Self-adjointness and spectral properties for the Dirac operator with Coulomb-type perturbations

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

and σ_k are the *Pauli matrices*

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

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  - essentially self-adjoint on $C_c^\infty(\mathbb{R}^3; \mathbb{C}^4)$,
  - self-adjoint on $H^1(\mathbb{R}^3; \mathbb{C}^4)$;
- H_0 is not positive:

$$\sigma(H_0) = \sigma_{ess}(H_0) = (-\infty, -m] \cup [m, +\infty).$$

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(A very basic) Question

Is $H = H_0 + \mathbb{V}$ self-adjoint (on the appropriate domain)?

Dirac-Coulomb Self-adjointness (unfair overview)

For $|\nu| \in \left[0, \frac{1}{2}\right)$: **[Kato, 1951].** For $f \in C_c^\infty(\mathbb{R}^3)^4$, the Hardy inequality

$$\frac{1}{4}\int_{\mathbb{R}^3} \frac{|f|^2}{|x|^2}\,dx \leq \int_{\mathbb{R}^3} |\nabla f|^2\,dx$$

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implies that the Coulomb potential is a (Kato) small perturbation: $H_0 + \nu/|x|$ is self-adjoint on $H^1(\mathbb{R}^3;\mathbb{C}^4)$ and essentially self-adjoint on $C_c^\infty(\mathbb{R}^3;\mathbb{C}^4)$.

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For $\sqrt{3}/2 < |\nu| < 1$ there are infinite self-adjoint extensions: among them there is a *distinguished* one! **[Klaus, Wüst, 1979]**

$$\psi \in \mathcal{D}(H_{\text{dist}}) \iff \int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|} \, dx < +\infty \iff \psi \in \dot{H}^{\frac{1}{2}}(\mathbb{R}^3; \mathbb{C}^4)$$

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$$\psi \in \mathcal{D}(H_{\text{dist}}) \iff \langle \mathbb{V}\psi, \psi \rangle_{L^2} < +\infty$$
$$\iff \langle -i\nabla\psi, \psi \rangle_{L^2} < +\infty.$$

Self-adjointness with matrix valued potentials

[Kato, 1951] holds for hermitian potentials $\mathbb{V} \in \mathbb{C}^{4\times 4}$ such that

$$|\mathbb{V}(x)| \leq a\frac{1}{|x|}, \quad \text{for } a < \frac{1}{2}.$$

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[Kato, 1981] and **[Arrizabalaga, Duoandikoetxea, Vega, 2013]** describe the distinguished extension for general matrix valued potentials such that

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Fundamental tool is the Hardy (Kato-Nenciu) inequality: for all $\psi \in C_c^\infty(\mathbb{R}^3; \mathbb{C}^4)$

$$\int_{\mathbb{R}^3} \frac{1}{|x|}|\psi|^2 \leq \int_{\mathbb{R}^3} |x||(-i\alpha\cdot\nabla + m\beta \pm \epsilon i)\psi|^2, \quad \epsilon \geq 0.$$

We remind that if $|\mathbb{V}(x)| \leq \frac{C}{|x|}$, with $C > 0$, if $H_0 + \mathbb{V}$ is self-adjoint then

$$\sigma_{ess}(H_0 + \mathbb{V}) = \sigma_{ess}(H_0) = (-\infty, -m] \cup [m, +\infty).$$

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In **[Dolbeault, Esteban, Séré, 2000]**, it is proved the validity of a min-max formula to determine the eigenvalues in the gap of the essential spectrum of the Dirac operator perturbed with Coulomb-like potentials $\mathbb{V}$ such that

$$\mathbb{V}(x) := V(x)\mathbb{I}_4, \qquad \lim_{|x|\to+\infty} |V(x)| = 0, \qquad -\frac{\nu}{|x|} - c_1 \leq V \leq c_2,$$

with $\nu \in (0,1)$ and $c_1, c_2 \geq 0$, $c_1 + c_2 - 1 < \sqrt{1-\nu^2}$.
As a consequence of their results, they proved the following Hardy-type inequality:

$$\int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \varphi|^2}{a + \frac{1}{|x|}} + \int_{\mathbb{R}^3} \left(a - \frac{1}{|x|} \right) |\varphi|^2 \geq 0, \qquad \text{for all } a > 0, \varphi \in C_c^\infty(\mathbb{R}^3)^2.$$

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Later, a later direct analytical proof was given in **[Dolbeault, Esteban, Loss, Vega, 2004]**.

Thanks to this inequality, in **[Esteban, Loss, 2007]** it is considered a general electrostatic potential $V : \mathbb{R}^3 \to \mathbb{R}$ such that for every $\varphi \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$

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

for some constant $c(V) \in (-1, 1)$, $\Gamma := \sup(V) < 1 + c(V)$, and for $\mathbb{V} := V\mathbb{I}_4$, they proved that the operator $H_0 + \mathbb{V}$ is self-adjoint on the appropriate domain.

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In particular, they could treat potentials such that

$$-\frac{\nu}{|x|} \leq V(x) < 1 + \sqrt{1 - \nu^2}, \quad \text{with } \nu \in (0, 1],$$

obtaining the distinguished extension in the case that $\nu < 1$, and giving a definition of distinguished extension in the critical case $\nu = 1$.

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The inequality was then used in **[Esteban, Lewin, Séré, 2017]**: they provided details on the domain of the distinguished extension and they showed the validity of a min-max formula for the eigenvalues in the spectral gap.

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The inequality was then used in **[Esteban, Lewin, Séré, 2017]**: they provided details on the domain of the distinguished extension and they showed the validity of a min-max formula for the eigenvalues in the spectral gap. (For a fair overview see **[C., Pizzichillo, 2018a]**).

Theorem ([C., Pizzichillo, Vega, 2018])

Let $m > 0$ and $a \in (-m, m)$. Let ψ be a distribution such that

$$\int_{\mathbb{R}^3} |(-i\alpha \cdot \nabla + m\beta - a)\psi|^2 |x| \, dx < +\infty.$$

Then $\psi \in L^2(|x|^{-1})^4$ and

$$\frac{m^2 - a^2}{m^2} \int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|} \, dx \leq \int_{\mathbb{R}^3} |(-i\alpha \cdot \nabla + m\beta - a)\,\psi|^2 |x| \, dx. \tag{1}$$

The inequality is sharp, in the sense that the constant on the left hand side can not be improved.

...

Theorem (addendum)

...

If $a \neq 0$, all the attainers are given by the elements of the two(complex)-parameter family $\{\psi_C^a\}_{C\in\mathbb{C}^2}$, with

$$\psi_C^a := \begin{cases} \dfrac{e^{-\sqrt{m^2-a^2}|x|}}{|x|^{1-\frac{a}{m}}} \cdot \begin{pmatrix} C \\ i\sqrt{\frac{m-a}{m+a}}\,\sigma\cdot\frac{x}{|x|}\cdot C \end{pmatrix} & \text{if } a>0, \\ \dfrac{e^{-\sqrt{m^2-a^2}|x|}}{|x|^{1+\frac{a}{m}}} \cdot \begin{pmatrix} -i\sqrt{\frac{m+a}{m-a}}\,\sigma\cdot\frac{x}{|x|}\cdot C \\ C \end{pmatrix} & \text{if } a<0, \end{cases} \in L^2(|x|^{-1})^4.$$

In the case that $a=0$, the inequality is attained by the functions ψ_C^a above, in the sense that

$$\lim_{\epsilon\to 0}\int_{\{|x|>\epsilon\}}\left[|x|\left|(-i\alpha\cdot\nabla+m\beta)\,\psi_C^0\right|^2-\frac{|\psi_C^0|^2}{|x|}\right]dx=0.$$

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With explicit computation:

$$\left(\boldsymbol{H_0} \mp \frac{\boldsymbol{\nu}}{|\boldsymbol{x}|} - \boldsymbol{a} \right) \psi_{\boldsymbol{C}}^{\boldsymbol{a}} = \mathbf{0}.$$

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(What about the vice-versa? Be patient!)

The two inequalities in the proof

The proof descends from the explicit computation of the following square:

$$
\begin{aligned}
0 &\le \int_{\mathbb{R}^3} |x| \left| (-i\alpha\cdot\nabla + m\beta - a)\psi - i\alpha\cdot\frac{x}{|x|}\Big(1-\frac{a}{m}\beta\Big)(1+2\mathbf{S}L)\frac{\psi}{|x|}\right|^2 dx \\
&= \int_{\mathbb{R}^3} |x| |(-i\alpha\cdot\nabla + m\beta - a)\psi|^2 \, dx - \frac{m^2-a^2}{m^2}\int_{\mathbb{R}^3} \frac{|(1+2\mathbf{S}L)\psi|^2}{|x|}\, dx,
\end{aligned}
$$

where the *spin angular momentum operator* $\mathbf{S}$ and the *orbital angular momentum* L are defined as

$$
\mathbf{S} = \frac{1}{2}\begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} \quad \text{and} \quad L := -ix\wedge\nabla.
$$

Moreover, since $|1+2\mathbf{S}L| \ge 1$,

$$
\int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|}\, dx \le \int_{\mathbb{R}^3} \frac{|(1+2\mathbf{S}L)\psi|^2}{|x|}\, dx.
$$

Thanks to the previous Theorem, for $a \in (-m, m)$

$$(H_0 - a)^{-1} : L^2(|x|)^4 \to L^2(|x|^{-1})^4, \quad \mathbf{u}(H_0 - a)^{-1}\mathbf{v} : L^2(\mathbb{R}^3)^4 \to L^2(\mathbb{R}^3)^4,$$

are well defined and bounded, with

$$\mathbf{u}(x) := |x|^{1/2}\mathbb{V}(x) \quad \text{and} \quad \mathbf{v}(x) := |x|^{-1/2}\mathbb{I}_4.$$

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Theorem (Birman-Schwinger principle)

Let $\mathbb{V}$ be a Hermitian matrix-valued potential such that $\sup_x |x||V(x)| < 1$, and let $\mathbf{u}, \mathbf{v}$ be defined as above. Let H_D be the distinguished realization and let $a \in (-m, m)$. Then

$$a \in \sigma_d(H_D) \iff -1 \in \sigma_d(\mathbf{u}(H_0 - a)^{-1}\mathbf{v}).$$

Moreover, the multiplicity of a as an eigenvalue of H_D coincides with the multiplicity of -1 as an eigenvalue of $\mathbf{u}(H_0 - a)^{-1}\mathbf{v}$.

For $\nu \in (0,1)$, the distinguished realization $H_\nu := H_0 - \frac{\nu}{|x|}$ verifies:

$$\sigma(H_\nu) = \sigma_d(H_\nu) \cup \sigma_{ess}(H_\nu) = \{a_1, a_2, \ldots\} \cup (-\infty, -m] \cup [m, +\infty), \quad (2)$$

and

$$\boldsymbol{m\sqrt{1-\nu^2} = a_1 = a_2 <} a_3 \leq \cdots \leq a_n \leq \cdots \leq m, \lim_{n\to+\infty} a_n = m.$$

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In **[Dolbeault, Esteban, Séré, 2000]**, they considered an *electric* potential $\mathbb{V} := V\mathbb{I}_4$, being $V = V(|x|)$ a *radially symmetric* function satisfying

$$\lim_{|x| \to +\infty} |V(x)| = 0, \qquad -\frac{\nu}{|x|} - c_1 \leq V \leq c_2$$

with $\nu \in (0,1)$ and $c_1, c_2 \geq 0$, $c_1 + c_2 - 1 < \sqrt{1-\nu^2}$. By means of **min-max** formulas, they proved that the distinguished self-adjoint realization H_D verifies (**??**), with

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In **[Esteban, Lewin, Séré, 2017]** they could generalise this result, removing the hypothesis of radial symmetry on $\mathbb{V}$ and for $\nu \in (0,1]$.

Let $a \in (-m, m)$ be an eigenvalue of $H_0 + \mathbb{V}$ with multiplicity $\mu(a)$ and let ψ be an associated eigenfunction, that is $(H_0 - a)\psi = -\mathbb{V}\psi$.

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Thanks to the Hardy-type inequality we have proved:

$$\nu^2 \int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|} \geq \int_{\mathbb{R}^3} |x||(H_0 - a)\psi|^2 \, dx \geq \tfrac{m^2 - a^2}{m^2} \int_{\mathbb{R}^3} \frac{|\psi|^2}{|x|} \, dx$$

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If $\boldsymbol{a = \pm m\sqrt{1 - \nu^2}}$, ψ is an attainer and so $\psi = \psi^a_C$, for $C \in \mathbb{C}^2$.

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Let $a \in (-m, m)$ be an eigenvalue of $H_0 + \mathbb{V}$ with multiplicity $\mu(a)$ and let ψ be an associated eigenfunction, that is $(H_0 - a)\psi = -\mathbb{V}\psi$.

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If $\boldsymbol{a = \pm m\sqrt{1-\nu^2}}$, ψ is an attainer and so $\psi = \psi_C^a$, for $C \in \mathbb{C}^2$. Then $0 = \left(H_0 \mp \frac{\nu}{|x|} - a\right)\psi_C^a = (H_0 + \mathbb{V} - a)\psi_C^a \implies$ $\boldsymbol{\mathbb{V}\psi_C^a = \mp \frac{\nu}{|x|}\psi_C^a}$, $\mu(a) \leq 2$.

Theorem ([C., Pizzichillo, Vega, 2018])

Let $\mathbb{V}$ be a Hermitian matrix valued potential such that $\sup_x |x||\mathbb{V}(x)| < 1$, and let H_D be the distinguished self-adjoint realization.

Let $a \in \sigma_d(H_D)$, let $\mu(a)$ be its multiplicity and let $\psi \in \mathcal{D}(H_D)$ be an associated eigenfunction. Then:

- $|a| \geq m\sqrt{1-\nu^2}$;
- $a = \pm m\sqrt{1-\nu^2}$ *if and only if* $\psi = \psi_C^a$ *for some* $C \in \mathbb{C}^2$*; in this case,* $\mathbb{V}\psi_C^a = \mp\frac{\nu}{|x|}\psi_C^a$ *and* $\mu(a) \leq 2$*;*
  if moreover $\mathbb{V}$ *is an electric potential, that is* $\mathbb{V} = V(x)\mathbb{I}_4$*, then* $V(x) = \mp\frac{\nu}{|x|}$.

...

Theorem (addendum)

...

- *in the case that* $a = \pm m\sqrt{1-\nu^2}$, *then* $\mu(a) = 2$ *if and only if*

$$\mathbb{V}(x) = \begin{cases} -\frac{\nu}{|x|}\mathbb{I}_4 + \begin{pmatrix} \mathrm{N}^2\sigma\cdot\frac{x}{|x|}\mathbf{W}^+(x)\sigma\cdot\frac{x}{|x|} & i\mathrm{N}\sigma\cdot\frac{x}{|x|}\mathbf{W}^+(x) \\ -i\mathrm{N}\mathbf{W}^+(x)\sigma\cdot\frac{x}{|x|} & \mathbf{W}^+(x) \end{pmatrix} & a > 0, \\ \frac{\nu}{|x|}\mathbb{I}_4 + \begin{pmatrix} \mathbf{W}^-(x) & i\mathrm{N}\mathbf{W}^-(x)\sigma\cdot\frac{x}{|x|} \\ -i\mathrm{N}\sigma\cdot\frac{x}{|x|}\mathbf{W}^-(x) & \mathrm{N}^2\sigma\cdot\frac{x}{|x|}\mathbf{W}^-(x)\sigma\cdot\frac{x}{|x|} \end{pmatrix} & a < 0, \end{cases}$$

where $\mathrm{N} = \sqrt{\frac{1-\sqrt{1-\nu^2}}{1+\sqrt{1-\nu^2}}}$, *and* $\mathbf{W}^+(x)$ *and* $\mathbf{W}^-(x)$ *are* 2×2 *Hermitian matrices whose eigenvalues are respectively* $\{\lambda_j^+(x)\}_{j=1,2}$ *and* $\{\lambda_j^-(x)\}_{j=1,2}$, *and they verify*

$$-\frac{\nu}{|x|}(1+\sqrt{1-\nu^2}) \le \lambda_j^-(x) \le 0 \le \lambda_j^+(x) \le \frac{\nu}{|x|}(1+\sqrt{1-\nu^2}).$$

Question

Can we extend these results to the general case when $\sup_x |x||\mathbb{V}(x)| \geq 1$?

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It is not clear what the distinguished extension is in this general case.

When $\sup_x |x||\mathbb{V}(x)| = 1$ it is no longer true that $\mathcal{D}(H_0 + \mathbb{V}) \subset \mathcal{D}(r^{-1/2})^4$.
For example, when $\mathbb{V}(x) = \mathbb{V}_C(x) = \frac{1}{|x|}$

the ground state $\psi_C^0 \notin \mathcal{D}(r^{-1/2})^4$.

Distinguished extension via quadratic forms

We select a self-adjoint extension T by asking that $\mathcal{D}(T)$ is included in the domain of an appropriate quadratic form.

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Assume that $v := \sup_{x \in \mathbb{R}^3} |x||\mathbb{V}(x)| \leq 1$, and let

$$q(\psi) := \int_{\mathbb{R}^3} \left[|x||-i\alpha \cdot \nabla\psi|^2 - |x||\mathbb{V}\psi|^2 \right] dx, \qquad \text{for all } \psi \in C_c^\infty(\mathbb{R}^3; \mathbb{C}^4).$$

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Thanks to the Kato-Nenciu inequality

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

this form is symmetric and non-negative, and hence closable: we denote its closure q (with abuse of notation) and its maximal domain $\mathcal{Q}$.

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this form is symmetric and non-negative, and hence closable: we denote its closure q (with abuse of notation) and its maximal domain $\mathcal{Q}$.
If $v < 1$, then for all $\psi \in \mathcal{Q}$, $\int \frac{|\psi(x)|^2}{|x|}\,dx < +\infty$, i.e. $\mathcal{D}(T) \subset \mathcal{Q}$ implies that T is the distinguished extension (**[Kato, 1981]**,**[Arrizabalaga, Duoandikoetxea, Vega, 2013]**).

Lemma ([C., Pizzichillo, 2018b])

For all $\psi \in C_c^\infty(\mathbb{R}^3)^4$ and $R > 0$:

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

Moreover, the inequality is sharp.

Consequently, for all $\psi \in \mathcal{Q}$:

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

In **[C., Pizzichillo, 2018b]** we describe all the self-adjoint realizations of the differential operator $H_0 + \mathbb{V}$, where

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

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We characterize all the self-adjoint extensions through the behaviour of the functions in the domain in the origin.
We construct a **boundary triple** for H_{max}
(remind that $\mathcal{D}(H_{max}) = \{\psi \in L^2(\mathbb{R}^3)^4 : H\psi \in L^2(\mathbb{R}^3)^4\}$).

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(remind that $\mathcal{D}(H_{max}) = \{\psi \in L^2(\mathbb{R}^3)^4 : H\psi \in L^2(\mathbb{R}^3)^4\}$).
Let

$$d := \sum_{\substack{k\in\setminus\{0\} \\ (k+\lambda)^2+\mu^2-\nu^2<1/4}} 2|k| < +\infty,$$

then $(\mathbb{C}^d, \Gamma^+, \Gamma^-)$ is a boundary triple for H_{max}, for appropriate $\Gamma^+, \Gamma^- : \mathcal{D}(H_{max}) \to \mathbb{C}^d$.

Let us consider $\mathbb{V}_C(x) = \frac{\nu}{|x|}$.

- If $0 < \nu < 1$ there exists $\gamma > 0$ such that for every $\psi \in \mathcal{D}(H_0 + \mathbb{V})$

$$\text{as } |x| \to 0: \quad \psi(x) \sim \frac{A|x|^{\gamma} + B|x|^{-\gamma}}{|x|} \sim \begin{cases} B|x|^{-\gamma-1}, & \text{if } B \neq 0, \\ A|x|^{\gamma-1}, & \text{if } B = 0, \end{cases}$$

  for some $A, B \in \mathbb{C}^4$.

- If $\nu = 1$, for every $\psi \in \mathcal{D}(H_0 + \mathbb{V})$ then

$$\text{as } |x| \to 0: \quad \psi(x) \sim \frac{A + B\log|x|}{|x|} \sim \begin{cases} \frac{B\log|x|}{|x|}, & \text{if } B \neq 0, \\ \frac{A}{|x|}, & \text{if } B = 0, \end{cases}$$

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There exists only one extension such that $B = 0$ for every function ψ: this is the distinguished one.

- If $\nu > 1$ there exists $\gamma > 0$ such that for every $\psi \in \mathcal{D}(H_0 + \mathbb{V})$

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No one appears to be distinguished in some sense.

Let us consider $\mathbb{V}_{am}(x) = \frac{\lambda}{|x|}(i\alpha \cdot \frac{x}{|x|}\beta)$.

- If $0 < \lambda < 1$ there exists $\gamma > 0$ such that for every $\psi \in \mathcal{D}(H_0 + \mathbb{V})$

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  for some $A, B \in \mathbb{C}^4$. The distinguished extension is the unique one such that $B = 0$ for all ψs.

- If $\lambda = 1$, for every $\psi \in \mathcal{D}(H_0 + \mathbb{V})$ then

$$\text{as } |x| \to 0: \quad \psi(x) \sim \frac{A}{|x|}$$

  for some $A \in \mathbb{C}^4$. No one appears to be distinguished.

Theorem ([C., Pizzichillo, 2018b])

Let

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

and assume that

$$\sup_{x\in\mathbb{R}^3} |x||\mathbb{V}(x)| \leq 1, \quad \mathbb{V}(x) \neq \pm\frac{i\alpha\cdot\frac{x}{|x|}\beta}{|x|}. \tag{4}$$

Then, there exists only one self-adjoint extension $\mathring{H}_{min} \subset T \subset H_{max}$ *such that* $\mathcal{D}(T) \subset \mathcal{Q}$.

This is a positive result: we give the definition of *distinguished* extension by means of quadratic forms in a bigger class than in **[Esteban, Loss, 2008]**, **[Esteban, Lewin, Séré, 2017]**.

This is a negative result: the condition $\mathcal{D}(T) \subset \mathcal{Q}$ does not appear to select an extension in the general case that $\sup_{x\in\mathbb{R}^3}|x||\mathbb{V}(x)| \leq 1$, since it does not in the case

$$\mathbb{V}(x) = \pm\frac{i\alpha\cdot\frac{x}{|x|}\beta}{|x|}.$$

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[C.,Pizzichillo, 2018a] Biagio Cassano, and Fabio Pizzichillo. *“Self-adjoint extensions for the Dirac operator with Coulomb-type spherically symmetric potentials.”* Letters in Mathematical Physics 108.12 (2018): 2635-2667.

[C.,Pizzichillo, 2018b] Biagio Cassano, and Fabio Pizzichillo. *“Boundary triples for the Dirac operator with Coulomb-type spherically symmetric perturbations.”* To appear in Journal of Mathematical Physics, arXiv preprint arXiv:1810.01659 (2018).

[C., Pizzichillo, Vega, 2018] Biagio Cassano, Fabio Pizzichillo, and Luis Vega. *“A Hardy-type inequality and some spectral characterizations for the Dirac-Coulomb operator.”* arXiv preprint arXiv:1810.01309 (2018).

The Dirac-Coulomb operator

The Dirac-Coulomb operator describes spin–$\frac{1}{2}$ particles in the external electrostatic field of an atomic nucleus of atomic number Z.
In fact

$$H_0 + \mathbb{V}_C(x) = -ic\hbar\alpha \cdot \nabla + \beta mc^2 + \frac{c\nu}{|x|}\mathbb{I}_4, \quad \nu = \frac{e^2 Z}{\hbar c} = Z\alpha_f,$$

where

- c is the speed of light,
- $\hbar$ is the Plank's constant,
- e is the charge of the electron,
- Z is the atomic number,
- $\alpha_f = (137.035\dots)^{-1}$ is the fine-structure constant.

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We set $\hbar = c = e = 1$.

We write

$$\psi \in \mathcal{D}(H_{max}) = \{\psi \in L^2(\mathbb{R}^3)^4 : H\psi \in L^2(\mathbb{R}^3)^4\},$$

$$\psi(x) = \sum_{j,m_j,k_j} \frac{1}{|x|}\left(f^+_{m_j,k_j}(|x|)\Phi^+_{m_j,k_j}\left(\frac{x}{|x|}\right) + f^-_{m_j,k_j}(|x|)\Phi^-_{m_j,k_j}\left(\frac{x}{|x|}\right)\right).$$

We have

$$H_{max} \cong \bigoplus_{j=\frac{1}{2},\frac{3}{2},\dots}^{\infty} \bigoplus_{m_j=-j}^{j} \bigoplus_{k_j=\pm(j+1/2)} h^*_{m_j,k_j},$$

$$h^*_{m_j,k_j}(f^+, f^-) := \begin{pmatrix} m + \frac{\nu+\mu}{r} & -\partial_r + \frac{k_j+\lambda}{r} \\ \partial_r + \frac{k_j+\lambda}{r} & -m + \frac{\nu-\mu}{r} \end{pmatrix} \begin{pmatrix} f^+ \\ f^- \end{pmatrix}.$$

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If $\boldsymbol{\delta_{k_j} \geq \frac{1}{4}}$ then $h^*_{m_j,k_j}$ is symmetric.
If $\boldsymbol{0 < \delta_{k_j} < 1/4}$ then

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

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

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

we set

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

If $\delta_{k_j} = 0$ then

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

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

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

we set

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

If $\delta_{k_j} < 0$ then

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

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

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

we set

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

For $j = \frac{1}{2}, \frac{3}{2}, \dots, \infty$; $m_j = -j, \dots, j$; $k_j = \pm(j + 1/2)$;
let $I := \{(j, m_j, k_j) : (k_j + \lambda)^2 + \mu^2 - \nu^2 < 1/4\}$ and $\boldsymbol{d} := \# I$.

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

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

Theorem ([C., Pizzichillo, 2018b])

$(\mathbb{C}^d, \Gamma^+, \Gamma^-)$ *is a boundary triple for* H_{max}.