Dirac operators with strong Coulomb singularity: domain and min-max levels

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The free Dirac operator

For $\psi \in \mathcal{C}_c^\infty((\mathbb{R}^3, \mathbb{C}^4)$, let

$$D_0 \, \psi = (-i \sum_{k=1}^{3} \alpha_k \partial_k + \beta)\psi = (-i\boldsymbol{\alpha} \cdot \nabla + \beta)\psi$$

$\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are 4×4 self-adjoint matrices satisfying the CAR

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij}, \qquad \alpha_i \beta + \beta \alpha_i = 0.$$

D_0 is symmetric for the scalar product on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, and it is essentially self-adjoint. Its closure (still denoted D_0) has domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and

$$(D_0)^2 = -\Delta + 1\,.$$

It is *unbounded from below*:

$$\sigma(D_0) = (-\infty; -1] \cup [1; +\infty).$$

Subcritical Dirac-Coulomb operators

Let us assume that $V = V_1 + V_2 + V_3$ with $V_2 \in L^3(\mathbb{R}^3, \mathbb{R})$, $V_3 \in L^\infty(\mathbb{R}^3, \mathbb{R})$ and $|V_1(x)| \le \nu/|x|$, $0 \le \nu < 1$ (subcritical potential).

For $\psi \in \mathcal{C}_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$, let $D_V\,\psi = (D_0 + V)\psi$. Then:

- D_V has a distinguished self-adjoint extension (still denoted D_V) characterized by the condition $\mathcal{D}(D_V) \subset H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$.
- Let $V_\epsilon := \min(\max(V(x), -1/\epsilon), 1/\epsilon)$. Then D_{V_ϵ} converges to D_V in the norm resolvent sense when $\epsilon \to 0$.
- If $\lim_{R\to\infty} \|V_3(x)\mathbf{1}_{|x|>R}\|_\infty = 0$, then $\sigma_{\rm ess}(D_V) = (-\infty, -1] \cup [1, \infty)$.
- If $0 \le \nu < \sqrt{3}/2$, then D_V is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$ and its closure has domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$.

These results were obtained in the 70's and early 80's (Schmincke, Wust, Nenciu, Klaus-Wust, Landgren-Rejto-Klaus, Kato).

Eigenvalues in the spectral gap

If $\nu < 1$ then $\sigma(D_{-\nu/|x|}) \cap (-1,1) = \{\mu_1 \leq \mu_2 \leq \cdots \to 1\}$ and the ground state ψ_1 is the eigenvector of eigenvalue

$$\mu_1 = \sqrt{1-\nu^2}\,.$$

More generally, when $-\nu/|x| \leq V$ and $\sup(V) < 1 + \sqrt{1-\nu^2}$ with $0 < \nu < 1$, one expects that $\sigma(D_V) \cap [\sqrt{1-\nu^2}, 1)$ is either empty, finite, or an infinite sequence of eigenvalues converging to 1.

Since D_0 is not bounded below, the standard Rayleigh-Ritz min-max characterization of these eigenvalues is not valid. This fact is a source of numerical instabilities.

Talman's principle '86

Assume that $-\frac{\nu}{|x|} \le V$ and $\sup(V) < 1 + \sqrt{1-\nu^2}$ with $0 < \nu < 1$.
Talman's claim is

$$\mu_1(V) = \inf_{\varphi \in C_c^\infty(\mathbb{R}^3,\mathbb{C}^2)\setminus\{0\}} \ \sup_{\substack{\psi = \binom{\varphi}{\chi} \\ \chi \in C_c^\infty(\mathbb{R}^3,\mathbb{C}^2)}} \frac{(\psi, D_V \psi)}{(\psi,\psi)}$$

-Proof by Griesemer-Lewis-Siedentop '99 when $-2 < V \le 0$.

-Proof by Dolbeault, Esteban, S. '00 when $\nu < \frac{\sqrt{3}}{2}$. The proof was incomplete when $\frac{\sqrt{3}}{2} \le \nu < 1$.

-Proof by Morozov-Müller '15 when $0 < \nu < 1$ with C_c^∞ replaced by $H^{1/2}$.

Abstract min-max principle (Dolbeault-Esteban-S. 00')

Let $\mathcal{H}$ be a Hilbert space and $A : \mathcal{D}(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator.

Let F be a core, i.e. a dense subspace of $\mathcal{D}(A)$ for the norm $\| \cdot \|_{\mathcal{D}(A)}$.

Let $\mathcal{H}_\pm = \Lambda_\pm \mathcal{H}$ be two orthogonal subspaces of $\mathcal{H}$, with $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$.

Define $F_\pm := \Lambda_\pm F$. Assume that each $F_\pm$ is in $\mathcal{D}(|A|^{1/2})$ and that:

(i) $a_- := \sup_{x_- \in F_- \setminus \{0\}} \frac{(x_-, A x_-)}{\|x_-\|^2_{\mathcal{H}}} < +\infty$.

Let

$$\lambda_k = \inf_{\substack{V \text{ subspace of } F_+ \\ \dim V = k}} \sup_{x \in (V \oplus F_-) \setminus \{0\}} \frac{(x, Ax)}{||x||^2_{\mathcal{H}}}, \qquad k \geq 1.$$

If:

(ii) $\lambda_1 > a_-$

then λ_k is the k-th eigenvalue μ_k of A in the interval (a_-, b) if it exists, where $b = \inf\ (\sigma_{\mathrm{ess}}(A) \cap (a_-, +\infty))$.

Application to D_V

Assume $-\frac{\nu}{|x|} \leq V$ and $\sup(V) < 1 + \sqrt{1-\nu^2}$ with $0 < \nu < 1$. Let
$\Lambda_+ \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \varphi \\ 0 \end{pmatrix}$, $\Lambda_- \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} 0 \\ \chi \end{pmatrix}$.

The subspace $F = C_c^\infty(\mathbb{R}^3, \mathbb{C}^4)$ is a core when $\nu < \frac{\sqrt{3}}{2}$, but in general it is **not** a core when $\frac{\sqrt{3}}{2} \leq \nu < 1$.

Assumption (i) is easily checked, with $a_- < \sqrt{1-\nu^2}$.

Assumption (ii) is a consequence of the inequality

$$q_{\sqrt{1-\nu^2}}(\varphi) \geq 0 \,, \quad \forall \varphi \in C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2) \,, \quad \forall \nu \in [0,1]$$

where

$$q_E(\varphi) := \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \varphi(x)|^2}{1 - V(x) + E} \, dx + \int_{\mathbb{R}^3} (1 + V(x) - E) |\varphi(x)|^2 \, dx \,.$$

This inequality can be proved by a regularization and continuation argument, or more directly by expressing q_E as a sum of "squares", as done by Dolbeault-Esteban-Loss-Vega '04.

Another construction of the distinguished extension (Esteban-Loss '07)

Assume $-\frac{\nu}{|x|} \leq V$ and $\sup(V) < 1 + \sqrt{1-\nu^2}$ with $0 < \nu \leq 1$. Then the norms q_E, $-1 + \sup(V) < E < \sqrt{1-\nu^2}$, are all equivalent on $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$.

Let $\mathcal{H}_{+1}$ be the closure of $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$ for one of these norms. Let D_V^* be the adjoint of the minimal operator D_V. Here, minimal means with domain $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$. Let

$$\mathcal{D} := \left\{ \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in \mathcal{H}_{+1} \times L^2(\mathbb{R}^3, \mathbb{C}^2) \ : \ D_V^* \psi \in L^2(\mathbb{R}^3, \mathbb{C}^4) \right\} .$$

Then the restriction of D_V^* to $\mathcal{D}$ is a self-adjoint extension of the minimal operator D_V. Moreover, when $\nu < 1$, it coincides with the distinguished self-adjoint extension. In other words, $\mathcal{D} \subset H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ when $\nu < 1$.

A density result when $\nu < 1$ (Esteban-Lewin-S. '17)

Assume that

$$V(x) \geq -\frac{1}{|x|} \quad \text{and} \quad \sup(V) < 2$$

and let

$$\mathcal{V} = \Big\{ \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \cap H^1_{\rm loc}(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2) \ : \\ (2-V)^{-1/2} \sigma \cdot \nabla \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \Big\}. \quad (1)$$

Then $C^\infty_c(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$ is dense in $\mathcal{V}$ for the norm

$$\|\varphi\|_{\mathcal{V}} := \|(2-V)^{-1/2} \sigma \cdot \nabla \varphi\|_{L^2} + \|\varphi\|_{L^2} \, .$$

In addition, we have the continuous embedding $\mathcal{V} \subset H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$.

A variant of the Esteban-Loss construction when $\nu < 1$ (Esteban-Lewin-S. '17)

Assume that for some $0 \leq \nu < 1$

$$V(x) \geq -\frac{\nu}{|x|} \qquad \text{and} \qquad \sup(V) < 1 + \sqrt{1-\nu^2}.$$

Then the distinguished self-adjoint extension of the minimal operator D_V is also the unique extension with domain included in

$$\left\{\psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{V}\right\}.$$

More precisely, the domain of this extension is

$$\mathcal{D} = \left\{\psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{V},\ D_V^*\psi \in L^2(\mathbb{R}^3, \mathbb{C}^4)\right\}.$$

The case $\nu = 1$ (Esteban-Lewin-S. '17)

In the Coulomb case $V(x) = -|x|^{-1}$ we introduce

$$\mathcal{W}_{\mathrm{C}} = \left\{ \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \ : \ \frac{\sigma \cdot \nabla |x| \varphi}{|x|^{1/2}(1+|x|)^{1/2}} \in L^2(\mathbb{R}^3, \mathbb{C}^2) \right\}. \quad (2)$$

Then we assume that $V(x) \geq -|x|^{-1}$ and that $\sup(V) < 1$ and we introduce the space

$$\mathcal{W} = \left\{ \varphi \in \mathcal{W}_{\mathrm{C}} \ : \ \left(\frac{1}{1 - V(x)} - \frac{|x|}{1+|x|} \right)^{1/2} \sigma \cdot \nabla \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2), \right.$$
$$\left. \left(V(x) + \frac{1}{|x|} \right)^{1/2} \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \right\}. \quad (3)$$

Density in the case $\nu = 1$ (Esteban-Lewin-S. '17)

We assume that

$$V(x) \geq -\frac{1}{|x|} \qquad \text{and} \qquad \sup(V) < 1.$$

Then the space $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^2)$ is dense in $\mathcal{W}_{\rm C}$ and in $\mathcal{W}$ for their respective norms. Also, we have the continuous embeddings

$$\mathcal{W} \subset \mathcal{W}_{\rm C} \subset H^s(\mathbb{R}^3, \mathbb{C}^2)$$

for every $0 \leq s < 1/2$.

A variant of Esteban-Loss in the critical case (Esteban-Lewin-S. '17)

Assume that $V(x) \geq -\frac{1}{|x|}$ and $\sup(V) < 1$. Then:

(a) The minimal operator D_V has a unique self-adjoint extension with domain $\mathcal{D}$ satisfying $\mathcal{D} \subset \left\{ \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{W} \right\}$ and we have

$$\mathcal{D} = \left\{ \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^4) \ : \ \varphi \in \mathcal{W}, \ D_V^* \psi \in L^2(\mathbb{R}^3, \mathbb{C}^4) \right\}.$$

(b) Let $V_\epsilon(x) := \max(V(x), -1/\epsilon)$ or $V_\epsilon = (1-\epsilon)V$. Then the distinguished self-adjoint extension D_{V_ϵ} converges in the norm resolvent sense to the distinguished extension D_V defined in the previous item.

(c) If $V = -\frac{1}{|x|}$, the distinguished extension is the only extension such that $|x|\psi \in L^\infty(\mathbb{R}^3)$, for any eigenvector ψ of D_V.

Definition of the min-max levels

We introduce the two projections

$$\Lambda_T^+ \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \varphi \\ 0 \end{pmatrix}, \qquad \Lambda_T^- \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} 0 \\ \chi \end{pmatrix}$$

corresponding to the Talman decomposition, and the spectral projections

$$\Lambda_0^+ = \mathbb{1}(D_0 \geq 0), \qquad \Lambda_0^- = \mathbb{1}(D_0 \leq 0)$$

of the free Dirac operator. For a space $F \subseteq H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, we define the min-max levels

$$\lambda_{T/0,F}^{(k)} = \inf_{\substack{W \text{ subspace of } \Lambda_{T/0}^+ F \\ \dim W = k}} \sup_{\substack{\psi \in W \oplus \Lambda_{T/0}^- F \\ \psi \neq 0}} \frac{\langle \psi, D_V \psi \rangle}{\|\psi\|_{L^2}^2}, \qquad k \geq 1. \tag{4}$$

Min-max: freedom in the choice of F and critical case (Esteban-Lewin-S. '17)

Assume that $V(x) \geq -\frac{\nu}{|x|}$ and $\sup(V) < 1 + \sqrt{1-\nu^2}$ with $0 < \nu \leq 1$.

Take a subspace F such that $C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4) \subseteq F \subseteq H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$.

Then, the number $\lambda^{(k)}_{T,F}$ defined in (4), is independent of the subspace F. Moreover, if the distinguished self-adjoint extension D_V has at least k eigenvalues $\mu_1 \leq \cdots \leq \mu_k$ in $[\sqrt{1-\nu^2}, b)$ counted with multiplicity, with $b = \min(\sigma_{ess}(D_V) \cap [\sqrt{1-\nu^2}, \infty))$, then $\lambda^{(k)}_{T,F} = \lambda^{(k)}_{0,F} = \mu_k$. Otherwise $\lambda^{(k)}_{T,F} = \lambda^{(k)}_{0,F} = b$.

Method of proof: For $F = C_c^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$, apply the abstract theorem of Dolbeault-Esteban-S. to D_{V_ϵ}, then pass to the limit $\epsilon \to 0$ using the norm-resolvent convergence. For other subspaces F and $\lambda^{(k)}_{T,F}$, use the density results given above. For $\lambda^{(k)}_{0,F}$, just use the density of C_c^∞ in $H^{1/2}$.

THANK YOU!