Self-adjoint extensions of Dirac operators via Hardy-like inequalities

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In the units in which both the speed of light c and Planck's constant $\hbar$ are equal to 1, the Dirac operator in the presence of an external electrostatic potential V is given by

$$H_0 + V \quad \text{with} \quad H_0 := -i\,\alpha \cdot \nabla + \beta\ .$$

$\alpha_1, \alpha_2, \alpha_3$ and β are 4×4 complex matrices, whose standard form (in 2×2 blocks) is

$$\beta = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}, \quad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \qquad (k = 1, 2, 3)\ ,$$

where $\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ 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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For $\nu \in (0, \pi/2]$ one can use the pseudo-Friedrich extension method to define an extension which satisfies

$$\mathcal{D}(H_0 + V) \subset \mathcal{D}(|H_0|^{1/2}) = H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)\,.$$

This result is obtained by using Kato's inequality :

$$|H_0| \geq \frac{2}{\pi|x|}\,.$$

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Actually one can prove that $H_0 - \frac{\nu}{|x|}$ defined on $C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)$ is essentially self-adjoint iff $\nu < \sqrt{3}/2$ (Schmincke, 1972).

Case $\nu < 1$

– Various works of Schmincke and Wüst show “basically" (some other technical assumptions made) that if

$$\sup_{x \neq 0} |x|\,|V(x)| < 1\,,$$

there is a distinguished self-adjoint extension of T characterized by the fact that the domain is contained in $D(T^*) \cap D(r^{-1/2})$.

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– In 1978, Klaus and Wüst proved that the above extensions coincide.

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$$-\Delta \geq \frac{(N-2)^2}{4\,|x|^2}\,,$$

marks the limit for self-adjointness : one can find a distinguished self-adjoint extension for the operator $-\Delta - \frac{\mu}{|x|^2}{}_{|C_0^\infty(\mathbb{R}^3)}$ iff $\mu \leq \frac{(N-2)^2}{4}$.

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But in the case of the Dirac operator, $H_0 + V$ is not bounded below for any potential V, even for $V = 0$. Hence the corresponding quadratic form is never semi-definite nonnegative.

Hardy inequality for Dirac operators I

BUT there is a Hardy-like inequality for the Dirac operator as follows : for all $\varphi \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$,

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \frac{1}{|x|}} \; + \; |\varphi|^2 \right) dx \; \geq \; \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \; .$$

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There are two proofs for it :

(1) (Dolbeault-E.-Séré , 2000) : If

$$\lim_{|x| \to +\infty} V(x) = 0 \quad \text{and} \quad -\frac{\nu}{|x|} - c_1 \leq V \leq \Gamma = \sup(V) \; ,$$

with $\nu \in (0,1)$, $c_1, \Gamma \geq 0$, $c_1 + \Gamma - 1 < \sqrt{1 - \nu^2}$. Then,

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \lambda_1(V) - V} \; + \; \big(1 - \lambda_1(V) + V\big) \, |\varphi|^2 \right) dx \; \geq \; 0 \; ,$$

where $\lambda_1(V)$ denotes the smallest eigenvalue of $H_0 + V$ in the spectral gap $(-1, 1)$.

Hardy inequality for Dirac operators II

We apply the above to the potentials $V_\nu := -\nu/|x|\,,\ \nu \in (0,1)$. We get :

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\varphi|^2}{1+\sqrt{1-\nu^2}+\frac{\nu}{|x|}} \ + \ \left(1-\sqrt{1-\nu^2}\right)|\varphi|^2 \right) dx \ \geq \ \nu \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|}\, dx \ ,$$

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CONSEQUENCE : nonnegativity of the quadratic form

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}\varphi|^2}{1+\frac{1}{|x|}} \ + \ \left(1-\frac{1}{|x|}\right)\,|\varphi|^2 \right) dx \ .$$

Hardy inequality for Dirac operators with magnetic fields

Note that the above type of inequalities also hold in the case on an external magnetic field B with associated potential A : for all $\varphi \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$, for $V_\nu := -\nu/|x|\,, \;\; \nu \in (0,1)$,

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot (\boldsymbol{\nabla} - iA)\,\varphi|^2}{1 + \lambda_1^A(V_\nu) - V_\nu} \; + \; \big(1 - \lambda_1^A(V_\nu) + V_\nu\big)\,|\varphi|^2 \right) dx \;\geq\; 0\;,$$

where $\lambda_1^A(V_\nu)$ denotes the smallest eigenvalue of the magnetic Dirac-Coulomb operator

$$H_0^A + V_\nu \;= -i\,\alpha \cdot (\nabla - iA) + \beta - \nu/|x|$$

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Remark. For very intense magnetic fields, and even if ν is very small, $\lambda_1^A(V_\nu)$ can leave the gap $(-1,1)$ and then the inequality is not true anymore.

Some definitions I

Assumption (A) : $V \in L^2_{\mathrm{loc}}\mathbb{R}^3, \mathbb{R})$ is a function such that for some constant $c(V) \in (-1,1)$, $\Gamma := \sup_{\mathbb{R}^3} V < 1 + c(V)$ and for every $\varphi \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$,

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(The potentials $V_\nu := -\nu/|x|$, $\quad \nu \in (0, 1]$ satisfy the above assumption with $c(V_\nu) = \sqrt{1 - \nu^2}$)

For any γ in $(\Gamma, 1 + c(V))$, consider the quadratic form

$$b_\gamma(\varphi, \varphi) := \int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}\varphi|^2}{\gamma - V} \ + \ \big(2 - \gamma + V\big)\, |\varphi|^2 \right) dx$$

defined on $C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$. Note that by assumption **(A)**, this quadratic form is nonnegative and symmetric on $C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$. Therefore it is closable and we denote its closure by $\widehat{b}_\gamma$ and its form domain by $\mathcal{H}^\gamma_{+1}$.

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Definition : We denote by S_γ the unique selfadjoint operator associated with $\widehat{b}_\gamma$: for all $\varphi \in D(S_\gamma) \subset \mathcal{H}^\gamma_{+1}$,

$$\widehat{b}_\gamma(\varphi, \varphi) = (\varphi, S_\gamma \varphi) \; .$$

Some definitions II

S_γ is an isometric isomorphism from $\mathcal{H}^\gamma_{+1}$ to its dual $\mathcal{H}^\gamma_{-1}$.

Moreover, $\mathcal{H}^\gamma_{+1}$ is the operator domain of $S_\gamma^{1/2}$, and for all $\varphi \in \mathcal{H}^\gamma_{+1}$,

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$$(2 - \gamma + V)\varphi - i\sigma \cdot \nabla\chi \, , \qquad -i\sigma \cdot \nabla\varphi + (V - \gamma)\chi \; \in \; L^2(\mathbb{R}^3, \mathbb{C}^2) \; .$$

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The meaning of these two expressions is in the weak sense, i.e., the linear functional $(\eta, (2 - \gamma + V)\varphi) + (-i\sigma \cdot \nabla\eta, \chi)$, which is defined for all test functions, extends uniquely to a bounded linear on $L^2(\mathbb{R}^3, \mathbb{C}^2)$: $\forall \eta \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)$,

$$\exists\, C > 0, \ |(\eta, (2 - \gamma + V)\varphi) + (-i\sigma \cdot \nabla\eta, \chi)| \leq C\, ||\eta||_{L^2(\mathbb{R}^3, \mathbb{C}^2)} \ .$$

Likewise the same for $(\eta, (V - \gamma)\chi) + (-i\sigma \cdot \nabla\eta, \varphi)$. From this definition it is clear that the domain does not depend on γ.

Main theorem

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Because formally they are the two components of the operator $H_0 + V + (1-\gamma)$, since $H_0 + V$ acts on smooth functions $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ as :

$$(H_0 + V)\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} (V+1)\varphi - i\sigma\cdot\nabla\chi \\ -i\sigma\cdot\nabla\varphi + (V-1)\chi \end{pmatrix}$$

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Theorem : If V satisfies Assumption **(A)**, the operator H_0+V defined on $\mathcal{D}$ is self-adjoint. And it is the unique self-adjoint extension of $T := H_0 + V_{|C_0^\infty(\mathbb{R}^3,\mathbb{C}^4)}$ such that the domain is contained in $\mathcal{H}_{+1}\times L^2(\mathbb{R}^3,\mathbb{C}^2)$.

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Proposition : When $\nu\in(0,1)$, our extension coincides with those of Schmincke, Wüst and Nenciu and in this case, $\mathcal{D}\subset H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$.

Intermediate results I

Proposition : Under assumption **(A)** on the potential V,

$$\mathcal{H}_{+1} \subset \left\{ \varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2) \,:\, \frac{-i\sigma \cdot \nabla\varphi}{\gamma - V} \in L^2(\mathbb{R}^3, \mathbb{C}^2) \right\},$$

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where $\nabla \varphi$ denotes the distributional gradient of φ. Therefore, we have the 'scale of spaces' $\mathcal{H}_{+1} \subset L^2(\mathbb{R}^3, \mathbb{C}^2) \subset \mathcal{H}_{-1}$.

Idea of proof : If $\delta := \frac{(\gamma - \Gamma)(1 + c(V) - \gamma)}{1 + c(V) - \Gamma}$ (> 0),

$$b_\gamma(\varphi, \varphi) \geq \delta \int_{\mathbb{R}^3} |\varphi|^2 \, dx + \delta \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla \varphi|^2}{(\gamma - V)^2} \, dx \ ,$$

Intermediate results II

Proposition : For any F in $L^2(\mathbb{R}^3, \mathbb{C}^2)$ and for any $\gamma \in (\Gamma, 1 + c(V))$,

$$-i\sigma \cdot \nabla \left(\frac{F}{\gamma - V} \right) \in \mathcal{H}_{-1} \ ,$$

where, once again, the gradient is to be interpreted in the distributional sense.

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Idea of proof : By the definition of the distributional derivative, for every $\eta \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^2)$,

$$\left| \left(-i\sigma \cdot \nabla\eta, \frac{F}{\gamma - V} \right) \right| = \left| \left(\frac{-i\sigma \cdot \nabla\eta}{\gamma - V}, F \right) \right| \leq \|\eta\|_{\mathcal{H}_{+1}} \, \|F\|_2 \ . \tag{2}$$

Hence, the linear functional

$$\eta \to \left(-i\sigma \cdot \nabla\eta, \frac{F}{\gamma - V} \right) \tag{2}$$

extends uniquely to a bounded linear functional on $\mathcal{H}_{+1}$.

Proof of main theorem : symmetry

We have to prove that for both pairs (φ, χ), $(\tilde\varphi, \tilde\chi)$ in the domain,

$$\left((H_0 + V + 1 - \gamma) \begin{pmatrix} \varphi \\ \chi \end{pmatrix} , \begin{pmatrix} \tilde\varphi \\ \tilde\chi \end{pmatrix} \right) = (\,(V-\gamma)\chi - i\sigma\cdot\nabla\varphi, \tilde\chi\,) + (\,(2-\gamma+V)\varphi - i\sigma\cdot\nabla\chi, \tilde\varphi\,)$$

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We use the above propositions to show symmetry as follows : for $\varphi, \tilde{\varphi}$ smooth,

$$\left((H_0 + V + 1 - \gamma) \begin{pmatrix} \varphi \\ \chi \end{pmatrix}, \begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix} \right) = (S_\gamma \varphi, \tilde{\varphi}) + \left((V - \gamma) \left[\chi + \frac{-i\sigma \cdot \nabla\varphi}{V - \gamma} \right], \left[\tilde{\chi} + \frac{-i\sigma \cdot \nabla\tilde{\varphi}}{V - \gamma} \right] \right).$$

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and both expressions are continuous in $\varphi, \tilde{\varphi}$ with respect to the $\mathcal{H}_{+1}$-norm. So we can pass to the limit and so prove symmetry.

Proof of main theorem : surjectivity

For any F_1, F_2 in $L^2(\mathbb{R}^3, \mathbb{C}^2)$, there exists $\begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in \mathcal{D}$ such that

$$(H_0 + V + 1 - \gamma) \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} (V + 2 - \gamma)\varphi - i\sigma \cdot \nabla\chi \\ -i\sigma \cdot \nabla\varphi + (V - \gamma)\chi \end{pmatrix} = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}$$

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Since S_γ is an isomorphism, there exists a unique φ in $\mathcal{H}_{+1}$ such that

$$S_\gamma \varphi = F_1 - i\sigma \cdot \nabla \left(\frac{F_2}{\gamma - V} \right) .$$

Indeed, F_1 is in $L^2(\mathbb{R}^3, \mathbb{C}^2)$ and therefore in $\mathcal{H}_{-1}$. Moreover the second term is also in $\mathcal{H}_{-1}$ by the above proposition. Next define χ by

$$\chi = \frac{-F_2 - i\sigma \cdot \nabla\varphi}{\gamma - V} \quad \Longleftrightarrow \quad (V - \gamma)\chi - i\sigma \cdot \nabla\varphi = F_2$$

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End of the proof of surjectivity

$$F_1 = S_\gamma \varphi - i\sigma \cdot \nabla \left(\chi + \frac{i\sigma \cdot \nabla \varphi}{\gamma - V} \right)$$

is equivalent to : for all smooth η,

$$\begin{aligned}
(\eta, F_1) &= (\eta, S_\gamma \varphi) + \big(-i\sigma \cdot \nabla \eta,\ \chi + \frac{i\sigma \cdot \nabla \varphi}{\gamma - V} \big) \\
&= (S_\gamma \eta, \varphi) + \big(-i\sigma \cdot \nabla \eta, \frac{i\sigma \cdot \nabla \varphi}{\gamma - V} \big) + (-i\sigma \cdot \nabla \eta, \chi) \\
&= \big(S_\gamma \eta - i\sigma \cdot \nabla \big(\frac{i\sigma \cdot \nabla \eta}{\gamma - V} \big), \varphi \big) + (-i\sigma \cdot \nabla \eta, \chi) \\
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&= ((V + 2 - \gamma)\eta, \varphi) + (-i\sigma \cdot \nabla \eta, \chi)
\end{aligned}$$

and in the weak sense, this means that

$$F_1 = (V + 2 - \gamma)\varphi - i\sigma \cdot \nabla \chi$$

Proof of main theorem : injectivity + uniqueness of the extension

Assuming that $(H_0 + V + 1 - \gamma) \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and since

$\chi = \frac{-F_2 - i\sigma \cdot \nabla \varphi}{\gamma - V}$ and $S_\gamma \varphi = F_1 - i\sigma \cdot \nabla \left(\frac{F_2}{\gamma - V} \right)$,

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It remains to show the uniqueness part in our theorem. Assume that $C_c^\infty(\mathbb{R}^3, \mathbb{C}^4) \subset \hat{\mathcal{D}}$ is another selfadjoint extension such that whenever $(\varphi, \chi) \in \hat{\mathcal{D}}$, $\varphi \in \mathcal{H}_{+1}$. Since $H_0 + V$ is selfadjoint on this domain, for all $(\tilde\varphi, \tilde\chi) \in C_c^\infty(\mathbb{R}^3, \mathbb{C}^4)$

$$\left(\begin{pmatrix} \tilde\varphi \\ \tilde\chi \end{pmatrix},\ (\,H_0 + V + 1 - \gamma\,)\begin{pmatrix} \varphi \\ \chi \end{pmatrix}\right) = \left((\,H_0 + V + 1 - \gamma\,)\begin{pmatrix} \tilde\varphi \\ \tilde\chi \end{pmatrix},\ \begin{pmatrix} \varphi \\ \chi \end{pmatrix}\right)$$

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$$\left(\begin{pmatrix}\tilde\varphi \\ \tilde\chi\end{pmatrix},\; (\,H_0 + V + 1 - \gamma\,)\begin{pmatrix}\varphi \\ \chi\end{pmatrix}\right) = \left((\,H_0 + V + 1 - \gamma\,)\begin{pmatrix}\tilde\varphi \\ \tilde\chi\end{pmatrix},\; \begin{pmatrix}\varphi \\ \chi\end{pmatrix}\right)$$

$$= \left(\begin{pmatrix}(V + 2 - \gamma)\tilde\varphi - i\sigma\cdot\nabla\tilde\chi \\ -i\sigma\cdot\nabla\tilde\varphi + (V - \gamma)\tilde\chi\end{pmatrix},\; \begin{pmatrix}\varphi \\ \chi\end{pmatrix}\right) = \left\langle\begin{pmatrix}\tilde\varphi \\ \tilde\chi\end{pmatrix}, \begin{pmatrix}(V + 2 - \gamma)\varphi - i\sigma\cdot\nabla\chi \\ -i\sigma\cdot\nabla\varphi + (V - \gamma)\chi\end{pmatrix}\right\rangle_{C_0^\infty, (C_0^\infty)'}$$

Thus, $\hat{\mathcal{D}} \subset \mathcal{D}$ and hence $\hat{\mathcal{D}} = \mathcal{D}$.

Remark about the finiteness of the energy

In the limit case $V(x) = -\frac{1}{|x|}$, the domain $\mathcal{D}$ is not contained anymore in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, but the total energy is still finite :

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \frac{1}{|x|}} \; + \; (1 - \frac{1}{|x|}) \, |\varphi|^2 \right) dx \; < \; +\infty$$

even if

$$\int_{\mathbb{R}^3} \frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \frac{1}{|x|}} \; dx \quad , \qquad \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \; = \; +\infty$$

THE END