Hardy inequalities and Dirac Operators

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Results in collaboration with: M. J. Esteban, E. Séré, M. Loss $\frac{\text{STANDARD HARDY INEQUALITY}}{\text{Let } u \in H^1(\mathbb{R}^N) \text{ and consider}}$

$$\int_{\mathbb{R}^N} \left| \nabla u + \frac{N-2}{2} \frac{x}{|x|^2} u \right|^2 dx \ge 0.$$

Develop this square and integrate by parts using the identity $\nabla \cdot \left(\frac{x}{|x|^2}\right) = \frac{N-2}{|x|^2}$

$$\int_{\mathbb{R}^N} |\nabla u|^2 \, dx \ge \frac{1}{4} (N-2)^2 \, \int_{\mathbb{R}^N} \frac{|u|^2}{|x|^2} \, dx$$

It is optimal (take appropriate truncations of $x \mapsto |x|^{-(N-2)/2}$): the operator $-\Delta - \frac{A}{|x|^2}$ is nonnegative if and only if $A \leq \frac{1}{4}(N-2)^2$. Optimality has to be taken with care: improvements with l.o.t. in L^2 by Brezis-Vazquez, in $W^{1,q}$ with q < 2 by Vazquez-Zuazua, and logarithmic terms by Adimurthi & al. N = 3 from now on.

Some notations

Free Dirac operator:

 $H_{0} = -i \alpha \cdot \nabla + \beta, \quad \text{with } \alpha_{1}, \ \alpha_{2}, \ \alpha_{3}, \ \beta \in \mathcal{M}_{4 \times 4}(\mathbb{C})$ $\beta = \begin{pmatrix} \mathbb{I} & 0\\ 0 & -\mathbb{I} \end{pmatrix}, \ \alpha_{i} = \begin{pmatrix} 0 & \sigma_{i}\\ \sigma_{i} & 0 \end{pmatrix}$

Pauli matrices:

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

Decomposition into upper / lower component: $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$

$$H_0 \Psi = \begin{pmatrix} R\chi + \varphi \\ R\varphi - \chi \end{pmatrix}$$
, with $R = -i \sigma \cdot \nabla$

Two of the main properties of H_0 are:

$$H_0^2 = -\Delta + 1$$

and

$$\sigma(H_0) = (-\infty, -1] \cup [1, +\infty) .$$

Denote by Y^{\pm} the spaces $\Lambda^{\pm}(H^{1/2}(\mathbb{R}^3, \mathbb{C}^4))$, where Λ^{\pm} are the positive and negative spectral projectors on $L^2(\mathbb{R}^3, \mathbb{C}^4)$ corresponding to the free Dirac operator: Λ^+ and $\Lambda^- = \mathbb{I}_{L^2} - \Lambda^+$ have both infinite rank and satisfy

$$H_0 \Lambda^+ = \Lambda^+ H_0 = \sqrt{1 - \Delta} \Lambda^+ = \Lambda^+ \sqrt{1 - \Delta} ,$$
$$H_0 \Lambda^- = \Lambda^- H_0 = -\sqrt{1 - \Delta} \Lambda^- = -\Lambda^- \sqrt{1 - \Delta} .$$
With $R = -i \sigma \cdot \nabla$, $R^2 = -\Delta$.

4

HARDY INEQUALITY FOR THE OPERATOR R

Proposition 1 With the above notations, for any $\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$,

$$\int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1 + \frac{1}{|x|}} \, dx \, + \, \int_{\mathbb{R}^3} |\varphi|^2 \, dx \, \ge \, \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx$$

This is a consequence of the following inequality, which is slightly more general: for all $\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$ and all $\nu \in (0, 1]$,

$$\nu \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} + \sqrt{1 - \nu^2} \int_{\mathbb{R}^3} |\varphi|^2 \le \int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{\frac{\nu}{|x|} + 1 + \sqrt{1 - \nu^2}} + \int_{\mathbb{R}^3} |\varphi|^2$$

Replace
$$\varphi(x)$$
 by $\varphi\left(rac{x}{\mu}
ight)$ and let $\mu
ightarrow 0$.

$$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} dx \le \int_{\mathbb{R}^3} |x| |(\sigma \cdot \nabla) \varphi|^2 dx \quad \text{for all} \quad \varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$$

Actually, taking $\phi = |x|^{1/2} \varphi$, this inequality has to be directly related to the standard Hardy inequality

$$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} = \int_{\mathbb{R}^3} \frac{|\phi|^2}{|x|^2} \le 4 \int_{\mathbb{R}^3} |\nabla \phi|^2 = 4 \int_{\mathbb{R}^3} \left| |x|^{1/2} \nabla \phi + \frac{1}{2} \frac{x}{|x|^{3/2}} \phi \right|^2$$
$$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} dx \le \int_{\mathbb{R}^3} |x| |\nabla \varphi|^2 dx$$

6

CONNECTION WITH THE SPECTRUM OF THE DIRAC OPERATOR

Let $\lambda_1(V)$ be the lowest eigenvalue of $H_0 + V$ in the gap (-1, 1) of the continuous spectrum of $H_0 + V$ (under appropriate assumptions on V). Let $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$ be the corresponding eigenfunction. $(H_0 + V)\Psi = \lambda_1(V)\Psi$ means, for $R = -ic(\sigma \cdot \nabla)$

$$\begin{cases} R\chi = (\lambda_1(V) - c^2 - V)\varphi \\ R\varphi = (\lambda_1(V) + c^2 - V) \chi \end{cases}$$

which can be solved by

$$\begin{cases} \chi = (\lambda_1(V) + c^2 - V)^{-1} R \varphi \\ R \left(\frac{R \varphi}{\lambda_1(V) + c^2 - V} \right) = (\lambda_1(V) - c^2 - V) \varphi \end{cases}$$

Multiplying by φ and integrating with respect to $x \in \mathbb{R}^3$, we get :

$$\int_{\mathbb{R}^3} \frac{|R \varphi|^2}{\lambda_1(V) + c^2 - V} \, dx + \int_{\mathbb{R}^3} V |\varphi|^2 \, dx + (c^2 - \lambda_1(V)) \int_{\mathbb{R}^3} |\varphi|^2 \, dx = 0$$

Note that for any fixed ϕ

$$\lambda \mapsto \int_{\mathbb{R}^3} \frac{|R\phi|^2}{\lambda + c^2 - V} \, dx + \int_{\mathbb{R}^3} V|\phi|^2 \, dx \, + (c^2 - \lambda) \int_{\mathbb{R}^3} |\phi|^2 \, dx$$

is monotone decreasing. We shall see that $\lambda_1(V)$ and ϕ can be characterized as follows

$$\begin{split} \lambda_1(V) \text{ is the smallest } \lambda \text{ for which} \\ \int_{\mathbb{R}^3} \frac{|R\phi|^2}{\lambda + c^2 - V} \, dx + \int_{\mathbb{R}^3} V|\phi|^2 \, dx \, + (c^2 - \lambda) \int_{\mathbb{R}^3} |\phi|^2 \, dx \geq 0 \,\,\forall \phi \\ \text{ and } \varphi \text{ is the corresponding optimal function.} \end{split}$$

The generalized Hardy inequality is recovered with $\lambda = \sqrt{1 - \nu^2}$.

OTHER STANDARD HARDY TYPE INEQUALITIES

Define the spectral projectors:

 $\Lambda^{+} = \chi_{(0,+\infty)}(H_{0}) \text{ and } \Lambda^{-} = \chi_{(-\infty,0)}(H_{0})$ Using the Fourier transform $u(x) \mapsto \hat{u}(\xi)$, we get $\hat{H}_{0} = i \alpha \cdot \xi + \beta, \quad \hat{H}_{0}^{2} = |\xi|^{2} + 1,$ $H_{0}^{2} = -\Delta + 1.$ 1) Using $-\Delta \geq \frac{1}{4} \frac{1}{|x|^{2}}$ (Hardy inequality), $|H_{0}| = \Lambda^{+}H_{0}\Lambda^{+} - \Lambda^{-}H_{0}\Lambda^{-}$ satisfies

$$|H_0| \ge \frac{\kappa}{|x|} \quad \kappa = \frac{1}{2}$$

 $Z \alpha \leq \kappa$ with $\alpha^{-1} = 137.037...$ means $Z \leq 68$.

2) Kato's inequality.

$$|H_0| \ge \frac{\kappa}{|x|}$$
 $\kappa = \frac{2}{\pi} = 0.63662...$

 $Z \alpha \leq \kappa$ means $Z \leq 87$. Optimal [Herbst]. 3) An inequality for the Brown & Ravenhall operator [Burenkov, Evans, Perry, Siedentop, Tix]:

$$B := \Lambda^+ \left(H_0 - \frac{\kappa}{|x|} \right) \Lambda^+ \ge 0 \quad \kappa = \frac{2}{\frac{2}{\pi} + \frac{\pi}{2}} = 0.906037...$$

B was introduced by Bethe and Salpeter. κ is sharp. $Z\,\alpha \leq \kappa$ means $Z \leq 124.$

MIN-MAX CHARACTERIZATION OF THE DISCRETE SPECTRUM

Kato's inequality and related inequalities have no evident relation with the spectrum of H_0 : $\nu = \frac{2}{\pi}$ or $\nu = \frac{2}{2/\pi + \pi/2}$ are not critical for the (point) spectrum of $H_0 - \frac{\nu}{|x|}$. The operator

$$H_{\nu} := H_0 - \frac{\nu}{|x|}, \quad 0 < \nu < 1$$

has a self-adjoint extension with domain included in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and its spectrum is given by

$$\sigma(H_{\nu}) = (-\infty, -1] \cup \{\lambda_1^{\nu}, \lambda_2^{\nu}, \ldots\} \cup [1, \infty), \quad \lim_{\nu \to 1} \lambda_1^{\nu} = 0.$$

 H_{ν} is self-adjoint only for $\nu < 1$. The notion of "first eigenvalue" in (-1, 1) does not make sense for $\nu \ge 1$.

Assume that $V \in M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and $\exists \delta > 0$ such that

(*H*) $\pm \Lambda^{\pm} (H_0 + V) \Lambda^{\pm} \ge \delta \Lambda^{\pm} \sqrt{1 - \Delta} \Lambda^{\pm}$ in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ With $Y^{\pm} = \Lambda^{\pm} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$, define



Theorem 1 [J.D., Esteban, Séré] Under assumption (H), if $V \in L^{\infty}(\mathbb{R}^3 \setminus \overline{B}_{R_0})$ for some $R_0 > 0$ is such that $\lim_{R \to +\infty} \|V\|_{L^{\infty}(|x|>R)} = 0$, $\lim_{R \to +\infty} \sup_{|x|>R} V(x)|x|^2 = -\infty$, then $\{c_k(V)\}_{k\geq 1}$ is the non-decreasing sequence of eigenvalues of $H_0 + V$ in the interval [0, 1), counted with multiplicity, and

$$0 < \delta \le c_1(V) = \lambda_1(V) \le \dots c_k(V) = \lambda_k(V) \le \dots \le 1, \lim_{k \to +\infty} c_k(V) = 1$$

Griesemer and Siedentop proved an abstract result which implies the above min-max characterization for the eigenvalues of H_0 + V for a certain class of potentials V (which does not include singularities close to the Coulombic ones). This has

Remark. Any potential V such that $|V| \le a|x|^{-\beta} + C$ belongs to $M^3(\mathbb{R}^3) + L^{\infty}(\mathbb{R}^3)$ for all $a, C > 0, \beta \in (0, 1)$. If $|V| \le a|x|^{-1}$, then (H) is satisfied if $a < 2/(\pi/2 + 2/\pi) \approx 0.9$. Moreover, any $V \in L^{\infty}(\mathbb{R}^3)$ satisfies (H) if $||V||_{\infty} < 1$.

Remark. Assumption (H) implies that for all constants $\kappa > 1$, close to 1, there is a positive constant $\delta(\kappa) > 0$ such that :

$$\pm \Lambda^{\pm}(H_0 + \kappa V)\Lambda^{\pm} \geq \delta(\kappa)\Lambda^{\pm}$$
 in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$

FURTHER MIN-MAX RESULTS: TALMAN'S DECOMPOSITION

$$\mathcal{H}_{+}^{T} = L^{2}(\mathbb{R}^{3}, \mathbb{C}^{2}) \otimes \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\}, \quad \mathcal{H}_{-}^{T} = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} \otimes L^{2}(\mathbb{R}^{3}, \mathbb{C}^{2}) ,$$

so that, for any $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \in L^{2}(\mathbb{R}^{3}, \mathbb{C}^{4}),$

$$\Lambda^T_+\psi = \begin{pmatrix} \varphi \\ 0 \end{pmatrix}, \quad \Lambda^T_-\psi = \begin{pmatrix} 0 \\ \chi \end{pmatrix}.$$

Assume also that the potential V satisfies

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

with $\nu \in (0, 1)$ and $c_1, c_2 \in \mathbb{R}$. Finally, define the 2-spinor space $W := C_0^{\infty}(\mathbb{R}^3, \mathbb{C}^2)$, and the 4-spinor subspaces of $L^2(\mathbb{R}^3, \mathbb{C}^4)$

$$W_{+}^{T} := W \otimes \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} , \quad W_{-}^{T} := \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\} \otimes W$$

Theorem 2 [J.D., Esteban, Séré] Under the previous assumptions, all eigenvalues of $H_0 + V$ in the interval (-1, 1) are given by the following (eventually finite) sequence of real numbers



as long as they are contained in the interval (-1,1), assuming that the lowest of these min-max values is larger than -1.

In particular, $\lambda_1(V) = \inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}$ (Talman) where both φ and χ are in W and $\psi = {\varphi \choose \chi}$, as soon a the above inf-sup takes its values in (-1, 1). This theorem is a special case of an abstract result.

Abstract Min-Max Approach

Let \mathcal{H} be a Hilbert space and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator. $\mathcal{F}(A)$ is the form-domain of A. Let \mathcal{H}_+ , \mathcal{H}_- be two orthogonal Hilbert subspaces of \mathcal{H} such that $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Λ_{\pm} are the projectors on \mathcal{H}_{\pm} . We assume the existence of a core Fsuch that :

(i)
$$F_+ = \Lambda_+ F$$
 and $F_- = \Lambda_- F$ are two subspaces of $\mathcal{F}(A)$.
(ii) $a = \sup_{x_- \in F_- \setminus \{0\}} \frac{(x_-, Ax_-)}{\|x_-\|_{\mathcal{H}}^2} < +\infty$.

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

(iii) $c_1 > a$, $b = \inf (\sigma_{ess}(A) \cap (a, +\infty)) \in [a, +\infty]$. Definition: for $k \ge 1$, λ_k is the k^{th} eigenvalue of A in (a, b), counted with multiplicity, *if this eigenvalue exists*. If not, $\lambda_k = b$. **Theorem 3** [J.D., Esteban, Séré] Assume (i)-(ii)-(iii).

$$c_k = \lambda_k , \quad \forall k \ge 1$$

As a consequence, $b = \lim_{k \to \infty} c_k = \sup_k c_k > a$.

<u>References</u> on the min-max approach: Talman and Datta & Deviah for the computation of the first positive eigenvalue of Dirac operators with a potential. Other min-max approaches were proposed by Drake & Goldman and Kutzelnigg.

Esteban & Séré: Dirac operators with a Coulomb-like potential. Griesemer & Siedentop: first abstract theorem on the variational principle, under conditions (i), (ii), and two additional hypotheses instead of (iii): $(Ax, x) > a||x||^2 \forall x \in F_+ \setminus \{0\}$, the operator $(|A| + 1)^{1/2}P_-\Lambda_+$ is bounded. Here Λ_+ is the orthogonal projection of \mathcal{H} on \mathcal{H}_+ and P_- is the spectral projection of A for the interval $(-\infty, a]$, i.e. $P_- = \chi_{(-\infty, a]}(A)$. [Griesemer, Lewis & Siedentop]: an alternative approach which extends the results of Griesemer & Siedentop and applies to Dirac operators with potentials having Coulomb singularities.

Additional comment: the difficult part to apply the previous theorem is condition (iii): the first level of min-max has to be above the lower bound of the gap. A possible method consists in deriving an abstract continuation method when the family of operators depends continuously on a parameter, for instance ν in case of $H_{\nu} := H_0 - \frac{\nu}{|x|}$. This allows us to take any $\nu \in (0, 1)$ in the case of the Coulomb potential $V(x) = \frac{\nu}{|x|}$.

Proof: see the finite dimensional case (numerical approach).

A MIN-MAX APPROACH OF HARDY TYPE INEQUALITIES THE CASE OF TALMAN'S MIN-MAX

As a subproduct of our method, we obtain Hardy type inequalities. In the case of the decomposition based on the projectors of the free Dirac operator, one gets a Hardy type inequality. A simpler form is obtained in case of Talman's decomposition.

For every $\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)$ consider

$$\lambda(\varphi) = \sup_{\chi} \frac{(\psi, (H_0 + V) \psi)}{(\psi, \psi)} \quad \text{where} \quad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

This number is achieved by the function

$$\chi(\varphi) := \frac{-i (\sigma \cdot \nabla) \varphi}{1 - V + \lambda(\varphi)} = \frac{R\varphi}{1 - V + \lambda(\varphi)}$$

Moreover, $\lambda = \lambda(\varphi)$ is the unique solution to the equation

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

(uniqueness is an easy consequence of the monotonicity of both sides of the equation in terms of λ). Thus $\lambda_1(V)$ is the solution of the following minimization problem

$$\lambda_1(V) := \inf\{\lambda(\varphi) : \varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)\}.$$

This is by far simpler than working with Rayleigh quotients.

 $\lambda_1(V)$ is the best constant in the inequality

$$\int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1 + \lambda_1(V) - V} \, dx \, + \, \int_{\mathbb{R}^3} (1 - \lambda_1(V) + V) |\varphi|^2 \, dx \, \ge \, 0$$

For any $\nu \in (0,1)$, the first eigenvalue of $H_{\nu} := H_0 - \frac{\nu}{|x|}$ is explicit:

$$\lambda_1\left(-\frac{\nu}{|x|}\right) = \sqrt{1-\nu^2}$$

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

Moreover this inequality is achieved. In the limit $\nu \rightarrow 1$, we get the optimal (but not achieved) inequality:

$$\int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1 + \frac{1}{|x|}} \, dx \, + \, \int_{\mathbb{R}^3} |\varphi|^2 \, dx \quad \ge \quad \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx$$

This inequality is not invariant under scaling.

THE MIN-MAX ASSOCIATED WITH THE PROJECTORS OF THE FREE DIRAC OPERATOR: CORRESPONDING HARDY TYPE INEQUALITY Consider the splitting $\mathcal{H} = \mathcal{H}_{+}^{f} \oplus \mathcal{H}_{-}^{f}$, with $\mathcal{H}_{\pm}^{f} = \Lambda^{\pm}\mathcal{H}$, where $\Lambda^{+} = \chi_{(0,+\infty)}(H_{0}), \Lambda^{-} = \chi_{(-\infty,0)}(H_{0}), i.e.$

$$\Lambda^{\pm} = \frac{1}{2} \left(\mathbb{1} \pm \frac{\Pi_0}{\sqrt{1 - \Delta}} \right)$$

Theorem 4 If $\lim_{|x| \to +\infty} V(x) = 0$ and $-\frac{\nu}{|x|} - c_1 \leq V \leq c_2$ with $\nu \in (0, 1), c_1, c_2 \geq 0, c_1 + c_2 - 1 < \sqrt{1 - \nu^2}, then$ $c_k^f(V) = \lambda_k(V) \quad \forall k \geq 1.$

Case $\nu < \frac{1}{2}$: [Esteban, Séré], case $\nu < \frac{2}{\frac{2}{\pi} + \frac{\pi}{2}}$: [J.D., Esteban, Séré]

If
$$E \ge c_1^f(V)$$
, $Q_{E,\nu}^f(\psi_+) \ge 0$, $\forall \psi_+ \in \Lambda^+ \left(C_0^\infty(\mathbb{R}^3, \mathbb{C}^4) \right)$
 $Q_{E,\nu}^f(\psi_+) := ||\psi_+||_{H^{1/2}}^2 - (\psi_+, (E-V)\psi_+)$
 $+ \left(\Lambda^- |V|\psi_+, \left(\Lambda^- (\sqrt{1-\Delta} + E + |V|)\Lambda^- \right)^{-1} \Lambda^- |V|\psi_+ \right)$

Proposition 2 For all $\nu \in [0,1]$, $\psi_+ \in \Lambda^+ (C_0^{\infty}(\mathbb{R}^3, \mathbb{C}^4))$,

$$\begin{split} \nu \int_{\mathbb{R}^{3}} \frac{|\psi_{+}|^{2}}{|x|} dx + \sqrt{1 - \nu^{2}} \int_{\mathbb{R}^{3}} |\psi_{+}|^{2} dx \\ &\leq \int_{\mathbb{R}^{3}} (\psi_{+}, \sqrt{1 - \Delta} \psi_{+}) dx + \nu^{2} \int_{\mathbb{R}^{3}} \left(\Lambda^{-} \left(\frac{\psi_{+}}{|x|} \right), B^{-1} \Lambda^{-} \left(\frac{\psi_{+}}{|x|} \right) \right) dx \\ with \quad B := \Lambda^{-} \left(\sqrt{1 - \Delta} + \frac{\nu}{|x|} + \sqrt{1 - \nu^{2}} \right) \Lambda^{-} \end{split}$$

23

Taking functions with support near the origin, we find, after rescaling and passing to the limit, a new homogeneous Hardytype inequality. If

$$\Lambda_{\pm}^{0} := \frac{1}{2} \left(\mathbb{I} \pm \frac{\alpha \cdot \hat{p}}{|\hat{p}|} \right), \quad \hat{p} := -i\nabla$$

are the projectors associated with the zero-mass free Dirac operator, then for any $\psi_+ \in \Lambda^0_+ \left(C^{\infty}_0(\mathbb{R}^3, \mathbb{C}^4) \right)$,

$$\int_{\mathbb{R}^3} \frac{|\psi_+|^2}{|x|} dx \le \int_{\mathbb{R}^3} (\psi_+, |\hat{p}|\psi_+) dx + \int_{\mathbb{R}^3} \left(\Lambda^0_- \left(\frac{\psi_+}{|x|} \right), (B^0)^{-1} \Lambda^0_- \left(\frac{\psi_+}{|x|} \right) \right) dx$$

with $B^0 := \Lambda^0_- \left(|\hat{p}| + \frac{1}{|x|} \right) \Lambda^0_-$

GENERALIZED HARDY INEQUALITY: AN ANALYTICAL PROOF

Notes from a discussion with M. Loss. Related works based on commutators of M.J. Esteban, L. Vega, Adimurthi containing improvements like logarithmic terms.

Proposition 3 Let g be a bounded radial C^1 function such that $\lim_{x\to 0} |x| g(x)$ is finite. Then for any $\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$,

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

Proof. Let $\phi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$ and $\varepsilon = \pm 1$. In the case of the generalized Hardy inequality, take $g(x) = 1 + \frac{1}{|x|}$. From

$$\int_{\mathbf{R}^3} \left| \frac{1}{\sqrt{g}} \left(\sigma \cdot \nabla \phi \right) + \varepsilon \sqrt{g} \left(\sigma \cdot \frac{x}{|x|} \phi \right) \right|^2 \, dx \ge 0, \text{ we get}$$

$$\int_{\mathbb{R}^3} \frac{1}{g} |\sigma \cdot \nabla \phi|^2 dx + \int_{\mathbb{R}^3} g |\phi|^2 dx \ge \varepsilon \left(\phi, \left[\frac{1}{\sqrt{g}} (\sigma \cdot \nabla), \sqrt{g} \left(\sigma \cdot \frac{x}{|x|}\right)\right] \phi\right)_{L^2}$$

Let $L = ix \wedge \nabla$. A straightforward computation shows that

$$\begin{bmatrix} (\sigma \cdot \nabla), \left(\sigma \cdot \frac{x}{|x|} \right) \end{bmatrix} = \frac{2}{|x|} (1 + \sigma \cdot L)$$
$$\begin{bmatrix} \frac{1}{\sqrt{g}} (\sigma \cdot \nabla), \sqrt{g} \left(\sigma \cdot \frac{x}{|x|} \right) \end{bmatrix} = \frac{1}{2g} \left(\nabla g \cdot \frac{x}{|x|} \right) + \frac{2}{|x|} (1 + \sigma \cdot L) ,$$
$$\begin{bmatrix} \frac{1}{\sqrt{g}} \sigma \cdot \left(\nabla - \frac{x}{|x|} \frac{\partial}{\partial r} \right), \sqrt{g} \left(\sigma \cdot \frac{x}{|x|} \right) \end{bmatrix} = \frac{2}{|x|} (1 + \sigma \cdot L) .$$

Lemma 4 The spectrum of $(1+\sigma \cdot L)$ is $\mathbb{Z}\setminus\{0\}$ and $L^2(\mathbb{R}^3, \mathbb{C}^2) = \mathcal{H}_- \oplus \mathcal{H}_+$ with $\mathcal{H}_\pm = P_\pm L^2(\mathbb{R}^3, \mathbb{C}^2)$, $P_\pm = \frac{1}{2}\left(1 \pm \frac{1+\sigma \cdot L}{|1+\sigma \cdot L|}\right)$. As a consequence, for any nonnegative radial function h, if $\phi \in \mathcal{H}_\pm$, $\pm (\phi, h(1+\sigma \cdot L)\phi)_{L^2} \ge \int_{\mathbb{R}^3} h |\phi|^2 dx$

Let
$$\varphi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^2)$$
, $\varphi_{\pm} = P_{\pm}\varphi$. Apply Lemma 4 to φ_{\pm} with $\varepsilon = \pm 1$ (resp. to φ_{-} with $\varepsilon = -1$), $h = \frac{1}{|x|}$, $\nabla_{\!\!\perp} = \left(\nabla - \frac{x}{|x|}\frac{\partial}{\partial r}\right)$:
$$\int_{\mathbb{R}^3} \frac{1}{g} |\sigma \cdot \nabla_{\!\!\perp} \varphi_{\pm}|^2 dx + \int_{\mathbb{R}^3} g |\phi_{\pm}|^2 dx \ge \int_{\mathbb{R}^3} \frac{2}{|x|} |\varphi_{\pm}|^2 dx$$
For any radial function h ,

$$\int_{\mathbf{R}^{3}} h |\varphi|^{2} dx = \int_{\mathbf{R}^{3}} h |\varphi_{-}|^{2} dx + \int_{\mathbf{R}^{3}} h |\varphi_{+}|^{2} dx$$
$$\int_{\mathbf{R}^{3}} |\nabla \varphi|^{2} dx \ge \int_{\mathbf{R}^{3}} |\nabla_{\!\perp} \varphi_{-}|^{2} dx + \int_{\mathbf{R}^{3}} |\nabla_{\!\perp} \varphi_{+}|^{2} dx$$

<u>A NUMERICAL ALGORITHM FOR COMPUTING</u> <u>THE EIGENVALUES OF THE DIRAC OPERATOR</u>

In principle one has to look for the minima of the Rayleigh quotient

$$\frac{((H_0+V)\psi,\psi)}{(\psi,\psi)}$$

on "well chosen" subspaces of 4-spinors on which the above quotient is bounded from below. Direct approaches may face serious numerical difficulties. Our method is based on finding the best constant λ in the generalized Hardy inequality

$$\int_{\mathbb{R}^3} \frac{|R\phi|^2}{\lambda + 1 - V} \, dx + \int_{\mathbb{R}^3} V|\phi|^2 \, dx \, + (1 - \lambda) \int_{\mathbb{R}^3} |\phi|^2 \, dx \ge 0 \,\,\forall \phi$$

To do this, we minimize $\lambda = \lambda(\varphi)$, given by

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

w.r.t. φ . The discretized version of this equation on a finite dimensional space E_n of dimension n of 2-spinor functions is

$A^n(\boldsymbol{\lambda}) x_n \cdot x_n = \mathbf{0} ,$

where $x_n \in E_n$ and $A^n(\lambda)$ is a λ -dependent $n \times n$ matrix. If E_n is generated by a basis set $\{\varphi_i, \dots, \varphi_n\}$, the entries of the matrix $A^n(\lambda)$ are the numbers

$$\int_{\mathbb{R}^3} \left(\frac{\left(\left(\sigma \cdot \nabla \right) \varphi_i, \left(\sigma \cdot \nabla \right) \varphi_j \right)}{1 - V + \lambda} + \left(1 - \lambda + V \right) \left(\varphi_i, \varphi_j \right) \right) \, dx \; .$$

The matrix is monotone decreasing in λ . The ground state energy will then be approached from above by the unique λ for which the first eigenvalue of $A^n(\lambda)$ is zero.

The matrix $A^n(\lambda)$ is selfadjoint and has therefore n real eigenvalues:

 $\lambda_{1,n}(\lambda) < \lambda_{2,n}(\lambda) < ... \lambda_{1,n}(\lambda)$

which are all monotone decreasing functions of λ .

The equation

 $A^n(\boldsymbol{\lambda}) x_n \cdot x_n = \mathbf{0} ,$

means that x_n is an eigenvector associated to the eigenvalue $\lambda_{k,n}(\lambda) = 0$, for some k.

Minimizing λ is therefore equivalent to compute $\lambda_{1,n}$ as the solution of the equation

$\lambda_{1,n}(\boldsymbol{\lambda})=0$

The uniqueness of such a λ comes from the monotonicity.

Moreover, if the approximating finite spaces $(E_n)_{n \in \mathbb{N}}$ is an increasing family which generates $H^1(\mathbb{R}^3; \mathbb{C}^2)$, since for a fixed λ

$$\lambda_{1,n}(\lambda) \searrow \lambda_1(\lambda)$$
 as $n \to +\infty$

we also have

 $\lambda_{1,n} \searrow \lambda_1$ as $n \to +\infty$

This method has been tested on diatomic configurations (corresponding to a cylindrical symmetry) with B-splines basis sets. Approximations from above of the other eigenvalues of the Dirac operator, or excited levels, can also be computed by requiring successively that the second, third,... eigenvalues of $A^n(\lambda)$ are equal to zero.



Figure 1: Each eigenvalue $\mu_i(\lambda)$ of $A(\lambda)$, considered as a function of λ , is monotone decreasing. By looking for the zeros of the non continuous function $\lambda \mapsto \bar{\mu}(\lambda) = \inf_i |\mu_i(\lambda)|$, we obtain an efficient algorithm to compute all eigenvalues of the Dirac operator in the gap (-1, 1) and the corresponding eigenfunctions. The ground state of course corresponds to the smallest zero of $\bar{\mu}(\lambda)$ in (-1, 1). Moreover the method forbids variational collapse, no spurious states may appear and the only consequence of the approximation on a finite basis set is that eigenvalues are approximated from above.



Figure 2: Ground state of Th^{89+} corresponding to Z = 90, one atom, computed with $s_{\text{max}} = 10$, $z_{\text{max}} = 10$, h = 0.4.



Figure 3: Ground state of H_2^+ corresponding to Z = 1, two atoms, computed with $s_{\text{max}} = 700$, $z_{\text{max}} = 820$, h = 20.



Figure 4: Ground state of Th_2^{179+} corresponding to Z = 90, two atoms, computed with $s_{\text{max}} = 10$, $z_{\text{max}} = 12$, h = 0.4.