BOUNDARY TRIPLES FOR THE DIRAC OPERATOR WITH COULOMB-TYPE SPHERICALLY SYMMETRIC PERTURBATIONS

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ABSTRACT. We determine explicitely 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 behaviour 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.

1. 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}, v_{am}, the potentials $\mathbb{V}_{el}, \mathbb{V}_{sc}, \mathbb{V}_{am}$ are called respectively *electric*, *scalar*, and *anomalous magnetic* potential. This particular class of potentials has the property that, in

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the case that v_{el}, v_{sc}, v_{am} only depend on the radial variable, the action of $H_0+\mathbb{V}$ leaves invariant the *partial wave subspaces*(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 the Stone's theorem, see e.g. [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. [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 behaviour in the point of the functions in their domain. Referring to [5, 12] for a general overview on the theories of self-adjoint extensions, we cite here the theory of *boundary triples*, see [31, 5, 9, 25] 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 behaviour in the origin of the functions in the domain.

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

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

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 $C^\infty_c(\mathbb{R}^3)^4$ 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 [16, 28, 30, 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 [6, 14, 21, 23, 29, 35]. For $|\nu|\ge 1$ many self-adjoint extensions can be built, and for $|\nu|>1$ none appears to be *distinguished* in some suitable sense, see [17, 33, 36]. The definition of a distinguished extension for the case $|\nu|=1$ has been settled in [11], where it is considered a pontential $V:\mathbb{R}^3\to\mathbb{R}$ such that that for some constant $c(V)\in(-1,1)$, $\Gamma:=\sup(V)<1+c(V)$ and for every $\varphi\in C^\infty_c(\mathbb{R}^3)^2$,

$$\int_{\mathbb{R}^3}\left(\frac{|\sigma\cdot\nabla\varphi|^2}{1+c(V)-V}+(1+c(V)+V)\,|\varphi|^2\right)dx\ge 0. \tag{1.6}$$

In particular, for an electrostatic potential $\mathbb{V}(x):=V(x)\mathbb{I}_4$, $-\nu|x|^{-1}\le V(x)<1+\sqrt{1-\nu^2}$, $0<\nu\le 1$, 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 [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 [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 cut-off around the singularity.

The approach of [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

$$|\mathbb{V}(x)| \leq a\frac{1}{|x|} + b, \quad x \in \mathbb{R}^3 \setminus \{0\},$$

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

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

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:

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

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

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 [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 [7] and [32, Section 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

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

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

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

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 $j = \frac{1}{2}, \frac{3}{2}, \dots$; $m_j = -j, \dots, j$; $k_j = j + 1/2, -j - 1/2$:

$$\begin{aligned}
&\left(\frac{1}{2}, -\frac{1}{2}, 1\right), \left(\frac{1}{2}, \frac{1}{2}, 1\right), \left(\frac{1}{2}, -\frac{1}{2}, -1\right), \left(\frac{1}{2}, \frac{1}{2}, -1\right),\\
&\left(\frac{3}{2}, -\frac{3}{2}, 2\right), \left(\frac{3}{2}, -\frac{1}{2}, 2\right), \left(\frac{3}{2}, \frac{1}{2}, 2\right), \left(\frac{3}{2}, \frac{3}{2}, 2\right),\\
&\left(\frac{3}{2}, -\frac{3}{2}, -2\right), \left(\frac{3}{2}, -\frac{1}{2}, -2\right), \left(\frac{3}{2}, \frac{1}{2}, -2\right), \left(\frac{3}{2}, \frac{3}{2}, -2\right), \dots,\\
&\left(j, -j, j + \frac{1}{2}\right), \dots, \left(j, j, j + \frac{1}{2}\right), \left(j, -j, -j - \frac{1}{2}\right), \dots, \left(j, j, -j - \frac{1}{2}\right), \dots
\end{aligned} \tag{1.11}$$

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 [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:

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

where "$\cong$" means that the operators are unitarily equivalent, with

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

and

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

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 [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

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

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 [7, Theorems 1.1, 1.2, 1.3] we show that if $\delta_{k_j} \geq 1/4$ then t_{m_j,k_j} is essentially self-adjoint and if $\delta_{k_j} < 1/4$ that 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 parametrised 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 with the behaviour 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 [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 an other 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 consequence of Theorem 1.2, Proposition 1.5 and Theorem 1.12 in [5], or equivalently of Proposition 14.4 and Theorem 14.10 in [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-adoint 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 Remark 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 to label this 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 $f_{m_j,k_j} := \left(f^+_{m_j,k_j}, f^-_{m_j,k_j}\right) \in \mathcal{D}(h^*_{m_j,k_j})$. We select in the order (1.11) 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

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

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

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

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

being $D_{k_j} \in \mathbb{R}^{2\times 2}$ 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 [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 [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 [5, Proposition 1.14, Proposition 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 extension of $\mathring{H}_{min}$: the following theorem is 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 hold:*

(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-adoint 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, 1.3 in [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 $C^\infty_c(0,+\infty)^2$. Consequently, $\mathring{H}_{min}$ has deficiency indices (d,d), with d defined as in (1.16). We can now use the 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 can not 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 behaviour in the origin of the functions in their domain.

In the spirit of [4, 11, 22] in the next theorem 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 $q : C^\infty_c(\mathbb{R}^3;\mathbb{C}^4) \to \mathbb{R}$ 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 the following theorem, 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 possibile to use this criterium 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) and for all (j, m_j, k_j) *such that* $0 \neq \gamma_{k_j} = k_j + \lambda$,

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

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

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

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

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

or equivalently

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

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 in 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 [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 [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 [7, Remark 1.10].

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

- for $0 \leq |\nu| \leq \sqrt{3}/2$, 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 $\Gamma^\pm = \left(\Gamma^\pm_{-\frac12,1}, \Gamma^\pm_{\frac12,1}, \Gamma^\pm_{-\frac12,-1}, \Gamma^\pm_{\frac12,-1}\right)$. 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 $d = 4$, $\delta_1 = \delta_{-1} = 0$, $\Gamma^\pm = \left(\Gamma^\pm_{-\frac12,1}, \Gamma^\pm_{\frac12,1}, \Gamma^\pm_{-\frac12,-1}, \Gamma^\pm_{\frac12,-1}\right)$, 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-ajoint extension, as defined in [11]. More in general, in the case that $\mathbb{V}$ is as in (1.3), Theorem 1.9 selects the distinguished extension, as in [7, Propositions 1.7, 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 $R > 0$*

$$\int_{\mathbb{R}^3} |x||-i\alpha \cdot \nabla\psi(x)|^2 \, dx \geq \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|} \, dx + \frac{1}{4} \int_{\mathbb{R}^3} \frac{\left|\psi(x) - \frac{R}{|x|}\psi(R\frac{x}{|x|})\right|^2}{|x| \log^2(|x|/R)} \, dx. \tag{1.45}$$

Moreover, the inequality is sharp.

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

The paper is organized as follows: in Section 2 we prove Theorem 1.5 and in Section 3 we prove Lemma 1.13 and Theorem 1.9.

2. Proof of Theorem 1.5

We firstly prove the following lemma.

Lemma 2.1. *Let $j \in \{1/2, 3/2, \dots\}$, $m_j \in \{-j, \dots, j\}$, $k_j \in \{j + 1/2, -j - 1/2\}$ 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 Definition 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 $j \in \{1/2, 3/2, \dots\}$, $m_j \in \{-j, \dots, j\}$, $k_j \in \{j + 1/2, -j - 1/2\}$ are fixed. We distinguish various cases.

In the case $0 < \delta < \frac{1}{4}$, thanks to [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 $C^\infty_c(0,+\infty)^2 \subset \ker(\Gamma^+_{m_j,k_j}, \Gamma^-_{m_j,k_j})$.

Let us now consider the case that $\delta = 0$. Thanks to [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 lastly assume that $\delta < 0$. In this case, thanks to [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

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

Due to (1.33), one get (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 Definition 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 [7, Theorem 1.1]. Thanks to Lemma 2.1, we conclude that

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

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 Lemma 2.1.

Finally, since $C^\infty_c(\mathbb{R}^3\setminus\{0\})^4 \subseteq \ker(\Gamma^+,\Gamma^-)$, we deduce the condition (1.18). □

3. Proof of Theorem 1.9

In this Section we prove Lemma 1.13, the following Proposition 3.1 and finally Theorem 1.9.

Proof of Lemma 1.13. By direct computation (see for example [32, Equation (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 $\mathbf{S}$ is the *spin angular momentum operator*

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

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

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

It is standard (see for example [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 respectively symmetric and skew-symmetric on $C^\infty_c(\mathbb{R}^3)^4$, 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

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

Thanks to Proposition 2.4, *(iii)* in [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 [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,

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

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 firstly show that $\gamma_{k_j} \geq 0$ for all $j = 1/2, 3/2, \dots$, that is $(k+\lambda)^2 + \mu^2 - \nu^2 \geq 0$ for all $k \in \mathbb{Z}\setminus\{0\}$. Indeed, since $|x||\mathbb{V}(x)| = |\nu| + \sqrt{\mu^2+\lambda^2} \leq 1$, then $\nu^2 \leq 1 + \mu^2 + \lambda^2 - 2\sqrt{\mu^2+\lambda^2}$. Moreover, since $|\lambda| \leq 1$, then $M := \min_{k\in\mathbb{Z}\setminus\{0\}}(k+\lambda)^2 + \mu^2 - \nu^2 = (1-|\lambda|)^2 + \mu^2 - \nu^2$. Assume by contradiction that $M < 0$. Then $(1-|\lambda|)^2 + \mu^2 < \nu^2 \leq 1 + \mu^2 + \lambda^2 - 2\sqrt{\mu^2+\lambda^2}$, that is $|\lambda| > \sqrt{\mu^2+\lambda^2}$ and this is absurd. Incidentally we remark that $M = 0$ only if $\mu = 0$.

We denote

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

Following (1.11), we identify

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

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

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 Proposition 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

$$\psi(x) = \sum_{j=\frac{1}{2},\frac{3}{2},\dots}^{\infty} \sum_{m_j=-j}^{j} \sum_{k_j=\pm(j+1/2)} \frac{1}{r}\left(f^+_{m_j,k_j}(r)\Phi^+_{m_j,k_j}(\hat{x}) + f^-_{m_j,k_j}(r)\Phi^-_{m_j,k_j}(\hat{x})\right),$$
$$f_{m_j,k_j} = (f^+_{m_j,k_j}, f^-_{m_j,k_j}).$$

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 behaviour 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:

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

For all $(j, m_j, k_j) \in I_3$, we have that f_{m_j,k_j} verifies (1.28): since the logarithmic behaviour is not allowed by (3.2), we have necessarily that $\operatorname{Ran}(\Gamma^+_{m_j,k_j}, \Gamma^-_{m_j,k_j}) \subseteq \ker M_{k_j}$. 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 $s \sim (j, m_j, k_j) \in I_3$, $t \in \{1, \dots, d\}, t \ne s$.

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

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

that is (1.21). In order to show that (1.22), we show equivalently that $\det(AA^* + BB^*) \ne 0$ (see [1, Section 125, 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 $s = 1, \dots, d$. For $s \in I_1$ we have that $C_{ss} = (k_j + \lambda + \gamma_{k_j})^2 + (\mu - \nu)^2 \ge (k_j + \lambda + \gamma_{k_j})^2 = 4\gamma_{k_j}^2 > 0$. For $s \in I_2$ we have that $C_{ss} = (\mu + \nu)^2 + (k_j + \lambda + \gamma_{k_j})^2 \ge (k_j + \lambda - \gamma_{k_j})^2 > 0$. 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 to 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 [24, Section 2], [2, Theorem 4.6], [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. □

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