Critical threshold for electronic stability under the action of an intense magnetic field

Maria J. ESTEBAN

C.N.R.S. and University Paris-Dauphine

In collaboration with : Jean Dolbeault and Michael Loss

UIMP, SANTANDER, August 2011

Physical problem

Very strong magnetic fields could :

– destabilize matter, distorting atoms and molecules and forming polymer-like chains,

– facilitate the massive spontaneous appearance of positron-electron pairs,

Physical problem

Very strong magnetic fields could :

– destabilize matter, distorting atoms and molecules and forming polymer-like chains,

– facilitate the massive spontaneous appearance of positron-electron pairs,

– the best candidate for this to happen are the magnetars (neutron stars), in which huge gravitational collapses would facilitate the appearance of very intense magnetic fields,

Physical problem

Very strong magnetic fields could :

– destabilize matter, distorting atoms and molecules and forming polymer-like chains,

– facilitate the massive spontaneous appearance of positron-electron pairs,

– the best candidate for this to happen are the magnetars (neutron stars), in which huge gravitational collapses would facilitate the appearance of very intense magnetic fields,

Earth's magnetic field = 1 Gauss

Maximal field on Earth (MRI) = 1 Tesla = 10^4 Gauss

In new magnetars one expects fields of 10^{11} Tesla. In recent theories, up to 10^{16} Tesla in the heart of the magnetars.

Physical problem

Very strong magnetic fields could :

– destabilize matter, distorting atoms and molecules and forming polymer-like chains,

– facilitate the massive spontaneous appearance of positron-electron pairs,

– the best candidate for this to happen are the magnetars (neutron stars), in which huge gravitational collapses would facilitate the appearance of very intense magnetic fields,

Earth's magnetic field = 1 Gauss

Maximal field on Earth (MRI) = 1 Tesla = 10^4 Gauss

In new magnetars one expects fields of 10^{11} Tesla. In recent theories, up to 10^{16} Tesla in the heart of the magnetars.

OUR MODEL : an electron (driven by a Dirac operator) in a nuclear-like electrostatic field + an external constant magnetic field.

Real atoms and molecules can also be considered, but not today!

The free Dirac operator

$$\mathbf{H_0} = -\mathbf{i}\,\alpha\cdot\nabla + \beta\,, \qquad \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times 4}(\mathbb{C}) \qquad (c = m = \hbar = 1)$$

The free Dirac operator

$$\mathbf{H_0} = -\mathbf{i}\,\alpha \cdot \nabla + \beta\,, \qquad \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times 4}(\mathbb{C}) \qquad (c = m = \hbar = 1)$$

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

The free Dirac operator

$$\mathbf{H_0} = -\mathbf{i}\,\alpha \cdot \nabla + \beta\,, \qquad \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times 4}(\mathbb{C}) \qquad (c = m = \hbar = 1)$$

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

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

The free Dirac operator

$$\mathbf{H_0} = -\mathbf{i}\,\alpha\cdot\nabla + \beta\,, \qquad \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times 4}(\mathbb{C}) \qquad (c = m = \hbar = 1)$$

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

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

The two main properties of H_0 are:

$$\mathbf{H_0^2} = -\,\mathbf{\Delta} + \mathbb{I}, \qquad \sigma(\mathrm{H}_0) = (-\infty, -1] \cup [1, +\infty)$$

The free Dirac operator

$$\mathbf{H_0} = -\mathbf{i}\,\alpha\cdot\nabla + \beta\,, \qquad \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times 4}(\mathbb{C}) \qquad (c = m = \hbar = 1)$$

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

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

The two main properties of H_0 are:

$$\mathbf{H_0^2} = -\,\mathbf{\Delta} + \mathbb{1}, \qquad \sigma(\mathrm{H}_0) = (-\infty, -1] \cup [1, +\infty)$$

$\mathbf{H_0}$ acts on functions $\psi : \mathbb{R}^3 \to \mathbb{C}^4$

The free Dirac operator

$$\mathbf{H_0} = -\mathbf{i}\,\alpha\cdot\nabla + \beta\,, \qquad \alpha_1,\ \alpha_2,\ \alpha_3,\ \beta \in \mathcal{M}_{4\times 4}(\mathbb{C}) \qquad (c = m = \hbar = 1)$$

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

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

The two main properties of H_0 are:

$$\mathbf{H_0^2} = -\,\mathbf{\Delta} + \mathbb{1}, \qquad \sigma(\mathrm{H}_0) = (-\infty, -1] \cup [1, +\infty)$$

$\mathbf{H_0}$ acts on functions $\psi : \mathbb{R}^3 \to \mathbb{C}^4$

QUESTION : Spectrum of $\mathbf{H_0} + V$?

Eigenvalues of the Dirac operator without magnetic field

Let us first consider the case of Coulomb potentials $V_\nu := -\frac{\nu}{|x|},\ \nu > 0$.

Eigenvalues of the Dirac operator without magnetic field

Let us first consider the case of Coulomb potentials $V_\nu := -\frac{\nu}{|x|}, \ \nu > 0$.

$H_\nu := H_0 - \frac{\nu}{|x|}$ can be defined as a self-adjoint operator if $0 < \nu < 1$

(actually also (recent result) if $\nu = 1$).

Eigenvalues of the Dirac operator without magnetic field

Let us first consider the case of Coulomb potentials $V_\nu := -\frac{\nu}{|x|},\ \nu > 0$.

$H_\nu := H_0 - \frac{\nu}{|x|}$ can be defined as a self-adjoint operator if $0 < \nu < 1$

(actually also (recent result) if $\nu = 1$).

Its spectrum is given by:

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

$$0 < \lambda_1^\nu = \sqrt{1-\nu^2} \leq \cdots \leq \lambda_k^\nu \cdots < 1 \ .$$

and the fact that $\lambda_1(H_0 + V_\nu)$ belongs to $(-1, 1)$ is a kind of “stability condition" for the electron.

Magnetic case

When a external magnetic field B is present, one considers a magnetic potential $\mathbf{A}_B$ s. t. $curl\,\mathbf{A}_B = \mathbf{B}$.

Magnetic case

When a external magnetic field B is present, one considers a magnetic potential $\mathbf{A}_B$ s. t. $curl\, \mathbf{A}_B = \mathbf{B}$.

One has then to replace ∇ with $\nabla_B = \nabla - i\mathbf{A}_B$

Magnetic case

When a external magnetic field B is present, one considers a magnetic potential $\mathbf{A}_B$ s. t. $curl\,\mathbf{A}_B = \mathbf{B}$.

One has then to replace ∇ with $\nabla_B = \nabla - i\mathbf{A}_B$

$$\mathbf{H_B} = -\mathbf{i}\,\alpha \cdot \nabla_\mathbf{B} + \beta$$

Magnetic case

When a external magnetic field B is present, one considers a magnetic potential $\mathbf{A}_B$ s. t. $curl\, \mathbf{A}_B = \mathbf{B}$.

One has then to replace ∇ with $\nabla_B = \nabla - i\mathbf{A}_B$

$$\mathbf{H_B} = -\mathbf{i}\, \alpha \cdot \nabla_\mathbf{B} + \beta$$

If we consider $H_B + V$, if this operator is self-adjoint, if its essential spectrum is the set

$$(-\infty, -1] \cup [1, +\infty)$$

plus a discrete number of eigenvalues in the spectral gap $(-1, 1)$,

Magnetic case

When a external magnetic field B is present, one considers a magnetic potential $\mathbf{A}_B$ s. t. $curl\,\mathbf{A}_B = \mathbf{B}$.

One has then to replace ∇ with $\nabla_B = \nabla - i\mathbf{A}_B$

$$\mathbf{H_B} = -\mathbf{i}\,\alpha \cdot \nabla_\mathbf{B} + \beta$$

If we consider $H_B + V$, if this operator is self-adjoint, if its essential spectrum is the set

$$(-\infty, -1] \cup [1, +\infty)$$

plus a discrete number of eigenvalues in the spectral gap $(-1, 1)$,

Does $\lambda_1(B, V)$ ever leave the spectral gap $(-1, 1)$? and if yes, for which values of B ?

Eigenvalues below / in the middle of the continuous spectrum.

Spectrum of a self-adjoint operator A :

Eigenvalues below / in the middle of the continuous spectrum.

Spectrum of a self-adjoint operator A :

In the first case, $\lambda_1 = \min\limits_{x \neq 0} \dfrac{(Ax, x)}{||x||^2}$

Eigenvalues below / in the middle of the continuous spectrum.

Spectrum of a self-adjoint operator A :

In the first case, $\lambda_1 = \min\limits_{x \neq 0} \dfrac{(Ax, x)}{||x||^2}$

In the second case, $\lambda_1 = \min \ \max \dfrac{(Ax, x)}{||x||^2}$, $\lambda_1 = \max \ \min \dfrac{(Ax, x)}{||x||^2}$, $\ldots$

Abstract min-max theorem (Dolbeault, E., Séré, 2000)

Let $\mathcal{H}$ be a Hilbert space and $A : F = D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator defined on $\mathcal{H}$. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal subspaces of $\mathcal{H}$ satisfying: $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Define $F_\pm := P_\pm F$.

Abstract min-max theorem (Dolbeault, E., Séré, 2000)

Let $\mathcal{H}$ be a Hilbert space and $A : F = D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator defined on $\mathcal{H}$. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal subspaces of $\mathcal{H}$ satisfying: $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Define $F_\pm := P_\pm F$.

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

Abstract min-max theorem (Dolbeault, E., Séré, 2000)

Let $\mathcal{H}$ be a Hilbert space and $A : F = D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator defined on $\mathcal{H}$. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal subspaces of $\mathcal{H}$ satisfying: $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Define $F_\pm := P_\pm F$.

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

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

Abstract min-max theorem (Dolbeault, E., Séré, 2000)

Let $\mathcal{H}$ be a Hilbert space and $A : F = D(A) \subset \mathcal{H} \to \mathcal{H}$ a self-adjoint operator defined on $\mathcal{H}$. Let $\mathcal{H}_+$, $\mathcal{H}_-$ be two orthogonal subspaces of $\mathcal{H}$ satisfying: $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Define $F_\pm := P_\pm F$.

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

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

If (ii) $c_1 > a_-$,

then c_k is the k-th eigenvalue of A in the interval (a_-, b), where $b = \inf\,(\sigma_{\text{ess}}(A) \cap (a_-, +\infty))$.

Application to Dirac operators I

$$\psi : \mathbb{R}^3 \to \mathbb{C}^4 , \quad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \chi \end{pmatrix} , \quad \varphi, \chi : \mathbb{R}^3 \to \mathbb{C}^2$$

Application to Dirac operators I

$$\psi : \mathbb{R}^3 \to \mathbb{C}^4 , \quad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \chi \end{pmatrix} , \quad \varphi, \chi : \mathbb{R}^3 \to \mathbb{C}^2$$

Suppose that V satisfies

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

Application to Dirac operators I

$$\psi : \mathbb{R}^3 \to \mathbb{C}^4 , \quad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \varphi \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \chi \end{pmatrix} , \quad \varphi, \chi : \mathbb{R}^3 \to \mathbb{C}^2$$

Suppose that V satisfies

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

Then, for all $k \geq 1$,

$$\lambda_k(V) = \inf_{\substack{Y \text{ subspace of } C_o^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \dim Y = k}} \sup_{\varphi \in Y \setminus \{0\}} \sup_{\substack{\psi = \binom{\varphi}{\chi} \\ \chi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)}} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}$$

Application to Dirac operators II

The first eigenvalue of $H_0 + V$ in the spectral hole $(-1, 1)$ is given by

$$\lambda_1(V) := \inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}, \qquad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

Application to Dirac operators II

The first eigenvalue of $H_0 + V$ in the spectral hole $(-1, 1)$ is given by

$$\lambda_1(V) := \inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}, \qquad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

and

$$\lambda(\varphi) := \sup_{\substack{\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \\ \chi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)}} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}$$

Application to Dirac operators II

The first eigenvalue of $H_0 + V$ in the spectral hole $(-1, 1)$ is given by

$$\lambda_1(V) := \inf_{\varphi \neq 0} \sup_{\chi} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}, \qquad \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

and

$$\lambda(\varphi) := \sup_{\substack{\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \\ \chi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2)}} \frac{(\psi, (H_0 + V)\psi)}{(\psi, \psi)}$$

is the unique real number λ such that

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

Corollaries

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi)$$

Corollaries

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi)$$

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

Corollaries

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi)$$

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

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

and $\lambda_1(V)$ is the optimal constant in the above inequality.

Corollaries

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi)$$

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

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

and $\lambda_1(V)$ is the optimal constant in the above inequality.

Consequences:

- Robust and easy to implement algorithms.

Corollaries

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi)$$

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

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

and $\lambda_1(V)$ is the optimal constant in the above inequality.

Consequences:

- Robust and easy to implement algorithms.
- A new class of Hardy-like inequalities for the Dirac operator.

Corollaries

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi)$$

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

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

and $\lambda_1(V)$ is the optimal constant in the above inequality.

Consequences:

- Robust and easy to implement algorithms.
- A new class of Hardy-like inequalities for the Dirac operator.
- Very precise estimates for the magnetic case.

Towards a simple algorithm

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

Towards a simple algorithm

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

Let $A(\lambda)$ be the operator defined via the quadratic form and which acts on 2-spinors:

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

and consider its smallest eigenvalue, $\mu_1(\lambda)$.

Towards a simple algorithm

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

Let $A(\lambda)$ be the operator defined via the quadratic form and which acts on 2-spinors:

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

and consider its smallest eigenvalue, $\mu_1(\lambda)$.

Thanks to the monotonicity of $A(\lambda)$ with respect to λ, there exists a unique λ such that $\mu_1(\lambda) = 0$.

This λ is actually the first eigenvalue of A in the spectral gap $(-1, 1)$.

Discretization

Let us consider a n-dimensional space of functions from $\mathbb{R}^3$ into $\mathbb{C}^2$ spanned by $\varphi_1, \varphi_2, \ldots, \varphi_n$

Discretization

Let us consider a n-dimensional space of functions from $\mathbb{R}^3$ into $\mathbb{C}^2$ spanned by $\varphi_1, \varphi_2, \ldots, \varphi_n$

Define the $n \times n$ matrix $A_n(\lambda)$ whose entries are

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

Discretization

Let us consider a n-dimensional space of functions from $\mathbb{R}^3$ into $\mathbb{C}^2$ spanned by $\varphi_1, \varphi_2, \ldots, \varphi_n$

Define the $n \times n$ matrix $A_n(\lambda)$ whose entries are

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

Define $\mu_1^n(\lambda)$, the smallest eigenvalue of $A_n(\lambda)$

Discretization

Let us consider a n-dimensional space of functions from $\mathbb{R}^3$ into $\mathbb{C}^2$ spanned by $\varphi_1, \varphi_2, \ldots, \varphi_n$

Define the $n \times n$ matrix $A_n(\lambda)$ whose entries are

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

Define $\mu_1^n(\lambda)$, the smallest eigenvalue of $A_n(\lambda)$

Then, the unique zero of the map $\lambda \mapsto \mu_1^n(\lambda)$, λ_1^n, is an approximation of the first eigenvalue of $H + V$

Discretization

Let us consider a n-dimensional space of functions from $\mathbb{R}^3$ into $\mathbb{C}^2$ spanned by $\varphi_1, \varphi_2, \ldots, \varphi_n$

Define the $n \times n$ matrix $A_n(\lambda)$ whose entries are

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

Define $\mu_1^n(\lambda)$, the smallest eigenvalue of $A_n(\lambda)$

Then, the unique zero of the map $\lambda \mapsto \mu_1^n(\lambda)$, λ_1^n , is an approximation of the first eigenvalue of $H + V$

Somewhat related methods were introduced in the group of Baerends, in the Netherlands.

Some computations

We have used this method in:

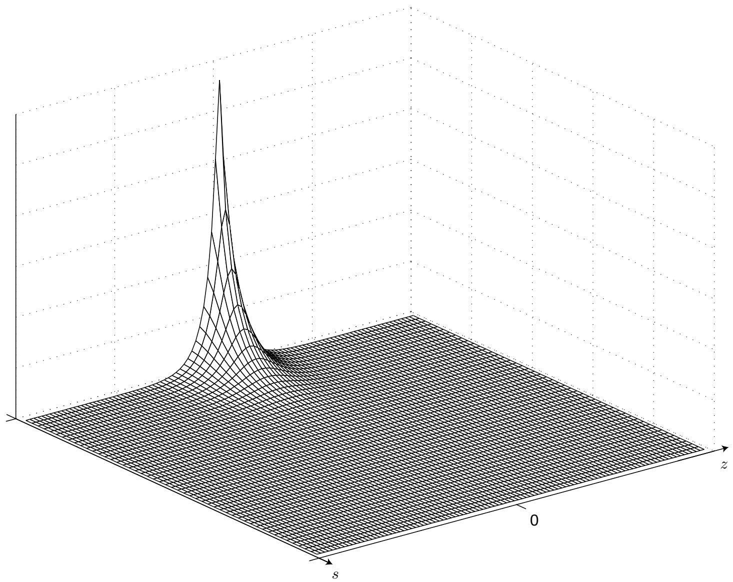
– **atomic computations** (basically a 1-d problem), for H, He^+, Cr^{23+} and Th^{89+}

Bases of Hermite polynomials or B-splines

– **Diatomic molecular computations** (in cylindrical coordinates a 2-d problem), for H_2^+ and Th_2^{179+}

B-splines

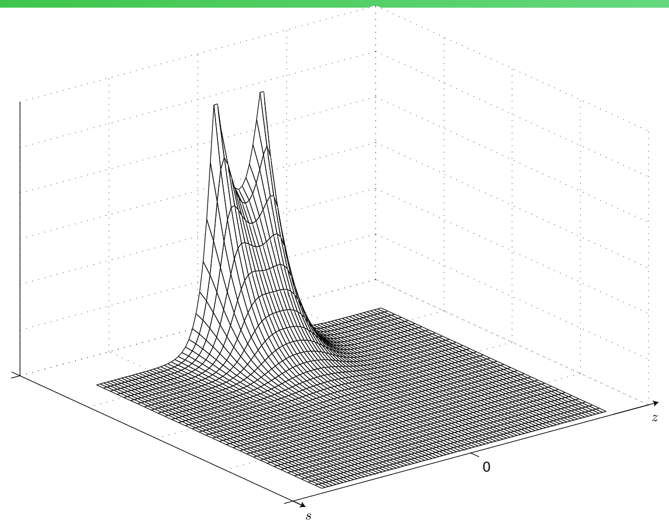
Some figures I



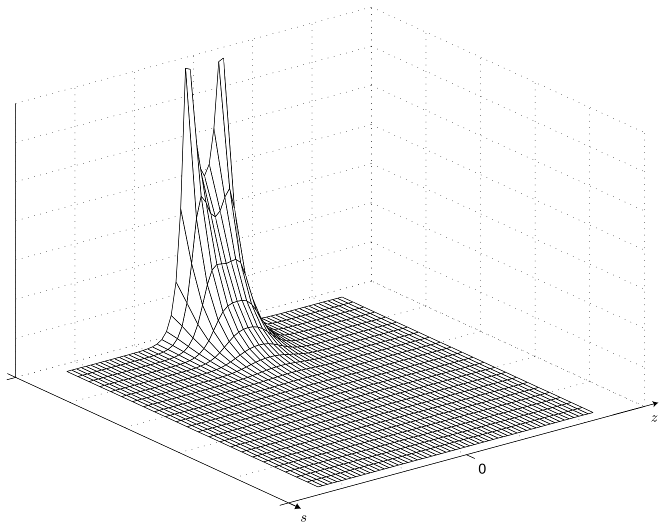
Ground state of Th^{89+} corresponding to $Z = 90$, an atom

J. Dolbeault, M.J. Esteban, E. Séré, M. Vanbreugel. *Phys. Rev. Letters* (2000)

Some figures II



Ground state of H_2^+ corresponding to $Z = 1$, two atoms



Ground state of Th_2^{179+} corresponding to $Z = 90$, two atoms

J. Dolbeault, M.J. Esteban, E. Séré. *Int. J. Quant. Chem.* (2003)

Hardy-like inequalities for Dirac operators I

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi) \ ; \quad \int_{\mathbb{R}^3} \left(\frac{|\sigma \cdot \nabla \varphi|^2}{1 - V + \lambda(\varphi)} + (1 - \lambda(\varphi)) \, |\varphi|^2 \right) dx = - \int_{\mathbb{R}^3} V \, |\varphi|^2 \, dx$$

Hardy-like inequalities for Dirac operators I

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2) \\ \varphi \neq 0}} \lambda(\varphi) \;\; ; \quad \int_{\mathbb{R}^3} \left(\frac{|\sigma \cdot \nabla \varphi|^2}{1 - V + \lambda(\varphi)} + (1 - \lambda(\varphi)) \, |\varphi|^2 \right) dx = - \int_{\mathbb{R}^3} V \, |\varphi|^2 \, dx$$

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

Hardy-like inequalities for Dirac operators I

$$\lambda_1(V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2) \\ \varphi\neq 0}} \lambda(\varphi) \ ; \quad \int_{\mathbb{R}^3} \left(\frac{|\sigma \cdot \nabla \varphi|^2}{1 - V + \lambda(\varphi)} + (1 - \lambda(\varphi))\, |\varphi|^2 \right) dx = - \int_{\mathbb{R}^3} V\, |\varphi|^2\, dx$$

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

We know that for $V_\nu = -\frac{\nu}{|x|}\,, \quad \nu \in (0,1)\,, \qquad \lambda_1(\nu/|x|) = \sqrt{1-\nu^2}$. From this,

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

Hardy-like inequalities for Dirac operators I

$$\lambda_1(V) = \inf_{\substack{\varphi\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \varphi\neq 0}} \lambda(\varphi)\ ; \quad \int_{\mathbb{R}^3}\left(\frac{|\sigma\cdot\nabla\,\varphi|^2}{1-V+\lambda(\varphi)}+(1-\lambda(\varphi))\,|\varphi|^2\right)dx = -\int_{\mathbb{R}^3} V\,|\varphi|^2\,dx$$

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

We know that for $V_\nu = -\frac{\nu}{|x|}\,,\quad \nu\in(0,1)\,,\qquad \lambda_1(\nu/|x|) = \sqrt{1-\nu^2}$. From this,

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

By taking the limit $\nu\to 1$, we get:

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

Hardy-like inequalities for Dirac operators II

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \frac{1}{|x|}} + |\varphi|^2 \right) dx \ \geq \ \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \,, \qquad \text{for all} \ \ \varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2) \,.$$

Hardy-like inequalities for Dirac operators II

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \frac{1}{|x|}} + |\varphi|^2 \right) dx \geq \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \,, \qquad \text{for all } \varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2) \,.$$

If we replace $\varphi(\cdot)$ by $\varepsilon^{-1}\varphi(\varepsilon^{-1}\cdot)$ and take the limit as $\varepsilon \to 0$, we obtain

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

$$\int_{\mathbb{R}^3} \left(\frac{|\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} \varphi|^2}{1 + \frac{1}{|x|}} + |\varphi|^2 \right) dx \geq \int_{\mathbb{R}^3} \frac{|\varphi|^2}{|x|} \, dx \,, \qquad \text{for all } \varphi \in H^1(\mathbb{R}^3, \mathbb{C}^2) \,.$$

If we replace $\varphi(\cdot)$ by $\varepsilon^{-1}\varphi(\varepsilon^{-1}\cdot)$ and take the limit as $\varepsilon \to 0$, we obtain

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

By taking $\varphi = (f, 0)$ with f purely real, we end up with

$$\int_{\mathbb{R}^3} |x| \, |\nabla f|^2 \geq \int_{\mathbb{R}^3} \frac{|f|^2}{|x|} \,, \qquad \text{for all } f \in H^1(\mathbb{R}^3, \mathbb{C}) \,,$$

which is itself equivalent to

$$\int_{\mathbb{R}^3} |\nabla u|^2 \, dx \geq \frac{1}{4} \int_{\mathbb{R}^3} \frac{|u|^2}{|x|^2} \, dx \qquad \text{for all } u \in H^1(\mathbb{R}^3, \mathbb{C}) \,.$$

Analytical proof of Hardy-Dirac inequalities

Consider the orbital angular momentum operator $\boldsymbol{L} = -i\,\boldsymbol{x} \wedge \boldsymbol{\nabla}$.
$\boldsymbol{L}$ acts only on the angular variables.

The spectrum of the operator $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ is the discrete set $\{\pm 1, \pm 2, \cdots\}$ (0 not included!). We denote by $P_{\pm}$ the projector related to $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ on $\mathbb{Z}^{\pm}$.

Analytical proof of Hardy-Dirac inequalities

Consider the orbital angular momentum operator $\boldsymbol{L} = -i\,\boldsymbol{x} \wedge \boldsymbol{\nabla}$.
$\boldsymbol{L}$ acts only on the angular variables.

The spectrum of the operator $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ is the discrete set $\{\pm 1, \pm 2, \cdots\}$ (0 not included!). We denote by $P_\pm$ the projector related to $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ on $\mathbb{Z}^\pm$.

Take $g = \left(1 + \sqrt{1-\nu^2} + \frac{\nu}{|x|}\right)^{-1/2}$ and a “good" h in

$$(**) \qquad \int_{\mathbb{R}^3} \left| \sqrt{g}\,(\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}) P_\pm \phi \pm \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})\,h}{\sqrt{g}}\, P_\pm \phi \right|^2 dx \geq 0\,,$$

develop the two squares and add them up.

Analytical proof of Hardy-Dirac inequalities

Consider the orbital angular momentum operator $\boldsymbol{L} = -i\,\boldsymbol{x} \wedge \boldsymbol{\nabla}$.
$\boldsymbol{L}$ acts only on the angular variables.

The spectrum of the operator $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ is the discrete set $\{\pm 1, \pm 2, \cdots\}$ (0 not included!). We denote by $P_\pm$ the projector related to $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ on $\mathbb{Z}^\pm$.

Take $g = \left(1 + \sqrt{1-\nu^2} + \frac{\nu}{|x|}\right)^{-1/2}$ and a “good" h in

$$(**) \qquad \int_{\mathbb{R}^3} \left| \sqrt{g}\, (\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}) P_\pm \phi \pm \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})\, h}{\sqrt{g}}\, P_\pm \phi \right|^2 dx \geq 0 \,,$$

develop the two squares and add them up.

We get (Dolbeault - E. - Loss - Vega) :

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

Analytical proof of Hardy-Dirac inequalities

Consider the orbital angular momentum operator $\boldsymbol{L} = -i\,\boldsymbol{x} \wedge \boldsymbol{\nabla}$.
$\boldsymbol{L}$ acts only on the angular variables.

The spectrum of the operator $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ is the discrete set $\{\pm 1, \pm 2, \cdots\}$ (0 not included!). We denote by $P_\pm$ the projector related to $1 + \boldsymbol{\sigma} \cdot \boldsymbol{L}$ on $\mathbb{Z}^\pm$.

Take $g = \left(1 + \sqrt{1-\nu^2} + \frac{\nu}{|x|}\right)^{-1/2}$ and a “good" h in

$$(**) \qquad \int_{\mathbb{R}^3} \left| \sqrt{g}\,(\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}) P_\pm \phi \pm \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})\,h}{\sqrt{g}} P_\pm \phi \right|^2 dx \ \geq\ 0\,,$$

develop the two squares and add them up.

We get (Dolbeault - E. - Loss - Vega) :

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

Since $\boldsymbol{L}$ acts only on the angular variables, we can add up the two inequalities $(**)$ without getting extra cross terms, only if g and h are radially symmetric! And we get $(*)$.

But multipolar potentials are not radially symmetric!

Application to magnetic Dirac operators

The smallest eigenvalue of $H_B + V = -i\,\alpha\cdot(\nabla - iA_B) + \beta$ in the spectral gap $(-1, 1)$ satisfies:

$$\lambda_1(B, V) = \inf_{\substack{\varphi\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \varphi\neq 0}} \lambda^B(\varphi)$$

Application to magnetic Dirac operators

The smallest eigenvalue of $H_B + V = -i\,\alpha \cdot (\nabla - iA_B) + \beta$ in the spectral gap $(-1,1)$ satisfies:

$$\lambda_1(B,V) = \inf_{\substack{\varphi \in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2) \\ \varphi \neq 0}} \lambda^B(\varphi)$$

$$\int_{\mathbb{R}^3} \Big(\frac{|\sigma \cdot \nabla_B \varphi|^2}{1 - V + \lambda^B(\varphi)} + (V + 1 - \lambda^B(\varphi))|\varphi|^2 \Big) dx \;=\; 0$$

Application to magnetic Dirac operators

The smallest eigenvalue of $H_B + V = -i\,\alpha\cdot(\nabla - iA_B) + \beta$ in the spectral gap $(-1,1)$ satisfies:

$$\lambda_1(B,V) = \inf_{\substack{\varphi\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \varphi\neq 0}} \lambda^B(\varphi)$$

$$\int_{\mathbb{R}^3}\Big(\frac{|\sigma\cdot\nabla_B\varphi|^2}{1-V+\lambda^B(\varphi)} + (V+1-\lambda^B(\varphi))|\varphi|^2\Big)dx \;=\; 0$$

$$\boxed{\int_{\mathbb{R}^3}\frac{|(\sigma\cdot\nabla_B)\varphi|^2}{1+\lambda_1(B,V_\nu)+\frac{\nu}{|x|}}\,dx + (1-\lambda_1(B,V_\nu))\int_{\mathbb{R}^3}|\varphi|^2\,dx \;\geq\; \int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\varphi|^2\,dx}$$

Application to magnetic Dirac operators

The smallest eigenvalue of $H_B + V = -i\,\alpha\cdot(\nabla - iA_B) + \beta$ in the spectral gap $(-1,1)$ satisfies:

$$\lambda_1(B,V) = \inf_{\substack{\varphi\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \varphi\neq 0}} \lambda^B(\varphi)$$

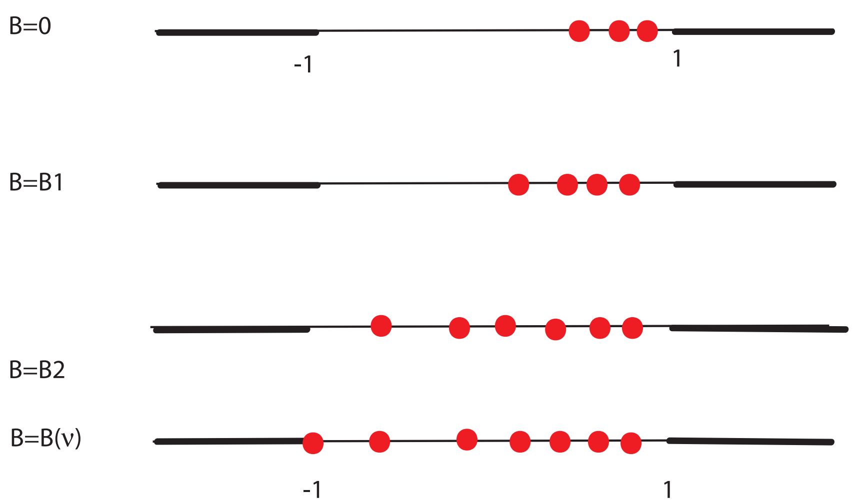
$$\int_{\mathbb{R}^3}\Big(\frac{|\sigma\cdot\nabla_B\varphi|^2}{1-V+\lambda^B(\varphi)} + (V+1-\lambda^B(\varphi))|\varphi|^2\Big)dx \;=\; 0$$

$$\boxed{\int_{\mathbb{R}^3}\frac{|(\sigma\cdot\nabla_B)\varphi|^2}{1+\lambda_1(B,V_\nu)+\frac{\nu}{|x|}}\,dx + (1-\lambda_1(B,V_\nu))\int_{\mathbb{R}^3}|\varphi|^2\,dx \;\geq\; \int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\varphi|^2\,dx}$$

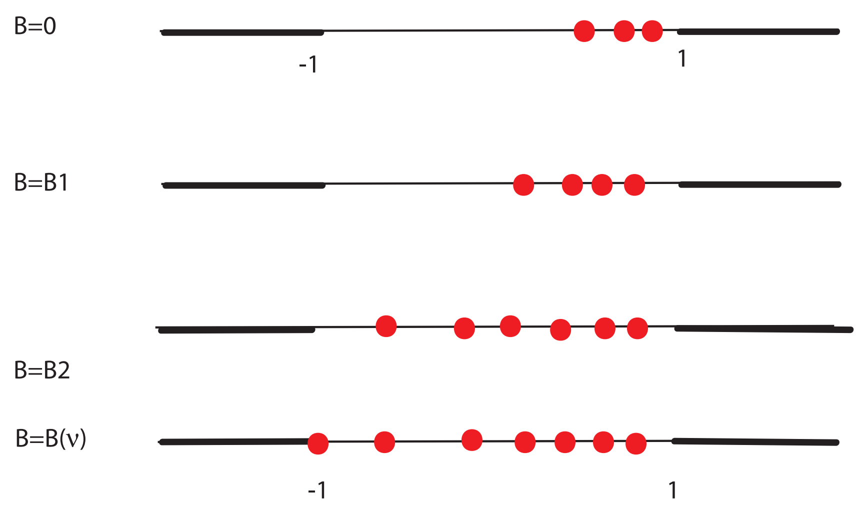
QUESTIONS : When do we have $\lambda_1(B,V)\in(-1,1)$?

If the eigenvalue $\lambda_1(B,V)$ leaves the interval $(-1,1)$, when ?

For a potential $V = V_\nu := -\frac{\nu}{|x|}, \quad \nu \in (0,1), \qquad 0 < B1 < B2 < B(\nu)$:



For a potential $V = V_\nu := -\frac{\nu}{|x|}, \quad \nu \in (0,1), \qquad 0 < B1 < B2 < B(\nu)$:



DEFINITION:

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

Some results (with J. Dolbeault and M. Loss)

$$V_\nu = -\frac{\nu}{|x|}, \quad \mathbf{A}_B(x) := \frac{B}{2}\begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix}, \quad \mathbf{B}(x) := \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix} \; ; \; \nu \in (0,1), \quad B \geq 0$$

Some results (with J. Dolbeault and M. Loss)

$$V_\nu = -\frac{\nu}{|x|}, \quad \mathbf{A}_B(x) := \frac{B}{2}\begin{pmatrix}-x_2\\ x_1\\ 0\end{pmatrix}, \quad \mathbf{B}(x) := \begin{pmatrix}0\\ 0\\ B\end{pmatrix}\ ;\ \nu \in (0,1), \ \ B \geq 0$$

- For $B = 0$, $\lambda_1(0, V_\nu) = \sqrt{1-\nu^2} \ \in (-1,1)$

Some results (with J. Dolbeault and M. Loss)

$$V_\nu = -\frac{\nu}{|x|}, \quad \mathbf{A}_B(x) := \frac{B}{2}\begin{pmatrix}-x_2\\ x_1\\ 0\end{pmatrix}, \quad \mathbf{B}(x) := \begin{pmatrix}0\\ 0\\ B\end{pmatrix}\ ;\ \nu \in (0,1), \ \ B \geq 0$$

- For $B = 0$, $\lambda_1(0, V_\nu) = \sqrt{1-\nu^2} \in (-1,1)$
- For all $B \geq 0$, $\lambda_1(B, V_\nu) < 1$

Some results (with J. Dolbeault and M. Loss)

$$V_\nu = -\frac{\nu}{|x|}, \quad \mathbf{A}_B(x) := \frac{B}{2}\begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix}, \quad \mathbf{B}(x) := \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix} \; ; \; \nu \in (0,1), \quad B \geq 0$$

- For $B = 0$, $\lambda_1(0, V_\nu) = \sqrt{1-\nu^2} \in (-1, 1)$
- For all $B \geq 0$, $\lambda_1(B, V_\nu) < 1$
- For all $\nu \in (0,1)$ there exists a critical field strength $B(\nu)$ such that

$$\lambda_1(B, V_\nu) \leq -1 \quad \text{if} \quad B \geq B(\nu)$$

Some results (with J. Dolbeault and M. Loss)

$$V_\nu = -\frac{\nu}{|x|}, \quad \mathbf{A}_B(x) := \frac{B}{2}\begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix}, \quad \mathbf{B}(x) := \begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix} \; ; \; \nu \in (0,1), \;\; B \geq 0$$

- For $B = 0$, $\lambda_1(0, V_\nu) = \sqrt{1-\nu^2} \in (-1,1)$
- For all $B \geq 0$, $\lambda_1(B, V_\nu) < 1$
- For all $\nu \in (0,1)$ there exists a critical field strength $B(\nu)$ such that

$$\lambda_1(B, V_\nu) \leq -1 \quad \text{if} \quad B \geq B(\nu)$$

- $\lim_{\nu \to 1} B(\nu) > 0\,,$ $\qquad \lim\limits_{\nu \to 0} \nu \log B(\nu) = \pi$

Some results (with J. Dolbeault and M. Loss)

$$V_\nu = -\frac{\nu}{|x|}, \quad \mathbf{A}_B(x) := \frac{B}{2}\begin{pmatrix}-x_2\\ x_1\\ 0\end{pmatrix}, \quad \mathbf{B}(x) := \begin{pmatrix}0\\0\\B\end{pmatrix}\ ;\ \nu \in (0,1), \quad B \geq 0$$

- For $B = 0$, $\lambda_1(0, V_\nu) = \sqrt{1-\nu^2} \in (-1, 1)$
- For all $B \geq 0$, $\lambda_1(B, V_\nu) < 1$
- For all $\nu \in (0,1)$ there exists a critical field strength $B(\nu)$ such that

$$\lambda_1(B, V_\nu) \leq -1 \quad \text{if} \quad B \geq B(\nu)$$

- $\lim_{\nu \to 1} B(\nu) > 0\,,$ $\qquad \lim\limits_{\nu \to 0} \nu \log B(\nu) = \pi$
- For ν small, the asymptotics of $B(\nu)$ can be calculated by an approximation in the first relativistic "Landau level".

How to determine $B(\nu)$?

$$\int_{\mathbb{R}^3} \frac{|(\sigma\cdot\nabla_B)\varphi|^2}{1+\lambda_1(B,V_\nu)+\frac{\nu}{|x|}}\,dx + (1-\lambda_1(B,V_\nu))\int_{\mathbb{R}^3}|\varphi|^2\,dx \geq \int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\varphi|^2\,dx$$

How to determine $B(\nu)$?

$$\int_{\mathbb{R}^3} \frac{|(\sigma\cdot\nabla_B)\varphi|^2}{1+\lambda_1(B,V_\nu)+\frac{\nu}{|x|}}\,dx + (1-\lambda_1(B,V_\nu))\int_{\mathbb{R}^3}|\varphi|^2\,dx \geq \int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\varphi|^2\,dx$$

and we are looking for $B_n \longrightarrow B(\nu)$ such that $\lambda_1(B_n,\nu) \longrightarrow -1$.

If everything were compact, we would be able to pass to the limit and obtain

$$\int_{\mathbb{R}^3} \frac{|x|\,|(\sigma\cdot\nabla_{B(\nu)})\varphi|^2}{\nu} - \int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\varphi|^2\,dx + 2\int_{\mathbb{R}^3}|\varphi|^2\,dx \geq 0$$

How to determine $B(\nu)$?

$$\int_{\mathbb{R}^3} \frac{|(\sigma\cdot\nabla_B)\varphi|^2}{1+\lambda_1(B,V_\nu)+\frac{\nu}{|x|}}\,dx\;+(1-\lambda_1(B,V_\nu))\int_{\mathbb{R}^3}|\varphi|^2\,dx\;\geq\;\int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\varphi|^2\,dx$$

and we are looking for $B_n \longrightarrow B(\nu)$ such that $\lambda_1(B_n,\nu)\longrightarrow -1$.

If everything were compact, we would be able to pass to the limit and obtain

$$\int_{\mathbb{R}^3}\frac{|x|\,|(\sigma\cdot\nabla_{B(\nu)})\varphi|^2}{\nu}-\int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\varphi|^2\,dx+2\int_{\mathbb{R}^3}|\varphi|^2\,dx\geq 0$$

Now define the functional

$$\mathcal{E}_{B,\nu}[\phi]:=\int_{\mathbb{R}^3}\frac{|x|}{\nu}\,|(\sigma\cdot\nabla_B)\,\phi|^2\,dx-\int_{\mathbb{R}^3}\frac{\nu}{|x|}\,|\phi|^2\,dx\ ,$$

If everything were compact and “nice",

$$\mu_{B(\nu),\nu}+2=0\ ;\qquad\qquad \mu_{B,\nu}:=\inf\left\{\mathcal{E}_{B,\nu}[\phi]\,;\quad\int_{\mathbb{R}^3}|\varphi|^2\,dx=1\right\}.$$

If everything were compact and “nice",

$$\mu_{B(\nu),\nu} + 2 = 0\ ; \qquad \mu_{B,\nu} := \inf\left\{\mathcal{E}_{B,\nu}[\phi]\ ; \quad \int_{\mathbb{R}^3} |\varphi|^2\,dx = 1\right\}.$$

If everything were compact and “nice",

$$\mu_{B(\nu),\nu} + 2 = 0 \; ; \qquad \mu_{B,\nu} := \inf \left\{ \mathcal{E}_{B,\nu}[\phi] \, ; \quad \int_{\mathbb{R}^3} |\varphi|^2 \, dx = 1 \right\} .$$

A very nice property is that the scaling $\phi_B := B^{3/4} \, \phi \left(B^{1/2} \, x \right)$ preserves the L^2 norm and $\mathcal{E}_{B,\nu}[\phi_B] = \sqrt{B} \, \mathcal{E}_{1,\nu}[\phi]$.

If everything were compact and “nice",

$$\mu_{B(\nu),\nu} + 2 = 0\ ; \qquad \mu_{B,\nu} := \inf\left\{\mathcal{E}_{B,\nu}[\phi]\ ; \quad \int_{\mathbb{R}^3} |\varphi|^2\, dx = 1\right\}.$$

A very nice property is that the scaling $\phi_B := B^{3/4}\,\phi\left(B^{1/2}\,x\right)$ preserves the L^2 norm and $\mathcal{E}_{B,\nu}[\phi_B] = \sqrt{B}\,\mathcal{E}_{1,\nu}[\phi]$.

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

we have $\mu_{B,\nu} = \sqrt{B}\,\mu(\nu)$.

THM : $\sqrt{B(\nu)}\,\mu(\nu) + 2 = 0$ which is equivalent to $B(\nu) = \frac{4}{\mu(\nu)^2}$.

If everything were compact and “nice",

$$\mu_{B(\nu),\nu} + 2 = 0 \; ; \qquad \mu_{B,\nu} := \inf \left\{ \mathcal{E}_{B,\nu}[\phi] \; ; \quad \int_{\mathbb{R}^3} |\varphi|^2 \, dx = 1 \right\}.$$

A very nice property is that the scaling $\phi_B := B^{3/4} \, \phi \left(B^{1/2} \, x \right)$ preserves the L^2 norm and $\mathcal{E}_{B,\nu}[\phi_B] = \sqrt{B} \, \mathcal{E}_{1,\nu}[\phi]$.

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

we have $\mu_{B,\nu} = \sqrt{B} \, \mu(\nu)$.

THM : $\sqrt{B(\nu)} \, \mu(\nu) + 2 = 0$ which is equivalent to $B(\nu) = \frac{4}{\mu(\nu)^2}$.

Now we would like to estimate $B(\nu)$. This can be done analytically or/and numerically. As we said before, analytically we have some estimates for ν close to 0 and to 1.

The Landau level approximation

Consider the class of functions $\mathcal{A}(B,\nu)$:

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

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

$$\phi(x) = \sum_\ell f_\ell(x_3)\,\phi_\ell(x_1,x_2)\,, \qquad z := x_3\,.$$

The Landau level approximation

Consider the class of functions $\mathcal{A}(B,\nu)$:

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

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

$$\phi(x) = \sum_\ell f_\ell(x_3)\,\phi_\ell(x_1,x_2)\,, \qquad z := x_3\,.$$

Now, we shall restrict the functional $\mathcal{E}_{B,\nu}$ to the first Landau level. In this framework, that we shall call the Landau level ansatz, we also define a critical field by

$$B_{\mathcal{L}}(\nu) := \inf\left\{B > 0\ :\ \liminf_{b \nearrow B} \lambda_1^{\mathcal{L}}(b,\nu) = -1\right\}\,,$$

where

$$\lambda_1^{\mathcal{L}}(b,\nu) := \inf_{\phi \in \mathcal{A}(B,\nu)\,,\ \Pi^\perp \phi = 0} \lambda[\phi,b,\nu]\,.$$

THEOREM : $B^{\mathcal{L}}(\nu) = \frac{4}{\mu^{\mathcal{L}}(\nu)^2}$, where

$$\mu^{\mathcal{L}}(\nu) := \inf_f \frac{\mathcal{L}_\nu[f]}{\|f\|^2_{L^2(\mathbb{R}^+)}} < 0 \, .$$

THEOREM : $B^{\mathcal{L}}(\nu) = \frac{4}{\mu^{\mathcal{L}}(\nu)^2}$, where

$$\mu^{\mathcal{L}}(\nu) := \inf_f \quad \frac{\mathcal{L}_\nu[f]}{\|f\|^2_{L^2(\mathbb{R}^+)}} < 0\,.$$

$$\mathcal{L}_\nu[f] = \frac{1}{\nu}\int_0^\infty b(z)\, f'^2\, dz - \nu \int_0^\infty a(z)\, f^2\, dz$$

$$b(z) = \int_0^\infty \sqrt{s^2+z^2}\, s\, e^{-s^2/2}\, ds \quad \text{and} \quad a(z) = \int_0^\infty \frac{s\, e^{-s^2/2}}{\sqrt{s^2+z^2}}\, ds\ .$$

THEOREM : $B^{\mathcal{L}}(\nu) = \frac{4}{\mu^{\mathcal{L}}(\nu)^2}$, where

$$\mu^{\mathcal{L}}(\nu) := \inf_f \frac{\mathcal{L}_\nu[f]}{\|f\|^2_{L^2(\mathbb{R}^+)}} < 0\,.$$

$$\mathcal{L}_\nu[f] = \frac{1}{\nu} \int_0^\infty b(z)\, f'^2\, dz - \nu \int_0^\infty a(z)\, f^2\, dz$$

$$b(z) = \int_0^\infty \sqrt{s^2 + z^2}\, s\, e^{-s^2/2}\, ds \quad \text{and} \quad a(z) = \int_0^\infty \frac{s\, e^{-s^2/2}}{\sqrt{s^2 + z^2}}\, ds\ .$$

COROLLARY. $\mu(\nu) \leq \mu^{\mathcal{L}}(\nu) < 0 \quad \Longrightarrow \quad B(\nu) \leq B^{\mathcal{L}}(\nu)\,.$

Final results

THEOREM. For $\nu \in (0, \nu_0)$, $$B^{\mathcal{L}}(\nu + \nu^{3/2}) \leq B(\nu) \leq B^{\mathcal{L}}(\nu)$$

Final results

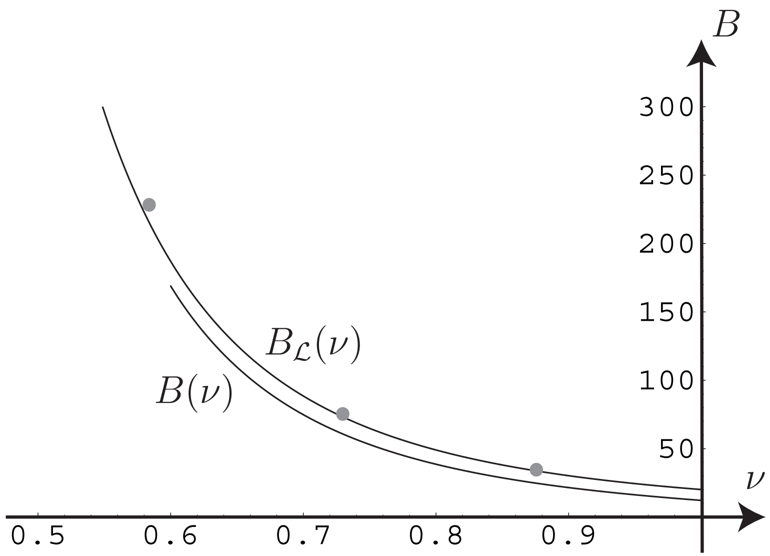
THEOREM. For $\nu \in (0, \nu_0)$, $\quad B^{\mathcal{L}}(\nu + \nu^{3/2}) \leq B(\nu) \leq B^{\mathcal{L}}(\nu)$

THEOREM. $\quad \lim_{\nu \to 0} \nu \log B^{\mathcal{L}}(\nu) = \pi \,.$

Final results

THEOREM. For $\nu \in (0, \nu_0)$, $\quad B^{\mathcal{L}}(\nu + \nu^{3/2}) \le B(\nu) \le B^{\mathcal{L}}(\nu)$

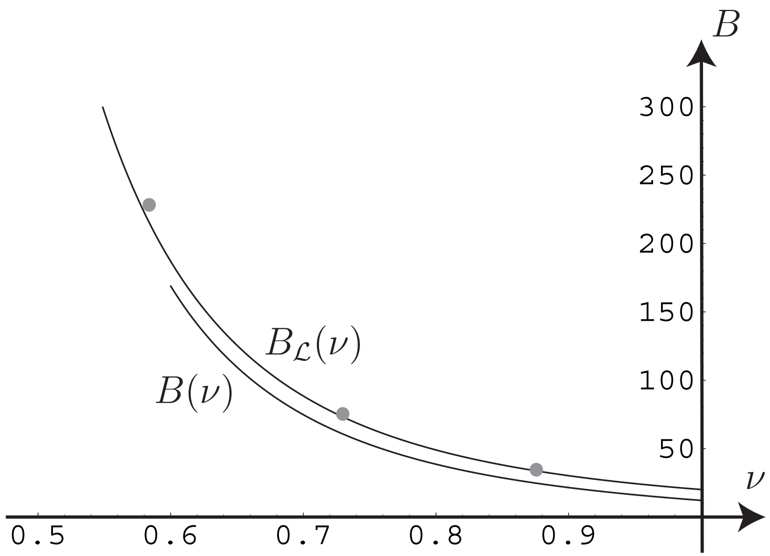
THEOREM. $\quad \lim_{\nu \to 0} \nu \log B^{\mathcal{L}}(\nu) = \pi \,.$



Final results

THEOREM. For $\nu \in (0, \nu_0)$, $$B^{\mathcal{L}}(\nu + \nu^{3/2}) \leq B(\nu) \leq B^{\mathcal{L}}(\nu)$$

THEOREM. $$\lim_{\nu \to 0} \nu \log B^{\mathcal{L}}(\nu) = \pi \,.$$



NUMERICAL OBSERVATION. For ν near 1, $B(\nu)$ is below $B^{\mathcal{L}}(\nu)$ by 30%.