^3, |x|^{-1}dx)$. On the other hand, since $\psi_j \to \psi$ almost everywhere, then $\chi_j \to \frac{\psi - \psi\left(R\frac{\cdot}{|\cdot|}\right)}{\log(|x|/R)}$ almost everywhere, and we conclude that $\chi_j \to \frac{\psi - \psi\left(R\frac{\cdot}{|\cdot|}\right)}{\log(|x|/R)}$ in $L^2(\mathbb{R}^3, |x|^{-1}dx)$. In conclusion, (3.3) holds for $\psi \in \mathcal{Q}$.

Consequently,

$$\int_{\{|x|<1\}} \frac{|\psi(x)|^2}{|x|\log^2(|x|/R)}\,dx \le 2\int_{\{|x|<1\}} \frac{\left|\psi(x) - \frac{R}{|x|}\psi\left(R\frac{x}{|x|}\right)\right|^2}{|x|\log^2(|x|/R)}\,dx + 2\int_0^1 \frac{\frac{R^2}{r^2}\int_{\{|x|=r\}}\left|\psi\left(R\frac{x}{|x|}\right)\right|^2 dS_x}{r\log^2(r/R)}\,dr.$$

The second term at right hand side is finite, since the numerator is constant with respect to $r \in (0, 1)$ and $(r\log^2 r)^{-1}$ is integrable in the origin, and the first term at right hand side is finite, as it is shown above. □

We can now finally prove Theorem 1.9.

Proof of Theorem 1.9. We first show that $\gamma_{k_j} \ge 0$ for all $j = 1/2, 3/2, \ldots$, that is, $(k+\lambda)^2 + \mu^2 - \nu^2 \ge 0$ for all $k \in \mathbb{Z}\backslash\{0\}$. Indeed, since $|x||\mathbb{V}(x)| = |\nu| + \sqrt{\mu^2+\lambda^2} \le 1$, then $\nu^2 \le 1 + \mu^2 + \lambda^2 - 2\sqrt{\mu^2+\lambda^2}$. Moreover, since $|\lambda| \le 1$, then $M := \min_{k\in\mathbb{Z}\backslash\{0\}}(k+\lambda)^2 + \mu^2 - \nu^2 = (1-|\lambda|)^2 + \mu^2 - \nu^2$. Assume by contradiction that $M < 0$. Then, $(1-|\lambda|)^2 + \mu^2 < \nu^2 \le 1 + \mu^2 + \lambda^2 - 2\sqrt{\mu^2+\lambda^2}$, that is, $|\lambda| > \sqrt{\mu^2+\lambda^2}$ and this is absurd. Incidentally, we remark that $M = 0$ only if $\mu = 0$.

We denote

$$\begin{aligned} I_1 &:= \{(j, m_j, k_j) \in I : 0 \ne \gamma_{k_j} = k_j + \lambda\}, \\ I_2 &:= \{(j, m_j, k_j) \in I : 0 \ne \gamma_{k_j} \ne k_j + \lambda\}, \\ I_3 &:= \{(j, m_j, k_j) \in I : \gamma_{k_j} = 0\}. \end{aligned}$$

Following (1.11), we identify

$$s \in \{1, \ldots, d\} \leftrightarrow (j, m_j, k_j) \in I.$$

Thanks to this, we have that $\{I_1, I_2, I_3\}$ is a partition of $\{1, \ldots, d\}$.

In the following, we determine $A, B \in \mathbb{C}^{d\times d}$ in such a way that $\mathcal{D}(T_{A,B}) \subseteq \mathcal{Q}$. Let ψ be a generic element in $\mathcal{D}(T_{A,B})$. Thanks to Theorem 3.1, the condition $\mathcal{D}(T_{A,B}) \subseteq \mathcal{Q}$ implies that ψ verifies (3.2). Following the notations of Theorem 1.5, we denote

$$\begin{aligned} \psi(x) &= \sum_{j=\frac12,\frac32,\ldots}^{\infty} \sum_{m_j=-j}^{j} \sum_{k_j=\pm(j+1/2)} \frac{1}{r}\left(f^+_{m_j,k_j}(r)\Phi^+_{m_j,k_j}(\hat{x}) + f^-_{m_j,k_j}(r)\Phi^-_{m_j,k_j}(\hat{x})\right), \\ f_{m_j,k_j} &= (f^+_{m_j,k_j}, f^-_{m_j,k_j}). \end{aligned}$$

For all $(j, m_j, k_j) \in I_1 \cap I_2$, we have that f_{m_j,k_j} verifies (1.25): since the singular behavior is not allowed by (3.2), we have necessarily that $A^- = 0$. Thanks to (1.27), we have that this is equivalent to (1.39) when $(j, m_j, k_j) \in I_1$ and equivalent to (1.40) when $(j, m_j, k_j) \in I_2$. We define the matrices A and B accordingly

$$\begin{aligned} &A_{ss} := k_j + \lambda + \gamma_{k_j}, \quad B_{ss} := \mu - \nu, && \text{for } s \sim (j, m_j, k_j) \in I_1 \\ &A_{ss} := \mu + \nu, \quad B_{ss} := -(k_j + \lambda - \gamma_{k_j}), && \text{for } s \sim (j, m_j, k_j) \in I_2, \\ &A_{st} = B_{st} = 0, && \text{for } s \sim (j, m_j, k_j) \in I_1 \cup I_2,\ 1 \le t \le d, t \ne s. \end{aligned}$$

For all $(j, m_j, k_j) \in I_3$, we have that f_{m_j,k_j} verifies (1.28): since the logarithmic behavior is not allowed by (3.2), we have necessarily that $\mathrm{Ran}(\Gamma^+_{m_j,k_j}, \Gamma^-_{m_j,k_j}) \subseteq \ker M_{k_j}$. This gives (1.41) and (1.42): they are equivalent since M has rank 1. Using the identification $s \sim (j, m_j, k_j)$, we define A and B accordingly

$$A_{ss} := k_j + \lambda, \quad B_{ss} := \mu - \nu \quad \text{for } ss \sim (j, m_j, k_j) \in I_3 \tag{3.4}$$

or equivalently

$$A_{ss} := \mu + \nu, \quad B_{ss} := -(k_j + \lambda) \quad \text{for } s \sim (j, m_j, k_j) \in I_3 \tag{3.5}$$

and $A_{st} = B_{st} = 0$ for $s \sim (j, m_j, k_j) \in I_3$, $t \in \{1, \ldots, d\}$, $t \neq s$.

In order to show that the extension that we have built is self-adjoint, we check the conditions (1.21) and (1.21) in Theorem 1.2: since A and B are real and diagonal and we have that

$$AB^* = AB = BA = BA^*,$$

that is (1.21). In order to show that (1.22), we show equivalently that $det(AA^* + BB^*) \neq 0$ (see Ref. 1, Sec. 125 and Theorem 4). Indeed, the matrix $AA^* + BB^*$ is diagonal and the elements of the diagonal equal $C_{ss} := (A_{ss})^2 + (B_{ss})^2$ for $s = 1, \ldots, d$. For $s \in I_1$, we have that $C_{ss} = (k_j + \lambda + \gamma_{k_j})^2 + (\mu - \nu)^2 \geq (k_j + \lambda + \gamma_{k_j})^2 = 4\gamma_{k_j}^2 > 0$. For $s \in I_2$, we have that $C_{ss} = (\mu + \nu)^2 + (k_j + \lambda + \gamma_{k_j})^2 \geq (k_j + \lambda - \gamma_{k_j})^2 > 0$. Finally, for $s \in I_3$, we have that $C_{ss} = (k_j + \lambda)^2 + (\mu - \nu)^2$ or $C_{ss} = (k_j + \lambda)^2 + (\nu + \mu)^2$: in both cases, $C_{ss} = 0$ if and only if $(\nu, \mu, \lambda) = (0, 0, 1)$ or $(\nu, \mu, \lambda) = (0, 0, -1)$, but this is excluded by (1.38).

The linear relation associated with A, B determines uniquely a unitary matrix $U \in \mathcal{U}(d)$ such that $T_{A,B} = T_U$, defined as in (1.37), see Ref. 24, Sec. 2; Ref. 2, Theorem 4.6; and Ref. 15, Theorem 3.1.4. This implies that $T_{A,B}$ is the unique self-adjoint extension with the required properties and concludes the proof. □

ACKNOWLEDGMENTS

This work was mainly developed while B.C. and F.P. were employed at *BCAM—Basque Center for Applied Mathematics*, and they were supported by ERCEA Advanced Grant No. 2014 669689—HADE, by the MINECO Project No. MTM2014-53850-P, by Basque Government Project No. IT-641-13 and also by the Basque Government through the BERC 2018-2021 program, and by Spanish Ministry of Economy and Competitiveness MINECO: BCAM Severo Ochoa excellence accreditation No. SEV-2017-0718. B.C. also acknowledges the Istituto Italiano di Alta Matematica "F. Severi" and the Czech Science Foundation (GAČR) within the Project No. 17-01706S. F.P. also has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (Grant Agreement MDFT No. 725528 of M.L.).

REFERENCES

[1] Akhiezer, N. and Glazman, I., *Theory of Linear Operators in Hilbert Space* (Courier Corporation, 2013), Vol. II.
[2] Arens, R., "Operational calculus of linear relations," Pac. J. Math. **11**, 9 (1961).
[3] Arrizabalaga, N., "Distinguished self-adjoint extensions of Dirac operators via Hardy-Dirac inequalities," J. Math. Phys. **52**(9), 092301 (2011).
[4] Arrizabalaga, N., Duoandikoetxea, J., and Vega, L., "Self-adjoint extensions of Dirac operators with Coulomb type singularity," J. Math. Phys. **54**(4), 041504 (2013).
[5] Brüning, J., Geyler, V., and Pankrashkin, K., "Spectra of self-adjoint extensions and applications to solvable Schrödinger operators," Rev. Math. Phys. **20**(01), 1–70 (2008).
[6] Burnap, C., Brysk, H., and Zweifel, P., "Dirac Hamiltonian for strong Coulomb fields," Il Nuovo Cimento B **64**(2), 407–419 (1981).
[7] Cassano, B. and Pizzichillo, F., "Self-adjoint extensions for the Dirac operator with Coulomb-type spherically symmetric potentials," Lett. Math. Phys. **108**, 2635–2667 (2018).
[8] Cassano, B., Pizzichillo, F., and Vega, L., "A Hardy-type inequality and some spectral characterizations for the Dirac–Coulomb operator," preprint arXiv:1810.01309 (2018).
[9] de Oliveira, C. R., *Intermediate Spectral Theory and Quantum Dynamics* (Springer Science & Business Media, 2008), Vol. 54.
[10] Esteban, M. J., Lewin, M., and Séré, E., "Domains for Dirac-Coulomb min-max levels," Revista Matemática Iberoamericana (in press).
[11] Esteban, M. J. and Loss, M., "Self-adjointness for Dirac operators via Hardy-Dirac inequalities," J. Math. Phys. **48**(11), 112107 (2007).
[12] Facchi, P., Garnero, G., and Ligabò, M., "Self-adjoint extensions and unitary operators on the boundary," Lett. Math. Phys. **108**(1), 195–212 (2018).
[13] Gallone, M., "Self-adjoint extensions of Dirac operator with Coulomb potential," in *Advances in Quantum Mechanics* (Springer, 2017), pp. 169–185.
[14] Gallone, M. and Michelangeli, A., "Self-adjoint realisations of the Dirac-Coulomb Hamiltonian for heavy nuclei," Anal. Math. Phys. **9**, 585–616 (2018).
[15] Gorbachuk, N., *Boundary Value Problems for Operator Differential Equations* (Springer Science & Business Media, 2012), Vol. 48.
[16] Gustafson, K. and Rejto, P., "Some essentially self-adjoint Dirac operators with spherically symmetric potentials," Isr. J. Math. **14**(1), 63–75 (1973).
[17] Hogreve, H., "The overcritical Dirac–Coulomb operator," J. Phys. A: Math. Theor. **46**(2), 025301 (2012).
[18] Kato, T., "Fundamental properties of Hamiltonian operators of Schrödinger type," Trans. Am. Math. Soc. **70**(2), 195–211 (1951).
[19] Kato, T., "Holomorphic families of Dirac operators," Math. Z. **183**(3), 399–406 (1983).
[20] Kato, T., *Perturbation Theory for Linear Operators* (Springer Science & Business Media, 2013), Vol. 132.
[21] Klaus, M. and Wüst, R., "Characterization and uniqueness of distinguished self-adjoint extensions of Dirac operators," Commun. Math. Phys. **64**(2), 171–176 (1979).
[22] Müller, D., "Minimax principles, Hardy-Dirac inequalities, and operator Cores for two and three dimensional Coulomb-Dirac operators," Doc. Math. **21**, 1151–1169 (2016).
[23] Nenciu, G., "Self-adjointness and invariance of the essential spectrum for Dirac operators defined as quadratic forms," Commun. Math. Phys. **48**(3), 235–247 (1976).
[24] Pankrashkin, K., "Resolvents of self-adjoint extensions with mixed boundary conditions," Rep. Math. Phys. **58**(2), 207–221 (2006).
[25] Pavlov, B. S., "The theory of extensions and explicitly-soluble models," Russ. Math. Surv. **42**(6), 127 (1987).

[26] Reed, M., and Simon, B., *Fourier Analysis*, Methods of Modern Mathematical Physics (Academic Press, New York, 1975), Vol. 2.
[27] Reed, M., and Simon, B., *Functional Analysis*, Methods of Modern Mathematical Physics (Academic Press, New York, 1980), Vol. 1.
[28] Rellich, F. and Jörgens, K., *Eigenwerttheorie partieller Differentialgleichungen: Vorlesung, gehalten an der Universität Göttingen* (Mathematisches Institut der Universität Göttingen, 1953).
[29] Schmincke, U.-W., "Distinguished selfadjoint extensions of Dirac operators," Math. Z. **129**(4), 335–349 (1972).
[30] Schmincke, U.-W., "Essential selfadjointness of Dirac operators with a strongly singular potential," Math. Z. **126**(1), 71–81 (1972).
[31] Schmüdgen, K., *Unbounded Self-Adjoint Operators on Hilbert Space* (Springer Science & Business Media, 2012), Vol. 265.
[32] Thaller, B., *The Dirac Equation* (Springer-Verlag Berlin, 1992), Vol. 31.
[33] Voronov, B. L., Gitman, D. M., and Tyutin, I. V., "The Dirac Hamiltonian with a superstrong Coulomb field," Theor. Math. Phys. **150**(1), 34–72 (2007).
[34] Weidmann, J., "Oszillationsmethoden für systeme gewöhnlicher Differentialgleichungen," Math. Z. **119**(4), 349–373 (1971).
[35] Wüst, R., "Distinguished self-adjoint extensions of Dirac operators constructed by means of cut-off potentials," Math. Z. **141**(1), 93–98 (1975).
[36] Xia, J., "On the contribution of the Coulomb singularity of arbitrary charge to the Dirac Hamiltonian," Trans. Am. Math. Soc. **351**(5), 1989–2023 (1999).