About a non-homogeneous Hardy-inequality and its relation with the spectrum of Dirac operators

Jean Dolbeault, Maria J. Esteban, Eric Séré

CEREMADE (UMR CNRS 7534)
Université Paris-Dauphine
F-75775 Paris Cedex 16
E-mail: dolbeaul, esteban, sere@ceremade.dauphine.fr

Abstract. A non-homogeneous Hardy-like inequality has recently been found to be closely related to the knowledge of the lowest eigenvalue of a large class of Dirac operators in the gap of their continuous spectrum.

Hardy inequalities and Coulomb singularities

The relationship between usual Hardy inequalities and spectra of elliptic operators is quite well known: the classical Hardy inequality in $\mathbb{R}^N$

$$
(1) \qquad -\Delta \;\geq\; \frac{(N-2)^2}{4}\;\frac{1}{|x|^2}
$$

and the fact that the constant $(N-2)^2/4$ is optimal tells us that the operator $-\Delta - \frac{A}{|x|^2}$ is nonnegative if and only if $A \leq \frac{1}{4}(N-2)^2$. When this condition is not satisfied, the spectrum of $-\Delta - \frac{A}{|x|^2}$ is actually the whole real line. In the rest of these notes, we shall assume that $N = 3$.

In the case of the Dirac operator, no clear Hardy inequality is available because this operator is not semibounded. In some well chosen units, the

Dirac operator is given by

$$H_0 = -i\,\alpha \cdot \nabla + \beta\ ,$$

with

$$\alpha_1, \alpha_2, \alpha_3, \beta \in \mathcal{M}_{4\times 4}(\mathbb{C})\ , \quad \beta = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & -\mathbb{I} \end{pmatrix}\ , \quad \alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}\ ,$$

where σ_i are the Pauli matrices

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

Two of the main properties of H_0 are:

(2) $$H_0^2 = -\Delta + 1\ ,$$

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 $\Lambda^\pm$ 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

$$H_0\,\Lambda^+ \ = \ \Lambda^+ H_0 \ = \ \sqrt{1-\Delta}\ \Lambda^+ \ = \ \Lambda^+ \sqrt{1-\Delta}\ ,$$

$$H_0\,\Lambda^- \ = \ \Lambda^- H_0 \ = \ -\sqrt{1-\Delta}\ \Lambda^- \ = \ -\Lambda^- \sqrt{1-\Delta}\ .$$

As a straightforward consequence, one has the two following Hardy-like inequalities.

Proposition 1 *There exists a positive constant K such that the following inequalities hold for any $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$:*

$$(H_0\,\Lambda^+\psi, \Lambda^+\psi) \ \geq \ K \int_{\mathbb{R}^3} |\psi|^2 \, \frac{dx}{|x|}\ ,$$

$$(H_0\,\Lambda^-\psi, \Lambda^-\psi) \ \leq \ -K \int_{\mathbb{R}^3} |\psi|^2 \, \frac{dx}{|x|}\ .$$

The first question is now to determine the best possible value of K. Because of the property (1) and (2), it is clear that $K \geq 1/2$. Kato proved that $K \geq \frac{2}{\pi}$ and Tix in [15], Burenkov and Evans in [1] improved this lower bound as far as $K \geq \frac{2}{2/\pi + \pi/2}$, as we shall see below. Let us note that we may write

$$|H_0| = \Lambda^+ \, H_0 \, \Lambda^+ - \Lambda^- \, H_0 \, \Lambda^- \, ,$$

and rephrase Proposition 1 as follows:

$$(\psi, |H_0| \, \psi) \quad \geq \quad K \int_{\mathbb{R}^3} |\psi|^2 \, \frac{dx}{|x|} \, , \quad \forall \, \psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4) \, .$$

With these notations, the Hardy-like inequality known as Kato's inequality is, on $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$,

$$|H_0| \quad \geq \quad \frac{2}{\pi} \frac{1}{|x|} \, ,$$

while the one derived in [15, 1] corresponds to:

$$(3) \qquad\qquad |H_0| \quad \geq \quad \frac{2}{(2/\pi + \pi/2)} \frac{1}{|x|} \, .$$

However, these inequalities have no relation with the spectrum of H_0 and indeed the numbers $\nu = \frac{2}{\pi}$ or $\nu = \frac{2}{2/\pi + \pi/2}$ are not critical when one looks at the (point) spectrum of the operator $H_0 - \frac{\nu}{|x|}$. The analysis of the operator $H_\nu := H_0 - \frac{\nu}{|x|}$ yields that for $0 < \nu < 1$, the operator H_ν can be defined as a self-adjoint operator with domain included in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and its spectrum is given by

$$\sigma(H_\nu) = (-\infty, -1] \cup \{\lambda_1^\nu, \lambda_2^\nu, \ldots\} \cup (1, \infty) \, ,$$

with

$$\lim_{\nu \to 1} \lambda_1^\nu = 0$$

(see [11, 12, 10, 16, 14]). Note that H_ν is self-adjoint only for $\nu < 1$ and speaking of its "first eigenvalue" in the interval $(-1, 1)$ does not make sense for $\nu \geq 1$. In our previous works [7, 3], we used the above inequalities to derive a min-max characterization of the eigenvalues of Dirac operators, but actually there is an alternative approach which is much sharper and goes as follows [4]:

$$(4) \quad \int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1 + \frac{1}{|x|}} \, dx + \int_{\mathbb{R}^3} |\varphi|^2 \, dx \quad \geq \quad \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \, , \quad \forall \, \varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \, .$$

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This inequality is Hardy-like, but it is not scale invariant, as are the usual and more classical Hardy inequalities. As we will see at the end of these notes, this inequality is directly related to the spectral properties of the Dirac-Coulomb operators H_ν for $0 < \nu < 1$.

A min-max approach of Hardy inequalities

Assume that the potential V belongs to $M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ (where $M^3(\mathbb{R}^3)$ is the Marcinkiewicz space which is also sometimes denoted by $L^{3,\infty}(\mathbb{R}^3)$) and assume also that there is a positive constant δ such that

$$(5) \qquad \Lambda^+ \left(H_0 + V \right) \Lambda^+ \geq \delta \sqrt{1 - \Delta} \, , \quad \Lambda^- \left(H_0 + V \right) \Lambda^- \leq - \delta \sqrt{1 - \Delta}$$

in $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Next, define the sequence

$$(6) \qquad \lambda_k(V) \quad = \quad \inf_{\substack{F \subset Y^+ \\ F \text{ vector space} \\ \dim F = k}} \quad \sup_{\substack{\psi \in F \oplus Y^- \\ \psi \neq 0}} \quad \frac{((H_0 + V)\psi, \psi)}{(\psi, \psi)} \, .$$

Theorem 2 *([3]) Let V be a scalar potential satisfying assumption (5). Assume also that $V \in L^\infty(\mathbb{R}^3 \setminus \overline{B}_{R_0})$ for some $R_0 > 0$ and that we have :*

$$\lim_{R \to +\infty} \|V\|_{L^\infty (|x| > R)} = 0 \, , \qquad \lim_{R \to +\infty} supess_{|x| > R} V(x) |x|^2 = -\infty \, .$$

Then $\lambda_k(V)$ as defined in (6) is an eigenvalue of $H_0 + V$, $\{\lambda_k(V)\}_{k \geq 1}$ is the non-decreasing sequence of eigenvalues of $H_0 + V$ in the interval $[0, 1)$, counted with multiplicity, and

$$0 < \delta \leq \lambda_1(V) \leq \lambda_k(V) < 1 \, , \quad \lim_{k \to +\infty} \lambda_k(V) \ = \ 1 \, .$$

Note that Griesemer and Siedentop in [9] also proved an abstract result which, when applied to Dirac operators, implies the above min-max characterization for the eigenvalues of $H_0 + V$. However, the class of potentials that they could deal with was quite different from ours and did not include singularities close to the Coulombic ones. This work was later improved in [8].

Remark 3 *Assume that V belongs to $M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Then V is $|H_0|$-bounded. In particular, any potential V such that $|V| \leq a|x|^{-\beta} + C$ is $|H_0|$-bounded for all a, $C > 0$, $\beta \in (0, 1]$. If $|V| \leq a|x|^{-1}$, then by (3), V satisfies (5) if $a < 2/(\pi/2 + 2/\pi) \approx 0.9$. Moreover, any $V \in L^\infty(\mathbb{R}^3)$ satisfies (5) if $\|V\|_\infty < 1$.*

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Remark 4 *Assumption (5) implies that for all constants $\kappa > 1$, close to 1, there is a positive constant $\delta(\kappa) > 0$ such that :*

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

Let us rewrite the Dirac operator in physical units, in the context of atomic physics. Consider the case a point-like nuclear charge Z, that is the case of an electron in a singular nuclear potential of charge Z. Then $\nu < \bar{\nu} = 2/(\pi/2 + 2/\pi)$ is equivalent to $Z \leq 124$. This is below what we know to be the best possible range: $Z \leq 137$ (or $\bar{\nu} = 1$), by explicit computations for the so-called hydrogenoid atoms. In [4] we improve the above result by using a different method which relies on spectral arguments instead of direct variational techniques. We proved that the above min-max characterization could indeed be extended to potentials with singularities as bad as $V_\nu(x) = \nu/|x|$, for all $0 < \nu < 1$, which corresponds to the optimal range in which the operator H_ν has a well defined self-adjoint extension.

Further min-max results

Consider

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

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

$$(7) \qquad \qquad \lim_{|x|\to+\infty} V(x) = 0 ,$$

$$(8) \qquad \qquad -\frac{\nu}{|x|} - c_1 \leq V \leq c_2 = \sup(V) ,$$

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 $L^2(\mathbb{R}^3, \mathbb{C}^4)$

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

Then the eigenvalues of $H_0 + V$ in the interval $(-1, 1)$ are all given by the elements of the following (eventually finite) sequence of real numbers

$$\inf_{\substack{F \subset W_+^T \\ F \text{ vector space} \\ \dim F = k}} \quad \sup_{\substack{\psi \in F \oplus W_-^T \\ \psi \neq 0}} \quad \frac{((H_0 + V)\,\psi, \psi)}{(\psi, \psi)} \ ,$$

that are contained in the interval $(-1, 1)$, provided that the lowest of these min-max values is larger than -1. In particular, under assumptions (7) and (8) on V, we have

$$(9) \qquad \lambda_1(V) \quad = \quad \inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)} \ ,$$

where both φ and χ are in W and $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$, as soon a the above inf-sup takes its values in $(-1, 1)$.

This procedure to find the eigenvalues of Dirac operators was first proposed in a heuristic way by Talman ([13]) and Datta-Deviah ([2]), and later proved to be rigorous for a class of bounded potentials in [9] by Griesemer and Siedentop. In [4] we proved that the result holds for a much larger class of potentials, including the ones with Coulomb singularities. Griesemer, Lewis and Siedentop also improved the result of [9] in [8].

More inequalities

As a subproduct of our proof in [4], we obtained the following result. If for every $\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)$ we define the number

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

this number is achieved by the function

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

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

$$(10) \qquad \lambda \int_{\mathbb{R}^3} |\varphi|^2 \, dx \quad = \quad \int_{\mathbb{R}^3} \left(\frac{|(\sigma \cdot \nabla)\varphi|^2}{1 - V + \lambda} + (1 + V)|\varphi|^2 \right) dx$$

(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

$$(11) \qquad \lambda_1(V) := \inf\{\lambda(\varphi) \; : \; \varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)\} \; .$$

In other words, $\lambda_1(V)$ is the solution of a minimization problem on a set of numbers defined by the nonlinear constraint (10), which is by far simpler than working with Rayleigh quotients.

From all these considerations we infer that when V satisfies the above hypothesis, $\lambda_1(V)$ is the best constant in the inequality

$$(12) \int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1 + \lambda_1(V) - V} \, dx \; + \; \int_{\mathbb{R}^3} (1 - \lambda_1(V) + V)|\varphi|^2 \, dx \; \geq \; 0 \quad \forall \varphi \in W \; .$$

In particular, since for the potential $V_\nu(x) = -\nu/|x|$ and $\nu \in (0,1)$, we explicitly know the first eigenvalue of $H_0 + V_\nu$:

$$\int_{\mathbb{R}^3} \frac{|(\sigma \cdot \nabla)\varphi|^2}{1+\sqrt{1-\nu^2}+\frac{\nu}{|x|}} \, dx \; + (1-\sqrt{1-\nu^2})\int_{\mathbb{R}^3} |\varphi|^2 \, dx \quad \geq \quad \nu \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \quad \forall \varphi \in W.$$

Moreover this inequality is achieved. On the contrary, when we take the limit $\nu \to 1$ in the above inequality, we obtain the limiting, optimal (but not achieved) inequality (4), which we recall for completeness:

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

inequality which is not invariant under scaling: if we rescale it to enhance its meaning for functions being supported near the origin, we find a more classical (and homogeneous) Hardy inequality

$$\int_{\mathbb{R}^3} |x| \; |(\sigma \cdot \nabla)\varphi|^2 \, dx \geq \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \quad \forall \; \varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \; .$$

The best constant in the right hand side of the inequality is 1.

In the next section we show that the characterization of the first eigenvalue by the minimization problem (9) and its relation with the Hardy-like inequality (12) are a useful tool to write a quite efficient algorithm for the numerical computation of Dirac eigenvalues in the gap of the continuous spectrum.

A numerical algorithm

To numerically approximate the eigenvalues of the Dirac operator, one has to look for the minima of the Rayleigh quotient

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

on "well chosen" subspaces of 4-spinors on which the above quotient is bounded from below. Direct approaches may face serious numerical difficulties [6], which can be avoided using (10) and (11) as follows. First discretize (10) on a finite dimensional space E_n of dimension n of 2-spinor functions. The discretized version of (10) is

$$A^n(\lambda)\, x_n \cdot x_n = 0 \;,$$

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 $\{\varphi_i, \ldots \varphi_n\}$, the entries of the matrix $A^n(\lambda)$ are the numbers

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

which are all 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. This method has been tested on a basis of Hermite polynomials (see [5] for some numerical results). More efficient computations have been made recently on diatomic configurations (corresponding to a cylindrical symmetry) with B-splines basis sets, involving very sparse matrices [6]. 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.

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