Dirac equation: variational approach and applications

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October 14, 2013

Mathématiques pour le graphène, Grenoble, October 14-15, 2013

Outline

1. Eigenvalues of the Dirac operator and minmax characterizations
2. Hardy inequalities, completion of the square
3. Strong magnetic fields
4. Numerical schemes

Minmax characterizations of the eigenvalues of the Dirac operator

Joint work with:

Maria J. Esteban and Eric Séré

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: $\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$

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

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 $\Lambda^\pm$ 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

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

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

$R = -i\,\sigma\cdot\nabla$, $R^2 = -\Delta$

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

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

H_ν is self-adjoint only for $\nu < 1$. The notion of "first eigenvalue" in $(-1, 1)$ or "ground state" does not make sense for $\nu \geq 1$.

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

$$(H) \qquad \pm\,\Lambda^\pm\,(H_0 + V)\,\Lambda^\pm \geq \delta\,\Lambda^\pm\sqrt{1-\Delta}\,\Lambda^\pm \quad \text{in } H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$$

With $Y^\pm = \Lambda^\pm H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$, define

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

Theorem

[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 $\lim_{R\to+\infty} \|V\|_{L^\infty(|x|>R)} = 0$, $\lim_{R\to+\infty} \operatorname{supess}_{|x|>R} V(x)|x|^2 = -\infty$, 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

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

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).

Remark. Any potential V such that $|V| \leq a|x|^{-\beta} + C$ belongs to $M^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for all a, $C > 0$, $\beta \in (0,1)$. If $|V| \leq a|x|^{-1}$, 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 :*

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

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 $\psi = \binom{\varphi}{\chi} \in L^2(\mathbb{R}^3,\mathbb{C}^4)$,

$$\Lambda_+^T\psi = \begin{pmatrix}\varphi\\0\end{pmatrix}\,,\quad \Lambda_-^T\psi = \begin{pmatrix}0\\\chi\end{pmatrix}$$

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

[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

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

assuming that the lowest of these min-max values is larger than -1

(Talman)

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

where both φ and χ are in W and $\psi = \binom{\varphi}{\chi}$, as soon a the above inf-sup takes its values in $(-1, 1)$ and $W_+^T \oplus W_-^T$ is a core

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 $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. $\Lambda_\pm$ are the projectors on $\mathcal{H}_\pm$. We assume the existence of a core F such that :

(i) $F_+ = \Lambda_+ F$ and $F_- = \Lambda_- F$ are two subspaces of $\mathcal{F}(A)$.

(ii) $a = \sup_{x_- \in F_- \setminus \{0\}} \frac{(x_-, Ax_-)}{\|x_-\|^2_{\mathcal{H}}} < +\infty$.

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

(iii) $\quad c_1 > a$, $b = \inf\,(\sigma_{\rm ess}(A) \cap (a, +\infty)) \in [a, +\infty]$.

Definition: for $k \geq 1$, λ_k is the $k^{\rm th}$ eigenvalue of A in (a, b), counted with multiplicity, *if this eigenvalue exists*. If not, $\lambda_k = b$.

Theorem

[J.D., Esteban, Séré] Assume (i)-(ii)-(iii).

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

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

References 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

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: a 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 $H_\nu := H_0 - \frac{\nu}{|x|}$

Thuis motivates the search for an adapted Hardy inequality

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

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

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

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

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

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

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

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

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

This inequality is not invariant under scaling

A numerical algorithm for computing the eigenvalues of the Dirac operator

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

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

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

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

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

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

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:

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

which are all monotone decreasing functions of λ.
The equation

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

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

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

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

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

we also have

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

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

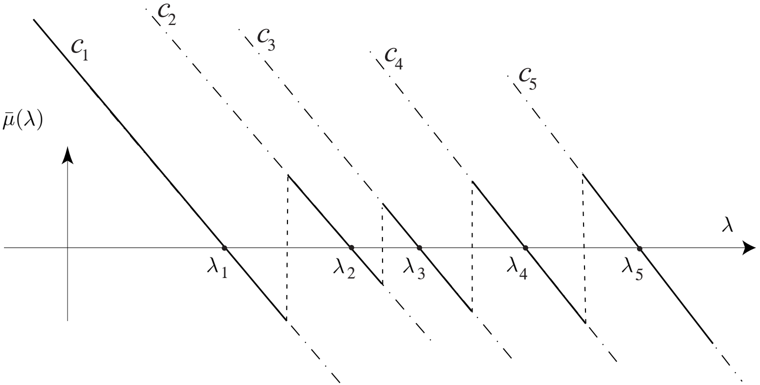


Figure: Each eigenvalue $\mu_i(\lambda)$ of $A(\lambda)$, considered as a function of λ, is monotone decreasing. By looking for the zeros of the non-continuous function $\lambda \mapsto \bar\mu(\lambda) = \inf_i |\mu_i(\lambda)|$, we obtain an efficient algorithm to compute all eigenvalues of the Dirac operator in the gap $(-1, 1)$ and the corresponding eigenfunctions. The ground state of course corresponds to the smallest zero of

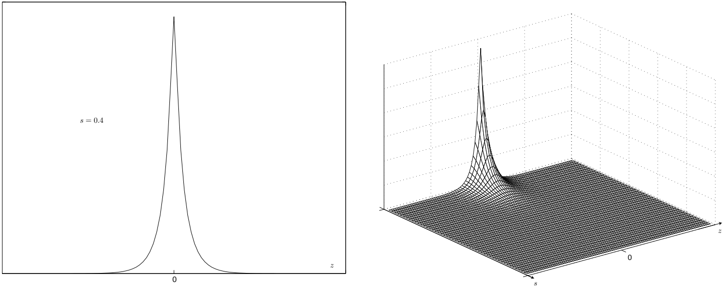


Figure: Ground state of Th^{89+} corresponding to $Z = 90$, one atom, computed with $s_{\max} = 10$, $z_{\max} = 10$, $h = 0.4$

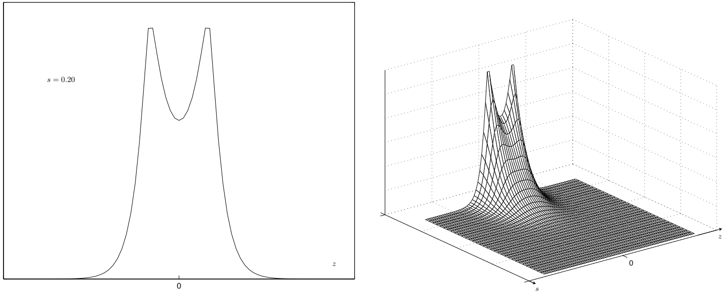
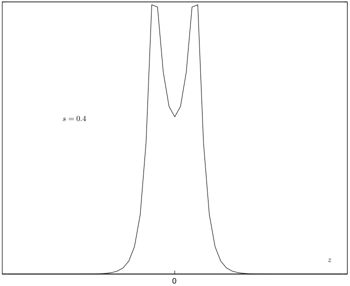


Figure: Ground state of H_2^+ corresponding to $Z = 1$, two atoms, computed with $s_{\max} = 700$, $z_{\max} = 820$, $h = 20$



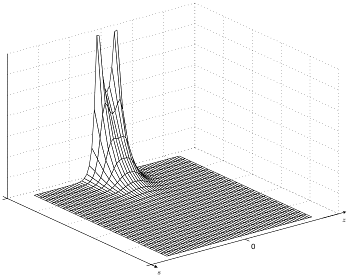


Figure: Ground state of Th_2^{179+} corresponding to $Z = 90$, two atoms, computed with $s_{\max} = 10$, $z_{\max} = 12$, $h = 0.4$

Two important issues

1. The issue of spurious eigenvalues: [Lewin-Séré (2009)] Spectral pollution and how to avoid it
2. The issue of the self-adjointness of the Dirac-Coulomb operator up to $\nu = 1$: [Esteban-Loss (2007)] Self-adjointness for Dirac operators via Hardy-Dirac inequalities

General min-max results, sign-changing potentials

Let $\mathcal{H}$ be a Hilbert space with scalar product $(\cdot,\cdot)$, and $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator. We denote by $\mathcal{F}(A)$ the form-domain of A. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal Hilbert subspaces of $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$

We denote by Λ^+, Λ^- the projectors on $\mathcal{H}_+$, $\mathcal{H}_-$. We assume the existence of a core F (*i.e.* a subspace of $D(A)$ which is dense for the norm $\|\cdot\|_{D(A)}$), such that :

(i) $F_+ = \Lambda^+ F$ and $F_- = \Lambda^- F$ are two subspaces of $\mathcal{F}(A)$.

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

(ii$^+$) $a^+ := \inf_{x_+ \in F_+ \setminus \{0\}} \frac{(x_+, Ax_+)}{\|x_+\|^2_{\mathcal{H}}} > -\infty$.

We consider the two sequences of min-max and max-min levels $(\lambda_k^+)_{k\geq 1}$ and $(\lambda_k^-)_{k\geq 1}$ defined by

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

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

Let $b^- := \inf\{\sigma_{\rm ess}(A) \cap (a^-, \infty)\}$, $b^+ := \sup\{\sigma_{\rm ess}(A) \cap (-\infty, a^+)\}$

$$(\mathrm{iii}^-) \qquad k_0^+ := \min\{k \geq 1\,,\ \lambda_k^+ > a^-\}$$

$$(\mathrm{iii}^+) \qquad k_0^- := \min\{k \geq 1\,,\ \lambda_k^- < a^+\}$$

Theorem

If (i)-(ii$^-$)-(iii$^-$) *hold, for any* $k \geq k_0^+$, *either* λ_k^+ *is the* $(k - k_0 + 1)$*-th eigenvalue of* A *in the interval* (a^-, b^-) *or it is equal to* b^-. *If* (i)-(ii$^+$)-(iii$^+$) *hold, for any* $k \geq k_0^-$, *either* λ_k^- *is the* $(k - k_0 + 1)$*-th eigenvalue of* A *(in reverse order) in the interval* (b^+, a^+) *or it is equal to* b^+

Consider a 1-parameter family of self-adjoint operators $A_\tau := A_0 + \tau\, V$, $\tau \in [0, \bar\tau] = \mathcal{I}$, V is a bounded scalar potential, $A_0 : D(A_0) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator. Let $\mathcal{H}_+$, $\mathcal{H}_-$, Λ^+ and Λ^- be above Assume further that there is a space $F \subset \mathcal{H}$ such that, for all $\tau \in \mathcal{I}$, F is a core for A_τ and the following hypotheses hold:

(j) $F_+ = \Lambda^+ F$ and $F_- = \Lambda^- F$ are two subspaces of $\mathcal{F}(A_\tau)$

(jj$^-$) There is $a^- \in \mathbb{R}$ such that $\sup_{\tau\in\mathcal{I},\, x_-\in F_-\setminus\{0\}} \frac{(x_-, A_\tau\, x_-)}{\|x_-\|^2_{\mathcal{H}}} \le a^-$

(jj$^+$) There is $a^+ \in \mathbb{R}$ such that $\inf_{\tau\in\mathcal{I},\, x_+\in F_+\setminus\{0\}} \frac{(x_+, A_\tau\, x_+)}{\|x_+\|^2_{\mathcal{H}}} \ge a^+$

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

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

$$a_1^- := \inf_{\tau\in\mathcal{I}} \left[\inf\left(\sigma(A_\tau)\cap(a^-, +\infty)\right)\right]$$

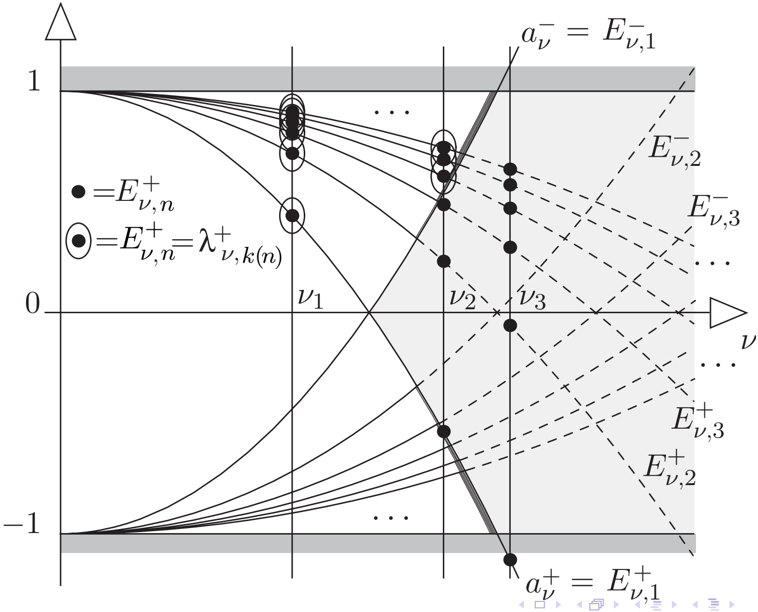
$$a_1^+ := \sup_{\tau\in\mathcal{I}} \left[\sup\left(\sigma(A_\tau)\cap(-\infty, a^+)\right)\right]$$

A continuation principle...

Theorem

Under the above assumptions,

- *if for some* $k_0^+ \geq 1$, $\lambda^{0,+}_{k_0^+} > a^-$ *and if* $a_1^- > a^-$, *for all* $k \geq k_0^+$, *the numbers* $\lambda_k^{\tau,+}$ *are either eigenvalues of* $A_0 + \tau\, V$ *in the interval* (a^-, b^-) *or* $\lambda_k^{\tau,+} = b^-$
- *If for some* $k_0^- \geq 1$, $\lambda^{0,-}_{k_0^-} < a^+$ *and* $a_1^+ < a^+$, *for all* $k \geq k_0^-$, *the numbers* $\lambda_k^{\tau,-}$ *are either eigenvalues of* $A_0 + \tau\, V$ *in the interval* (b^+, a^+) *or* $\lambda_k^{\tau,-} = b^+$


$a_\nu^- = E_{\nu,1}^-$
1
. . .
$E_{\nu,2}^-$
$=E_{\nu,n}^+$
$E_{\nu,3}^-$
$=E_{\nu,n}^+=\lambda_{\nu,k(n)}^+$
. . .
0
ν_1
ν_2
ν_3
ν
. . .
$E_{\nu,3}^+$
$E_{\nu,2}^+$
−1
. . .
$a_\nu^+ = E_{\nu,1}^+$

Hardy inequalities

Joint work with:

Maria J. Esteban and Eric Séré
Maria J. Esteban and Roberta Bosi
Maria J. Esteban, J. Duoandikoetxea and L. Vega

Standard Hardy inequality

Let $u \in H^1(\mathbb{R}^N)$ 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 $A \le \frac{1}{4}(N-2)^2$.
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. and many other
$N = 3$ from now on

Hardy inequality for the operator P

Proposition

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

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

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 $\nu \in (0, 1]$,

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

Replace $\varphi(x)$ by $\varphi\left(\frac{x}{\mu}\right)$ and let $\mu \to 0$.

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

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

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

$$\int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|}\,dx \le \int_{\mathbb{R}^3} |x|\,|\nabla\varphi|^2\,dx$$

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 $P = -i\,c\,(\sigma \cdot \nabla)$

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

which can be solved by

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

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

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

Note that for any fixed ϕ

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

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

$\lambda_1(V)$ is the smallest λ for which

$$\int_{\mathbb{R}^3} \frac{|P\,\phi|^2}{\lambda + c^2 - V}\; dx + \int_{\mathbb{R}^3} V|\phi|^2\;\; dx \; + (c^2 - \lambda) \int_{\mathbb{R}^3} |\phi|^2\;\; dx \geq 0 \;\forall\, \phi$$

and φ is the corresponding optimal function.

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

Other standard Hardy type inequalities

Define the spectral projectors:

$$\Lambda^+ = \chi_{(0,+\infty)}(H_0) \quad \text{and} \quad \Lambda^- = \chi_{(-\infty,0)}(H_0)$$

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

$$|H_0| \geq \frac{\kappa}{|x|} \qquad \kappa = \frac{1}{2}$$

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

2) *Kato's inequality.*

$$|H_0| \geq \frac{\kappa}{|x|} \quad \kappa = \frac{2}{\pi} = 0.63662\ldots$$

$Z\,\alpha \leq \kappa$ means $Z \leq 87$. Optimal [Herbst]

3) An inequality for the Brown & Ravenhall operator [Burenkov, Evans, Perry, Siedentop, Tix]:

$$\Lambda^+ \left(H_0 - \frac{\kappa}{|x|} \right) \Lambda^+ \geq 0 \quad \kappa = \frac{2}{\frac{2}{\pi} + \frac{\pi}{2}} = 0.906037\ldots$$

The above operator (l.h.s.) was introduced by Bethe and Salpeter.
κ is sharp. $Z\,\alpha \leq \kappa$ means $Z \leq 124$

Dirac operator: corresponding Hardy type inequality

Consider the splitting $\mathcal{H} = \mathcal{H}^f_+ \oplus \mathcal{H}^f_-$, with $\mathcal{H}^f_\pm = \Lambda^\pm \mathcal{H}$, where $\Lambda^+ = \chi_{(0,+\infty)}(H_0)$, $\Lambda^- = \chi_{(-\infty,0)}(H_0)$, *i.e.*

$$\Lambda^\pm = \frac{1}{2}\left(\mathbb{I} \pm \frac{H_0}{\sqrt{1-\Delta}}\right)$$

Theorem (J.D., Esteban, Séré)

If $\lim_{|x|\to+\infty} V(x) = 0$ *and* $-\frac{\nu}{|x|} - c_1 \le V \le c_2$ *with* $\nu \in (0,1)$, $c_1, c_2 \ge 0$, $c_1 + c_2 - 1 < \sqrt{1-\nu^2}$, *then*

$$c_k^f(V) = \lambda_k(V) \quad \forall\, k \ge 1$$

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

Proposition

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

$$\nu \int_{\mathbb{R}^3} \frac{|\psi_+|^2}{|x|}\, dx + \sqrt{1-\nu^2} \int_{\mathbb{R}^3} |\psi_+|^2\, dx$$
$$\leq \int_{\mathbb{R}^3} (\psi_+, \sqrt{1-\Delta}\, \psi_+)\, dx + \nu^2 \int_{\mathbb{R}^3} \left(\Lambda^- \left(\frac{\psi_+}{|x|}\right), B^{-1} \Lambda^- \left(\frac{\psi_+}{|x|}\right)\right) dx$$

with $B := \Lambda^- \left(\sqrt{1-\Delta} + \frac{\nu}{|x|} + \sqrt{1-\nu^2}\right) \Lambda^-$

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

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

are the projectors associated with the zero-mass free Dirac operator, then for any $\psi_+ \in \Lambda^0_+\left(C^\infty_0(\mathbb{R}^3, \mathbb{C}^4)\right)$

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

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

Generalized Hardy inequality: an analytical proof

[J.D.-Esteban-Loss-Vega] Related works based on commutators of M.J. Esteban, L. Vega, Adimurthi containing improvements like logarithmic terms.

Proposition

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

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

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

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

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

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

$$\left[(\sigma \cdot \nabla), \left(\sigma \cdot \frac{x}{|x|} \right) \right] = \frac{2}{|x|} (1 + \sigma \cdot L)$$

$$\left[\tfrac{1}{\sqrt{g}} (\sigma \cdot \nabla), \sqrt{g} \left(\sigma \cdot \tfrac{x}{|x|} \right) \right] = \tfrac{1}{2g} \left(\nabla g \cdot \tfrac{x}{|x|} \right) + \tfrac{2}{|x|} (1 + \sigma \cdot L) \,,$$

$$\left[\tfrac{1}{\sqrt{g}} \sigma \cdot \left(\nabla - \tfrac{x}{|x|} \tfrac{\partial}{\partial r} \right), \sqrt{g} \left(\sigma \cdot \tfrac{x}{|x|} \right) \right] = \tfrac{2}{|x|} (1 + \sigma \cdot L)$$

Lemma

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 $\phi\in\mathcal{H}_\pm$, $\qquad \pm\left(\phi, h\,(1+\sigma\cdot L)\,\phi\right)_{L^2}\geq\int_{\mathbb{R}^3}h\,|\phi|^2\,dx$

Let $\varphi\in H^{1/2}(\mathbb{R}^3,\mathbb{C}^2)$, $\varphi_\pm=P_\pm\varphi$. Apply Lemma **??** to φ_+ with $\varepsilon=+1$ (resp. to φ_- with $\varepsilon=-1$), $h=\frac{1}{|x|}$, $\nabla_\perp=\left(\nabla-\frac{x}{|x|}\frac{\partial}{\partial r}\right)$:

$$\int_{\mathbb{R}^3}\frac{1}{g}\left|\sigma\cdot\nabla_\perp\varphi_\pm\right|^2\,dx+\int_{\mathbb{R}^3}g\,\left|\phi_\pm\right|^2\,dx\geq\int_{\mathbb{R}^3}\frac{2}{|x|}\left|\varphi_\pm\right|^2dx$$

For any radial function h,

$$\int_{\mathbb{R}^3}h\,|\varphi|^2\,dx=\int_{\mathbb{R}^3}h\,|\varphi_-|^2\,dx+\int_{\mathbb{R}^3}h\,|\varphi_+|^2\,dx$$

$$\int_{\mathbb{R}^3}|\nabla\varphi|^2\,dx\geq\int_{\mathbb{R}^3}|\nabla_\perp\varphi_-|^2\,dx+\int_{\mathbb{R}^3}|\nabla_\perp\varphi_+|^2\,dx$$

Hardy inequality and Dirac: logarithmic improvements

[J.D.-Esteban-Loss-Vega] For some continuous functions $W > 1$ a.e. and constants $R > 0$ and $C(R) \leq 0$, the improved inequality

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \frac{W(|x|)}{|x|}} + |\varphi|^2 \right) dx \geq \int_{\mathbb{R}^3} \frac{W(|x|)}{|x|} |\varphi|^2 \, dx + C(R) \int_{S_R} |\varphi|^2 \, d\mu_R$$

holds for all $\varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2)$. Here μ_R is the surface measure induced by Lebesgue's measure on the sphere $S_R := \{x \in \mathbb{R}^3 \ : \ |x| = R\}$

$$W_\infty(x) = 1 + \frac{1}{8} \sum_{k=1}^{\infty} X_1(|x|)^2 \cdots X_k(|x|)^2 \, ,$$

where $X_1(s) := (a - \log(s))^{-1}$ for some $a > 1$, $X_k(s) := X_1 \circ X_{k-1})$. The functions X_k and W^∞ are well defined for $|x| = s < e^{a-1}$

Theorem

Assume that for some $R>0$ the improved inequality holds for every spinor $\varphi \in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)$, where W is a radially symmetric continuous function from $\mathbb{R}^+$ to $\mathbb{R}^+$. Assume moreover that $W(0)>0$ and W is nondecreasing in a neighbourhood of 0^+. Then $W(0)\le 1$,

$$\limsup_{s\to+\infty} W(s)/s \le 1$$

and for all $k\ge 1$,

$$\liminf_{s\to 0^+}\left(W(s)-1-\frac{1}{8}\sum_{j=1}^{k} X_1^2(s)\cdots X_j^2(s)\right)X_1^{-2}(s)\cdots X_{k+1}^{-2}(s)\le\frac{1}{8}$$

As soon as $W\not\equiv 1$, $C(R)$ must be negative

Hardy inequalities for the Schrödinger operator and the IMS method

Our goal is to obtain estimates for the lowest eigenvalue of $-\Delta - \mu\, V_M(x)$, where $V_M(x) = \sum_{k=1}^M \frac{1}{|x-y_k|^2}$, $M \geq 2$ and $y_1, \ldots y_M$ are M points of $\mathbb{R}^N$. Notice that the Hamiltonian is essentially self-adjoint if $\mu \leq (N-2)^2/4 - 1$, otherwise one has to use the corresponding Friedrichs extension. Define d by

$$d := \min_{1 \leq j \neq k \leq M} |y_k - y_j|/2$$

Theorem

Consider $\mu \in (0, (N-2)^2/4]$. For any $M \geq 2$, there is a nonnegative constant $K_M < \pi^2$ such that, for any $u \in H^1(\mathbb{R}^N)$,

$$\int |\nabla u|^2\, dx + \frac{K_M + (M+1)\,\mu}{d^2} \int |u|^2\, dx \geq \mu \int V_M(x)\, |u|^2\, dx$$

Multipolar Hardy inequality for the Dirac operator

We consider an arbitrary configuration of poles $y_k \in \mathbb{R}^3$, and define the following quantities :

$$a := \frac{\nu\, M}{d}\,, \quad b := \frac{\big[1 - S(\nu)\big]^2}{\nu^2}\,, \quad c := 2\,\frac{1 - S(\nu)}{\nu^2}\,,$$

$$d^*(\nu) = \frac{1}{2}\, M\,\nu\, c + \pi\,\sqrt{c}\,,$$

$$\lambda^*(d,\nu,M) := \frac{1}{c}\left[1 + \sqrt{c\,\left(a^2\nu^{-2} - \pi^2\, d^{-2} - a\right) + 1 - a^2\,\nu^{-2}}\,\right] - 1 - \frac{a}{2}\,,$$

with $S(\nu) = \sqrt{1-\nu^2}$ and $d := \min_{i\neq k} |y_i - y_j|/2$

Theorem

With the above notations, for all $\nu \in (0,1)$, $M \geq 2$, if $d \geq d^*(\nu)$, then for all $\phi \in H^1(\mathbb{R}^3, \mathbb{C}^2)$ we have

$$\int_{\mathbb{R}^3} \frac{|\vec{\sigma}\cdot\nabla\,\phi|^2}{1 + \lambda^* + \nu\, W_M}\, dx + (1-\lambda^*)\int_{\mathbb{R}^3} |\phi|^2\, dx \geq \nu \int_{\mathbb{R}^3} W_M\, |\phi|^2\, dx$$

Strong magnetic fields

Joint work with:

Maria J. Esteban and Michael Loss

Outline

- Relativistic hydrogenic atoms in strong magnetic fields: min-max and critical magnetic fields
- Characterization of the critical magnetic field
- Proof of the main result
- A Landau level ansatz
- Numerical results

Relativistic hydrogenic atoms in strong magnetic fields

The Dirac operator for a hydrogenic atom in the presence of a constant magnetic field B in the x_3-direction is given by

$$H_B - \frac{\nu}{|x|} \quad \text{with} \quad H_B := \alpha \cdot \left[\frac{1}{i}\nabla + \frac{1}{2}B(-x_2, x_1, 0)\right] + \beta$$

$\nu = Z\alpha < 1$, Z is the nuclear charge number
The Sommerfeld fine-structure constant is $\alpha \approx 1/137.037$
The magnetic field strength unit is $\frac{m^2 c^2}{|q|\hbar} \approx 4.4 \times 10^9$ Tesla

1 Gauss $= 10^{-4}$ Tesla

To put this in perspective, here is a table of magnetic field strengths		
The Earths magnetic field, which deflects compass needles	measured at the N magnetic pole	0.6 Gauss
A common, hand-held magnet	like those used to stick papers on a refrigerator	100 Gauss
The magnetic field in strong sunspots	(within dark, magnetized areas on the solar surface)	4000 Gauss
The strongest, sustained (i.e., steady) magnetic fields achieved so far in the laboratory	generated by hulking huge electromagnets	4.5 X 10^5 Gauss
The strongest man-made fields ever achieved, if only briefly	made using focussed explosive charges; lasted only 4 - 8 microseconds.	10^7 Gauss
The strongest fields ever detected on non-neutron stars	found on a handful of strongly-magnetized, compact white dwarf stars. (Such stars are rare. Only 3% of white dwarfs have Mega-gauss or stronger fields.)	10^8 Gauss
Typical surface, polar magnetic fields of radio pulsars	the most familiar kind of neutron star; more than a thousand are known to astronomers	10^{12}-10^{13} Gauss
Magnetars	soft gamma repeaters and anomalous X-ray pulsars (These are surface, polar fields. Magnetar interior fields may range up to 10^{16} Gauss, with field lines probably wrapped in a toroidal, or donut geometry inside the star.)	10^{14}-10^{15} Gauss

[R.C. Duncan, Magnetars, soft gamma repeaters and very strong magnetic fields]

The ground state energy $\lambda_1(\nu, B)$ is the smallest eigenvalue in the gap

As $B \nearrow$, $\lambda_1(\nu, B) \to -1$: we define the critical magnetic field as the field strength $B(\nu)$ such that "$\lambda_1(\nu, B(\nu)) = -1$"

[J.D., Esteban, Loss, Annales Henri Poincaré 2007]

- Non perturbative estimates based on min-max formulations

Theorem

For all $\nu \in (0,1)$, there exists a constant $C > 0$ such that

$$\frac{4}{5\,\nu^2} \le \; B(\nu) \; \le \; \min\left(\frac{18\,\pi\,\nu^2}{[3\,\nu^2 - 2]_+^2}\;,\; e^{\,C/\nu^2}\right)$$

- Relativistic lowest Landau level

$$\lim_{\nu \to 0} \nu \log(B(\nu)) \; = \; \pi$$

Magnetic Dirac Hamiltonian

$H_B\,\psi - \frac{\nu}{|x|}\,\psi = \lambda\,\psi$ is an equation for complex spinors $\psi = \binom{\phi}{\chi}$ where $\phi, \chi \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ are the upper and lower components

$$P_B\chi + \phi - \frac{\nu}{|x|}\,\phi = \lambda\,\phi$$
$$P_B\phi - \chi - \frac{\nu}{|x|}\,\chi = \lambda\,\chi$$

with $P_B := -\,i\,\sigma\cdot(\nabla - i\,\mathrm{A}_B(x))$

$$\mathrm{A}_B(x) := \frac{B}{2}\begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix}\,, \quad \mathrm{B}(x) := \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix}$$

Min–max characterization of the ground state energy

If $\psi = \binom{\phi}{\chi}$ is an eigenfunction with eigenvalue λ, eliminate the lower component χ and observe

$$0 = J[\phi, \lambda, \nu, B] := \int_{\mathbb{R}^3} \left(\frac{|P_B \phi|^2}{1 + \lambda + \frac{\nu}{|x|}} + (1 - \lambda)\, |\phi|^2 - \frac{\nu}{|x|}\, |\phi|^2 \right) d^3x$$

The function $\lambda \mapsto J[\phi, \lambda, \nu, B]$ is decreasing: define $\lambda = \lambda[\phi, \nu, B]$ to be the unique solution to

$$\text{either } J[\phi, \lambda, \nu, B] = 0 \quad \text{or} \quad -1$$

Theorem

Let $B \in \mathbb{R}^+$ and $\nu \in (0,1)$. If $-1 < \inf_{\phi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)} \lambda[\phi, \nu, B] < 1$,

$$\lambda_1(\nu, B) := \inf_{\phi} \lambda[\phi, \nu, B]$$

is the lowest eigenvalue of $H_B - \frac{\nu}{|x|}$ in the gap of its continuous spectrum, $(-1, 1)$

Characterization of the critical magnetic field

Using the scaling properties, we find an eigenvalue problem which characterizes the critical magnetic field

Notations

Magnetic Dirac operator with Coulomb potential $\nu/|x|$

$$H_B := \begin{pmatrix} \mathbb{I} - \nu/|x| & -i\,\sigma\cdot(\nabla - i\,\mathrm{A}) \\ -i\,\sigma\cdot(\nabla - i\,\mathrm{A}) & -\mathbb{I} - \nu/|x| \end{pmatrix} \tag{1}$$

where A is a magnetic potential corresponding to B, and $\mathbb{I}$ and σ_k are respectively the identity and the Pauli matrices

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

Let $\mathrm{B} = (0, 0, B)$, $\mathrm{A} = \mathrm{A}_B$. For any $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, define

$$P_B := -i\,\sigma\cdot(\nabla - i\,\mathrm{A}_B(x))\,, \quad \mathrm{A}_B(x) := \frac{B}{2}\begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix} \tag{3}$$

Consider the functional

$$J[\phi,\lambda,\nu,B] := \int_{\mathbb{R}^3} \left(\frac{|P_B\phi|^2}{1+\lambda+\frac{\nu}{|x|}} + (1-\lambda)\,|\phi|^2 - \frac{\nu}{|x|}\,|\phi|^2 \right) d^3x \qquad (4)$$

on the set of admissible functions

$$\mathcal{A}(\nu,B) := \{\phi\in C_0^\infty \;:\; \|\phi\|_{L^2}=1,\ \lambda\mapsto J[\phi,\lambda,\nu,B] \textit{ changes sign in } (-1,+\infty)\}$$

$\lambda=\lambda[\phi,\nu,B]$ is either the unique solution to $J[\phi,\lambda,\nu,B]=0$ if $\phi\in\mathcal{A}(\nu,B)$

$$\lambda_1(\nu,B) := \inf_{\phi\in\mathcal{A}(\nu,B)} \lambda[\phi,\nu,B] \qquad (5)$$

The critical magnetic field is defined by

$$B(\nu) := \inf\left\{ B>0 \;:\; \liminf_{b\nearrow B} \lambda_1(\nu,b) = -1 \right\} \qquad (6)$$

Auxiliary functional

$$\mathcal{E}_{B,\nu}[\phi] := \int_{\mathbb{R}^3} \frac{|x|}{\nu} \, |P_B \, \phi|^2 \, d^3x - \int_{\mathbb{R}^3} \frac{\nu}{|x|} \, |\phi|^2 \, d^3x \qquad (7)$$

$$\Longleftrightarrow \mathcal{E}_{B,\nu}[\phi] + 2 \, \|\phi\|^2_{L^2(\mathbb{R}^3)} = J[\phi, -1, \nu, B]$$

Scaling invariance

$$\mathcal{E}_{B,\nu}[\phi_B] = \sqrt{B} \, \mathcal{E}_{1,\nu}[\phi] \quad \phi_B := B^{3/4} \, \phi \left(B^{1/2} \, x \right) \qquad (8)$$

We define

$$\mu(\nu) := \inf_{0 \not\equiv \phi \in C_0^\infty(\mathbb{R}^3)} \frac{\mathcal{E}_{1,\nu}[\phi]}{\|\phi\|^2_{L^2(\mathbb{R}^3)}} \qquad (9)$$

Formally : $-1 = \lambda_1(\nu, B(\nu)), \quad \inf_{0 \not\equiv \phi \in C_0^\infty(\mathbb{R}^3)} J[\phi, -1, \nu, B] = 0$

$$\Longrightarrow \sqrt{B(\nu)} \, \mu(\nu) + 2 = 0$$

Main result

Theorem

For all $\nu \in (0,1)$,

$$\mu(\nu) := \inf_{0 \not\equiv \phi \in C_0^\infty(\mathbb{R}^3)} \frac{\mathcal{E}_{1,\nu}[\phi]}{\|\phi\|^2_{L^2(\mathbb{R}^3)}}$$

is negative, finite,

$$B(\nu) = \frac{4}{\mu(\nu)^2} \tag{10}$$

and $B(\nu)$ *is a continuous, monotone decreasing function of* ν *on* $(0,1)$

Proof of the main result

- Preliminary results
- Proof

Preliminary results

$$(\nu, \phi) \mapsto \nu\, \mathcal{E}_{1,\nu}[\phi] = \int_{\mathbb{R}^3} |x|\, |P_1\, \phi|^2\, d^3x - \int_{\mathbb{R}^3} \frac{\nu^2}{|x|}\, |\phi|^2\, d^3x \tag{11}$$

is a concave, bounded function of $\nu \in (0,1)$, for any $\phi \in C_0^\infty(\mathbb{R}^3)$

$$\phi(x) := \sqrt{\frac{B}{2\,\pi}}\, e^{-\frac{B}{4}(|x_1|^2+|x_2|^2)} \begin{pmatrix} f(x_3) \\ 0 \end{pmatrix} \quad \forall\, x = (x_1, x_2, x_3) \in \mathbb{R}^3 \tag{12}$$

$f \in C_0^\infty(\mathbb{R}, \mathbb{R})$ such that $f \equiv 1$ for $|x| \le \delta$, $\delta > 0$, and $\|f\|_{L^2(\mathbb{R}^+)} = 1$

$$\mathcal{E}_{B,\nu}[\phi] \le \frac{C_1}{\nu} + C_2\, \nu - C_3\, \nu \log B \tag{13}$$

$\phi_{1/B}(x) = B^{-3/4}\, \phi\left(B^{-1/2}\, x\right)$, $\quad \mathcal{E}_{1,\nu}[\phi_{1/B}] = B^{-1/2}\, \mathcal{E}_{B,\nu}[\phi] < 0$

Lemma

On the interval $(0,1)$, the function $\nu \mapsto \mu(\nu)$ is continuous, monotone decreasing and takes only negative real values

Proofs

$$\tilde{B}(\nu) = \sup\left\{B > 0 \;:\; \inf_{\phi}\left(\mathcal{E}_{B,\nu}[\phi] + 2\,\|\phi\|^2_{L^2(\mathbb{R}^3)}\right) \geq 0\right\} = \frac{4}{\mu(\nu)^2} \quad (14)$$

$$\mathcal{E}_{B,\nu}[\phi] + 2\,\|\phi\|^2_{L^2(\mathbb{R}^3)} \geq J[\phi, \lambda_1(\nu, B), \nu, B] \geq J[\phi, \lambda[\phi, \nu, B], \nu, B] = 0 \quad (15)$$

$$\Longrightarrow B(\nu) \leq \tilde{B}(\nu)$$

Proofs

Let $B=B(\nu)$ and consider $(\nu_n)_{n\in\mathbb{N}}$ such that $\nu_n\in(0,\nu)$,
$\lim_{n\to\infty}\nu_n=\nu$,
$\lambda^n:=\lambda_1(\nu_n,B)>-1$ and $\lim_{n\to\infty}\lambda^n=-1$
Let ϕ_n be the optimal function associated to λ^n: $J[\phi_n,\lambda^n,\nu_n,B]=0$

Let $\chi\geq 0$ on $\mathbb{R}^+$ such that $\chi\equiv 1$ on $[0,1]$, $0\leq\chi\leq 1$ and $\chi\equiv 0$ on $[2,\infty)$, and $\chi_n(x):=\chi(|x|/R_n)$, $\lim_{n\to\infty}R_n=\infty$, $\tilde\phi_n:=\phi_n\,\chi_n$

$$P_B\,\phi_n=\underbrace{(P_B\,\tilde\phi_n)\,\chi_n}_{=a}+\underbrace{\left[-(P_0\,\chi_n)\,\phi_n\right]}_{=b} \qquad (16)$$

Using $|a|^2\geq\frac{|a+b|^2}{1+\varepsilon}-\frac{|b|^2}{\varepsilon}$, we get

$$|P_B\,\phi_n|^2\geq\frac{|(P_B\,\tilde\phi_n)\,\chi_n|^2}{1+\varepsilon_n}-\frac{|(P_0\,\chi_n)\,\phi_n|^2}{\varepsilon_n} \qquad (17)$$

1) The function $\tilde{\phi}_n$ is supported in the ball $B(0, 2\,R_n)$: with $\mu_n := (1+\varepsilon_n)\big[2(1+\lambda^n)R_n+\nu_n\big]$,

$$\frac{1}{1+\varepsilon_n}\int_{\mathbb{R}^3}\frac{|P_B\,\tilde{\phi}_n|^2}{1+\lambda^n+\frac{\nu_n}{|x|}}\,d^3x \geq \frac{1}{\mu_n}\int_{\mathbb{R}^3}|x|\,|P_B\,\tilde{\phi}_n|^2\,d^3x \qquad (18)$$

2) $\mathrm{Supp}(P_0\,\chi_n)\subset B(0,2\,R_n)\setminus B(0,R_n)$, $|P_0\,\chi_n|^2\leq\kappa\,R_n^{-2}$

$$\frac{1}{\varepsilon_n}\int_{\mathbb{R}^3}\frac{|(P_0\,\chi_n)\,\phi_n|^2}{1+\lambda^n+\frac{\nu_n}{|x|}}\,d^3x \leq \frac{\kappa}{\varepsilon_n\,R_n\big[(1+\lambda^n)\,R_n+\nu_n\big]}\int_{\mathbb{R}^3}|\phi_n|^2\,d^3x \qquad (19)$$

With $\eta_n = \kappa/(\varepsilon_n\, R_n\, ((1+\lambda^n)\, R_n + \nu_n)) + \nu_n/R_n$, we can write

$$0 = J[\phi_n, \lambda^n, \nu_n, B] \geq \frac{1}{\mu_n} \int_{\mathbb{R}^3} |x|\, |P_B\, \tilde{\phi}_n|^2\, d^3x - \nu_n \int_{\mathbb{R}^3} \frac{|\tilde{\phi}_n|^2}{|x|}\, d^3x + (1-\lambda^n-\eta_n) \int_{\mathbb{R}^3} |\tilde{\phi}_n|^2\, d^3x$$

Let $\tilde{\nu}_n = \sqrt{\mu_n\, \nu_n}$

$$\frac{1}{\tilde{\nu}_n} \int_{\mathbb{R}^3} |x|\, |P_B\, \tilde{\phi}_n|^2\, d^3x - \tilde{\nu}_n \int_{\mathbb{R}^3} \frac{|\tilde{\phi}_n|^2}{|x|}\, d^3x + 2 \int_{\mathbb{R}^3} |\tilde{\phi}_n|^2\, d^3x \leq \left[2 - \sqrt{\frac{\mu_n}{\nu_n}}\, (1-\lambda^n-\eta_n)\right] \int_{\mathbb{R}^3} |\tilde{\phi}_n|^2\, d^3x \to 0$$

$$\tilde{B}(\nu') \leq B = B(\nu) \quad \forall\, \nu' > \nu \tag{20}$$

By continuity, $\tilde{B}(\nu) \leq B(\nu)$ □

A Landau level ansatz

- Definition
- Characterization of the critical field (Landau level ansatz)
- Asymptotic behaviour as $\nu \longrightarrow 0_+$
- Comparison of the critical magnetic fields

Landau Levels

First Landau level for a constant magnetic field of strength B: the space of all functions ϕ which are linear combinations of the functions

$$\phi_\ell := \frac{B}{\sqrt{2\,\pi\,2^\ell\,\ell!}}\,(x_2 + i\,x_1)^\ell\,e^{-B\,s^2/4}\begin{pmatrix}1\\0\end{pmatrix}, \quad \ell\in\mathbb{N}, \quad s^2 = x_1^2 + x_2^2 \quad (21)$$

where the coefficients depend only on x_3, *i.e.*

$$\phi(x) = \sum_\ell f_\ell(x_3)\,\phi_\ell(x_1, x_2) \quad (22)$$

Π is the projection of ϕ onto the first Landau level. Critical field in the Landau level ansatz

$$B_{\mathcal{L}}(\nu) := \inf\left\{B > 0\ :\ \liminf_{b\nearrow B}\lambda_1^{\mathcal{L}}(\nu, b) = -1\right\}$$
$$\lambda_1^{\mathcal{L}}(\nu, B) := \inf_{\phi\in\mathcal{A}(\nu,B)\,,\ \Pi^\perp\phi=0}\lambda[\phi, \nu, B]$$

Characterization of the critical field (Landau level ansatz)

The counterpart of our main result holds in the Landau level ansatz. For any $\nu \in (0,1)$, if

$$\mu_{\mathcal{L}}(\nu) := \inf_{\phi \in \mathcal{A}(\nu, B)\,,\ \Pi^\perp \phi = 0} \mathcal{E}_{1,\nu}[\phi] \qquad (23)$$

then

$$B_{\mathcal{L}}(\nu) = \frac{4}{\mu_{\mathcal{L}}(\nu)^2} \qquad (24)$$

Goal: compare $\mu_{\mathcal{L}}(\nu)$ with $\mu(\nu)$

Cylindrical coordinates: $s=\sqrt{x_1^2+x_2^2}$ and $z=x_3$

If ϕ is in the first Landau level, then

$$\mathcal{E}_{1,\nu}[\phi]=\sum_\ell \frac{1}{\nu}\int_0^\infty b_\ell\, {f_\ell'}^2\, dz-\nu\int_0^\infty a_\ell\, f_\ell^2\, dz \tag{25}$$

$$a_\ell(z):=\left(\phi_\ell,\frac{1}{r}\,\phi_\ell\right)_{L^2(\mathbb{R}^2,\mathbb{C}^2)}=\frac{1}{2^\ell\,\ell!}\int_0^{+\infty}\frac{s^{2\ell+1}\,e^{-s^2/2}}{\sqrt{s^2+z^2}}\,ds \tag{26}$$

$$b_\ell(z):=(\phi_\ell,r\,\phi_\ell)_{L^2(\mathbb{R}^2,\mathbb{C}^2)}=\frac{1}{2^\ell\,\ell!}\int_0^{+\infty}s^{2\ell+1}\,e^{-s^2/2}\sqrt{s^2+z^2}\,ds \tag{27}$$

$$\Longrightarrow \mathcal{E}_{1,\nu}[\phi]\ge\frac{1}{\nu}\int_0^\infty b_0\,|f'|^2\,dz-\nu\int_0^\infty a_0\,f^2\,dz \tag{28}$$

Consider $\phi(x)=f(z)\,\frac{e^{-s^2/4}}{\sqrt{2\,\pi}}\binom{1}{0}$

$$\frac{1}{2}\,\mathcal{E}_{1,\nu}[\phi] = \frac{1}{\nu}\int_0^\infty b_0\, f'^2\, dz - \nu\int_0^\infty a_0\, f^2\, dz := \mathcal{L}_\nu[f] \tag{29}$$

$$b_0(z) = \int_0^\infty \sqrt{s^2+z^2}\, s\, e^{-s^2/2}\, ds \quad \text{and} \quad a_0(z) = \int_0^\infty \frac{s\, e^{-s^2/2}}{\sqrt{s^2+z^2}}\, ds \tag{30}$$

The minimization problem in the Landau level ansatz is now reduced to

$$\mu_{\mathcal{L}}(\nu) = \inf_f \frac{\mathcal{L}_\nu[f]}{\|f\|^2_{L^2(\mathbb{R}^+)}} \tag{31}$$

By definition of $\mu(\nu)$ and $\mu_{\mathcal{L}}(\nu)$, we have

$$\mu(\nu) \le \mu_{\mathcal{L}}(\nu) \tag{32}$$

It is a non trivial problem to estimate how close these two numbers are

Asymptotic behaviour (Landau level ansatz)

Observe that $b(z) \geq \frac{1}{a(z)}$ and let

$$\mathcal{L}_\nu^-[f] := \frac{1}{\nu}\int_0^\infty \frac{1}{a}\,f'^2\,dz - \nu\int_0^\infty a\,f^2\,dz \tag{33}$$

and

$$\mathcal{L}_\nu^+[f] := \frac{1}{\nu}\int_0^\infty b\,f'^2\,dz - \nu\int_0^\infty \frac{1}{b}\,f^2\,dz \tag{34}$$

with corresponding infima $\mu_{\mathcal{L}}^-(\nu)$ and $\mu_{\mathcal{L}}^+(\nu)$

Lemma

For any $\nu \in (0,1)$,

$$\mu_{\mathcal{L}}^-(\nu) \leq \mu_{\mathcal{L}}(\nu) \leq \mu_{\mathcal{L}}^+(\nu) \tag{35}$$

Lemma

With the above notations, $\lim_{\nu\to 0_+} \nu \log|\mu_{\mathcal{L}}(\nu)| = -\frac{\pi}{2}$

Comparison of the critical magnetic fields

Theorem

With the above notations, $\lim_{\nu \to 0_+} \frac{\log B(\nu)}{\log B_{\mathcal{L}}(\nu)} = 1$

Known: $\mu(\nu) \leq \mu_{\mathcal{L}}(\nu)$
$B(\nu) > 1$ for any $\nu \in (0, \bar{\nu})$ for some $\bar{\nu} > 0$: $\nu \in (0, \bar{\nu})$, then $\lambda_1(\nu, 1) > -1$ and therefore, for all ϕ,

$$\mathcal{E}_{1,\nu}[\phi] \geq \mathcal{F}_\nu[\phi] := \int_{\mathbb{R}^3} \frac{|\sigma \cdot \nabla_1 \phi|^2}{\lambda_1(\nu, 1) + 1 + \frac{\nu}{|x|}} \, d^3x - \int_{\mathbb{R}^3} \frac{\nu}{|x|} \, |\phi|^2 \, d^3x \qquad (36)$$

$\mathcal{G}_\nu \begin{pmatrix} \phi \\ \chi \end{pmatrix} := \left(H_B \begin{pmatrix} \phi \\ \chi \end{pmatrix}, \begin{pmatrix} \phi \\ \chi \end{pmatrix} \right)$ is concave in χ:

$$1 + \mathcal{F}_\nu[\phi] = \sup_\chi \frac{\mathcal{G}_\nu \binom{\phi}{\chi}}{\|\phi\|^2_{L^2(\mathbb{R}^3)} + \|\chi\|^2_{L^2(\mathbb{R}^3)}} \qquad (37)$$

$$\sup_\chi \frac{\mathcal{G}_\nu \binom{\phi}{\chi}}{\|\phi\|_{L^2(\mathbb{R}^3)} + \|\chi\|_{L^2(\mathbb{R}^3)}} \geq \sup_{\Pi^\perp \chi = 0} \frac{\mathcal{G}_\nu \binom{\phi}{\chi}}{\|\phi\|_{L^2(\mathbb{R}^3)} + \|\chi\|_{L^2(\mathbb{R}^3)}} \ldots \tag{38}$$

(estimate of the interaction term and Cauchy-Schwartz)

$$\ldots \geq \sup_\chi \frac{\mathcal{G}_{\nu+\nu^{3/2}} \binom{\Pi\phi}{\Pi\chi} + \mathcal{G}_{\nu+\sqrt{\nu}} \binom{\Pi^\perp \phi}{0}}{\|\Pi\phi\|_{L^2(\mathbb{R}^3)} + \|\Pi^\perp\phi\|_{L^2(\mathbb{R}^3)} + \|\Pi\chi\|_{L^2(\mathbb{R}^3)}} \tag{39}$$

(being perpendicular to the lowest Landau level raises the energy)

$$\ldots \geq \sup_\chi \frac{\mathcal{G}_{\nu+\nu^{3/2}} \binom{\Pi\phi}{\Pi\chi} + d(\nu)\, \|\Pi^\perp\phi\|^2_{L^2(\mathbb{R}^3)}}{\|\Pi\phi\|_{L^2(\mathbb{R}^3)} + \|\Pi^\perp\phi\|_{L^2(\mathbb{R}^3)} + \|\Pi\chi\|_{L^2(\mathbb{R}^3)}} \tag{40}$$

with $d(0) = \sqrt{2} > \sup_\chi \frac{\mathcal{G}_{\nu+\nu^{3/2}} \binom{\Pi\phi}{\Pi\chi}}{\|\Pi\phi\|_{L^2(\mathbb{R}^3)} + \|\Pi\chi\|_{L^2(\mathbb{R}^3)}}$ $\Longrightarrow \mu^-_{\mathcal{L}}(\nu + \nu^{3/2}) \leq \mu(\nu)$

Numerical results

- Computations in the Landau level ansatz
- General case (without Landau level ansatz)
- Conclusion

Computations in the Landau level ansatz

We minimize $\mathcal{L}_\nu[f]/\|f\|^2_{L^2(\mathbb{R}^+)}$ on the set of the solutions f_λ of

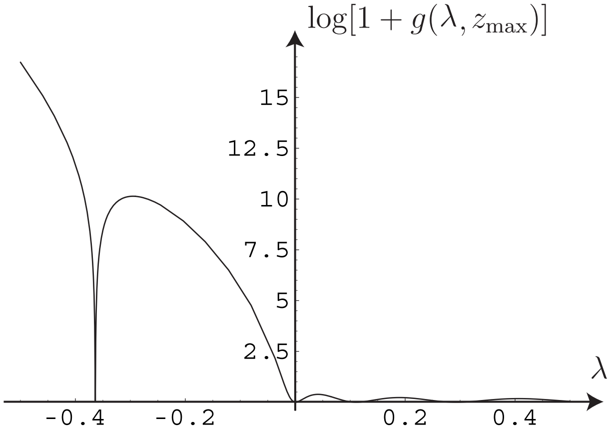
$$f'' + \frac{z\,a(z)}{b(z)}\,f' + \frac{\nu}{b(z)}\,(\lambda + \nu\,a(z))\,f = 0\,, \quad f(0) = 1\,,\ f'(0) = 0 \quad (41)$$

We notice that $b'(z) = z\,a(z)$, and, for any $z > 0$,

$$a(z) = e^{\frac{z^2}{2}}\sqrt{\frac{\pi}{2}}\,\mathrm{erfc}\left(\frac{z}{\sqrt{2}}\right) \quad \text{and} \quad b(z) = e^{\frac{z^2}{2}}\sqrt{\frac{\pi}{2}}\,\mathrm{erfc}\left(\frac{z}{\sqrt{2}}\right) + z \quad (42)$$

Shooting method: minimize $g(\lambda, z_{\max}) := |f_\lambda(z_{\max})|^2 + |f'_\lambda(z_{\max})|^2$
As $z_{\max} \to \infty$, the first minimum $\mu_{\mathcal{L}}(\nu, z_{\max})$ of $\lambda \mapsto g(\lambda, z_{\max})$ converges to 0 and thus determines $\lambda = \mu_{\mathcal{L}}(\nu)$

Landau level ansatz (2)



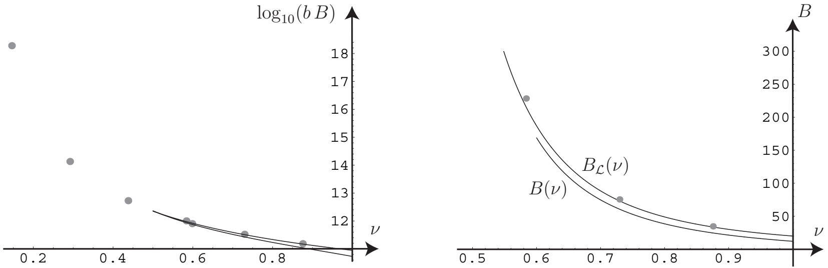
Plot of $\lambda \mapsto \log[1+g(\lambda,z_{\max})]$ with $z_{\max}=100$, for $\nu=0.9$

Landau level ansatz (3)

$b = \frac{m^2 c^2}{e \hbar} \approx 4.414 \cdot 10^9$ is the numerical factor to get the critical field in Tesla

ν	Z	$\mu_{\mathcal{L}}$	$B_{\mathcal{L}}(\nu)$	$\log_{10}(b\, B_{\mathcal{L}}(\nu))$
0.409	56.	-0.0461591	1877.35	12.9184
0.5	68.52	-0.0887408	507.941	12.3506
0.598	82.	-0.14525	189.596	11.9227
0.671	92.	-0.192837	107.567	11.6765
0.9	123.33	-0.363773	30.2274	11.1252
1	137.037	-0.445997	20.1093	10.9482

Landau level ansatz (4)



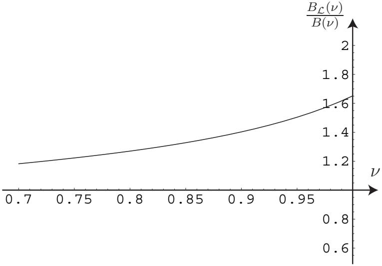
Left: values of the critical magnetic field in Tesla ($\log_{10}$ scale)
Right: values in dimensionless units
Ground state levels in the Landau level ansatz: upper curve
Levels obtained by a direct computation: lower curve
Dots correspond to the values computed by [Schlüter, Wietschorke, Greiner] in the Landau level ansatz

Computations without the Landau level ansatz

We numerically compute $B(\nu)$ in the general case, without ansatz
Discretization: B-spline functions of degree 1 on a logarithmic, variable step-size grid, in cylindrical symmetry give large but sparse matrices

ν	Z	λ_1	$B(\nu)$	$\log_{10}(b\,B(\nu))$
0.50	68.5185	-0.0874214	523.389	12.3637
0.60	82.2222	-0.153882	168.922	11.8725
0.70	95.9259	-0.231198	74.833	11.5189
0.80	109.63	-0.321875	38.6087	11.2315
0.90	123.333	-0.430854	21.5476	10.9782
1.00	137.037	-0.573221	12.1735	10.7302

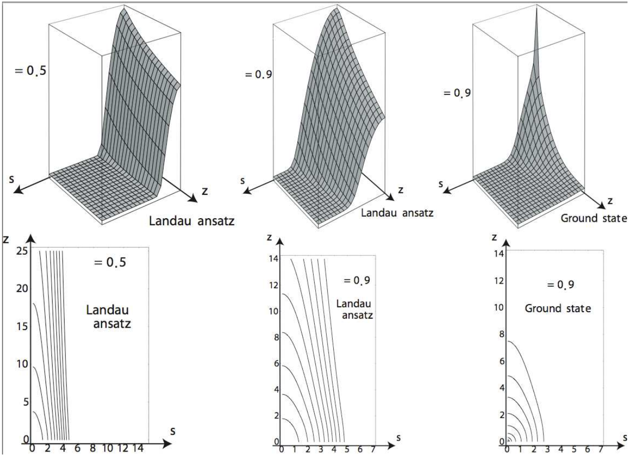
General case (2)



Ratio of the ground state levels computed in the Landau level ansatz vs. ground state levels obtained by a direct computation

- Orders of magnitude of the critical magnetic field, shape of the curve: ok in the Landau level ansatz
- Except maybe in the limit $\nu \to 0$, no justification of the Landau level ansatz: computed critical fields, shapes of the corresponding ground state differ

General case (3)



Conclusion

The Landau level ansatz, which is commonly accepted in non relativistic quantum mechanics as a good approximation for large magnetic fields, is a quite crude approximation for the computation of the critical magnetic field (that is the strength of the field at which the lowest eigenvalue in the gap reaches its lower end) in the Dirac-Coulomb model

Even for small values of ν, which were out of reach in our numerical study, it is not clear that the Landau level ansatz gives the correct approximation at first order in terms of ν

Accurate numerical computations involving the Dirac equation cannot simply rely on the Landau level ansatz.

More on numerical schemes

Joint work with:

[Maria J. Esteban and Michael Loss]
Lyonell Boulton (work in progress)

A variational formulation for computing the critical threshold

Let

$$H_B = \begin{pmatrix} \mathbb{I} + V_\nu & -i\sigma \cdot (\nabla - iA_B) \\ -i\sigma \cdot (\nabla - iA_B) & -\mathbb{I} + V_\nu \end{pmatrix}$$

be the magnetic Dirac operator with Coulomb potential

$$V_\nu(x,y,z) = -\frac{\nu}{\sqrt{x^2+y^2+z^2}} \qquad 0 < \nu < \sqrt{3}/2$$

and magnetic potential

$$A_B(x) = \frac{B}{2} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}$$

associated with a constant magnetic field $(0,0,B)$. Here $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \text{and} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The critical threshold is achieved at the value of $B > 0$, such that the smallest eigenvalue of H_B hits -1, the upper end of the negative essential spectrum of H_B
Let $P_B : \mathrm{Dom}(P_B) \longrightarrow L^2(\mathbb{R}^3)^2$ be a self-adjoint realisation of

$$P_B = -\,i\,\sigma\cdot(\nabla - i\,A_B)$$

$$\mathcal{E}_\nu[\phi,\psi] = \int_{\mathbb{R}^3} \frac{P_1\phi\cdot P_1\psi}{-V_\nu}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z + \int_{\mathbb{R}^3} V_\nu\phi\cdot\psi\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

and $\mathcal{E}_\nu[\phi] = \mathcal{E}_\nu[\phi,\phi]$. According to [D.-Esteban-Loss (2008)], the critical threshold is found to be

$$B(\nu) = \frac{4}{\mu(\nu)^2}$$

where

$$\mu(\nu) = \inf_{0\neq\phi\in C_0^\infty(\mathbb{R}^3)^2} \frac{\mathcal{E}_\nu[\phi]}{\|\phi\|^2_{L^2(\mathbb{R}^3)^2}}$$

Cylindrical coordinates

To a point $(x, y, z) \in \mathbb{R}^3$, we associate coordinates $(s, \theta, z) \in \mathbb{R}^+ \times [0, 2\pi) \times \mathbb{R}$ such that

$$x = s\,\cos\theta \qquad y = s\,\sin\theta \qquad s = \sqrt{x^2 + y^2}$$

and state the following useful formulae

$$\partial_x = \cos\theta\,\partial_s - \tfrac{1}{s}\,\sin\theta\,\partial_\theta \qquad \partial_s = \cos\theta\,\partial_x + \sin\theta\,\partial_y$$

$$\partial_y = \sin\theta\,\partial_s + \tfrac{1}{s}\,\cos\theta\,\partial_\theta \qquad \partial_\theta = -s\sin\theta\,\partial_x + s\,\cos\theta\,\partial_y$$

In these coordinates, P_B takes the form

$$P_B = -\,i \begin{pmatrix} \partial_z & e^{-i\theta}\left(\partial_s - \frac{i}{s}\,\partial_\theta - \frac{B\,s}{2}\right) \\ e^{i\theta}\left(\partial_s + \frac{i}{s}\,\partial_\theta + \frac{B\,s}{2}\right) & -\,\partial_z \end{pmatrix}$$

Spectral decomposition

Decompose

$$L^2(\mathbb{R}^3)^2 = \bigoplus_{m\in\{k+\frac{1}{2}:k\in\mathbb{Z}\}} \mathcal{L}_m$$

$$\mathcal{L}_m = \left\{ \phi(s\cos\theta, s\sin\theta, z) = \begin{pmatrix} c(s,z)\, e^{i(m-1/2)\theta} \\ d(s,z)\, e^{i(m+1/2)\theta} \end{pmatrix} : c, d \in L^2(\mathbb{R}^+ \times \mathbb{R}, \mathrm{d}\mu) \right\}$$

where $\mathrm{d}\mu = s\,\mathrm{d}s\,\mathrm{d}z$. For $\phi \in \mathcal{L}_m \cap \mathrm{Dom}\, P_B$,

$$P_B\phi = -i \begin{pmatrix} \left[\partial_z c + \partial_s d + \frac{m+1/2}{s}\, d - \frac{B\,s}{2}\, d\right] e^{i(m-1/2)\theta} \\ \left[\partial_s c - \partial_z d - \frac{m-1/2}{s}\, c + \frac{B\,s}{2}\, c\right] e^{i(m+1/2)\theta} \end{pmatrix}$$

Hence $\mathcal{L}_m$ is an invariant subspace of P_B and

$$P_{m,B} = -i \begin{pmatrix} \partial_z & (\partial_s + \frac{1}{2s}) + \frac{m}{s} - \frac{B\,s}{2} \\ (\partial_s + \frac{1}{2s}) - \frac{m}{s} + \frac{B\,s}{2} & -\partial_z \end{pmatrix}$$

Proposition

For any $\nu \in (0,1)$, the lowest eigenvalue of H_B is achieved by spinnors with $m = 1/2$

Upper bounds

$$\mu^h_{\mathrm{up}}(\nu) = \min_{0\neq\psi\in\mathcal{V}_h} \frac{\tilde{\mathcal{E}}_{1/2,\nu}[\psi]}{\|\psi\|^2_{L^2(\mathbb{R}^+\times\mathbb{R},\,\mathrm{d}\mu)^2}}$$

ν	upper bound B_ν	$\mu^h_{\mathrm{up}}(\nu)$
0.5	476.0356	-0.091666
0.55	267.9217	-0.12219
0.6	164.9883	-0.15571
0.65	108.1061	-0.19236
0.7	74.1462	-0.23227
0.75	52.6372	-0.27567
0.8	38.339	-0.32301
0.85	28.4239	-0.37514
0.9	21.2612	-0.43375
0.95	15.8311	-0.50266
1	11.3584	-0.59343

Table: Upper bounds for a triangulation of $(0,30)\times(-70,70)$. Here the NDOF$=87186$

Temple-Lehmann bounds

Consider an operator H acting on $L^2(\mathbb{R}^3)$ and let $\phi \in C_0^\infty(H) \cap C_0^\infty(H^2)$ such that $\|\phi\|_{L^2(\mathbb{R}^3)} = 1$. Then there exists a point λ_1 of the spectrum of H in the interval

$$((\phi, H\phi) - \delta_\phi, (\phi, H\phi) + \delta_\phi) \quad \text{where } \delta_\phi = \sqrt{(\phi, H^2\phi) - (\phi, H\phi)^2}$$

Proof. Consider

$$F[\lambda, \phi] := (\phi, H^2\phi) - 2\lambda(\phi, H\phi) + \lambda^2 = (\phi, (H-\lambda)^2\phi) \geq \mathrm{dist}(\lambda, \mathrm{spectrum}(H))^2$$

The function $\lambda \mapsto F[\lambda, \phi]$ reaches its minimum for $\lambda = (\phi, H\phi)$, which proves the result. □

Lower bounds

ν	B_ν	$\mu^h_{\rm lo}(\nu)$
0.5	246.9537	-0.12727
0.55	193.0395	-0.14395
0.6	128.6754	-0.17631
0.65	85.4486	-0.21636
0.7	57.1526	-0.26455
0.75	38.1625	-0.32375
0.8	25.1624	-0.39871
0.85	16.39	-0.49401
0.9	10.8415	-0.60742
0.95	7.669	-0.7222
1	7.7013	-0.72069

Table: Lower bounds for a triangulation of $(0,30)\times(-70,70)$. NDOF$=212744$

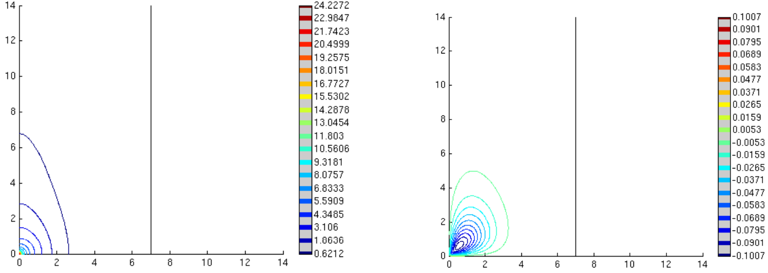


Figure: Upper and lower spinors

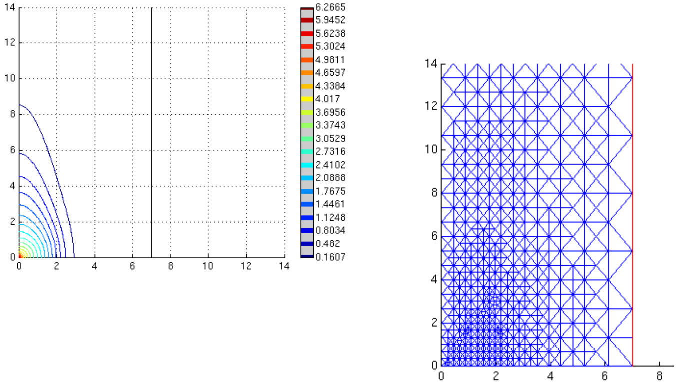


Figure: Logarithm of the density + 1 and mesh for this example. Here and above $\nu = .9$ and we use Lagrange elements of order 3 on a large thin rectangle.

Thank you for your attention !