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

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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

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ω is an eigenvalue of $\mathbf{H_0} + V$ with associated eigenfunction φ iff $\psi(t,x) := e^{-i\omega t}\varphi(x)$ is a solution of

$$i\psi_t + \mathbf{H_0}\psi + V\psi = 0 \quad \text{in} \quad \mathbb{R}\times\mathbb{R}^3$$

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Its spectrum is given by:

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

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

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

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

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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 $F_\pm := P_\pm F$.

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

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If (ii) $c_1 > a_-$, then c_k is the k-th eigenvalue of A in the interval (a_-, b), where $b = \inf\,(\sigma_{\mathrm{ess}}(A) \cap (a_-, +\infty))$.

Application to magnetic Dirac operators I

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Then, for all $k \geq 1$,

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

Application to magnetic Dirac operators II

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

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is the unique real number λ such that

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

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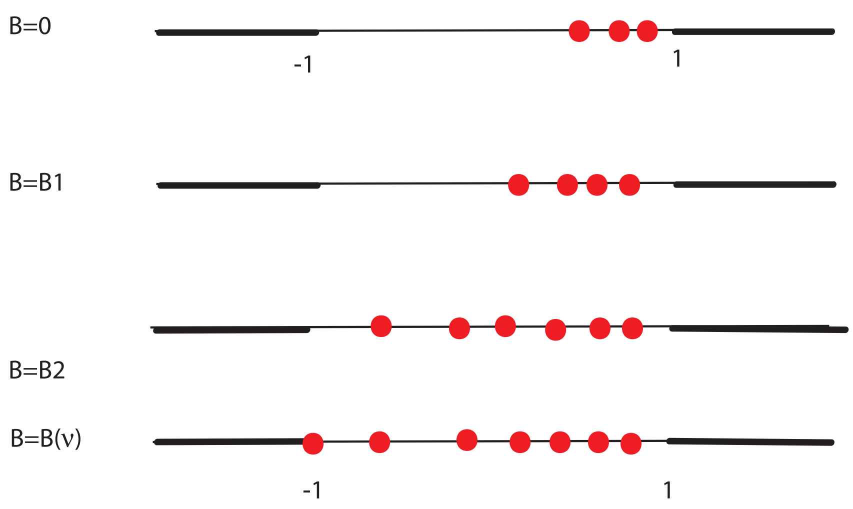
QUESTIONS : When do we have $\lambda_1(B,V)\in(-1,1)$?

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

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



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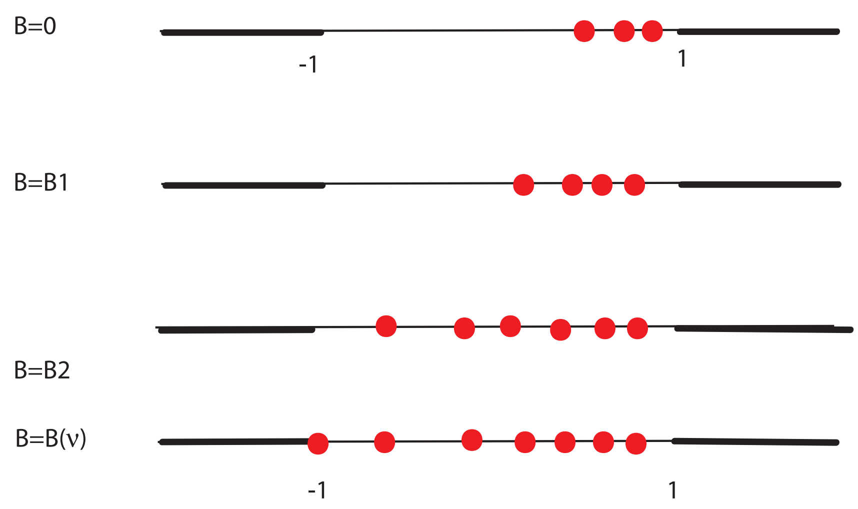

DEFINITION: $$B(\nu) := \inf \left\{ B > 0 \ : \ \liminf_{b \nearrow B} \lambda_1(B,\nu) = -1 \right\} . \qquad (1)$$

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

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

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- For ν small, the asymptotics of $B(\nu)$ can be calculated by an approximation in the first relativistic "Landau level".

How to determine $B(\nu)$?

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

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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 $B(\nu)$?

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

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

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

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",

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

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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 $\mathcal{E}_{B,\nu}[\phi_B] = \sqrt{B}\,\mathcal{E}_{1,\nu}[\phi]\;.$

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

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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 $\mathcal{A}(B,\nu)$:

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

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

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

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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

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

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

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

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

Final results

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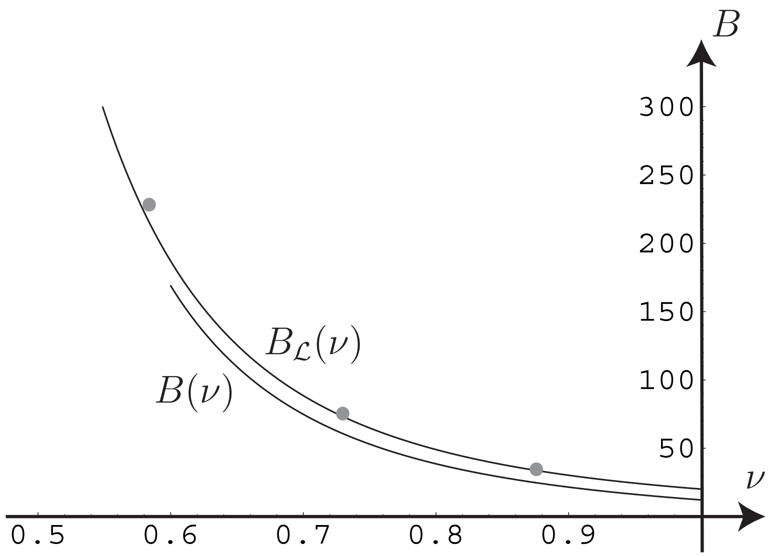

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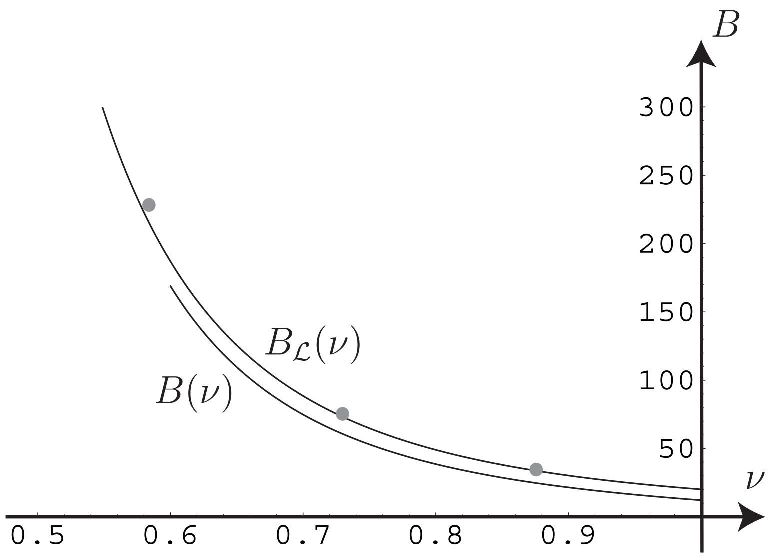

NUMERICAL OBSERVATION. For ν near 1, $B(\nu)$ is below $B^{\mathcal{L}}(\nu)$ by 30%.