Relativistic hydrogenic atoms in strong magnetic fields

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Outline of the talk

- Introduction
- Min–max characterization of the ground state energy
- Critical magnetic field
- Asymptotics for the critical magnetic field
- Numerical computations

Introduction

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

N.B. The earth's magnetic field is of the order of 1 Gauss $= 10^{-4}$ Tesla

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

As $B \nearrow$, $\lambda_1(\nu, B) \to -1$: Critical field strength $B(\nu)$ such that $\lambda_1(\nu, B(\nu)) = -1$

Our first main result is a rough estimate of

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

A non perturbative result based on min-max formulations

Relativistic lowest Landau level

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

Min–max characterization of the ground state energy

Magnetic Dirac Hamiltonian

$H_B\,\psi - \frac{\nu}{|x|}\,\psi = \lambda\,\psi$ is an equation for four complex functions $\psi = \binom{\phi}{\chi}$ 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 $P_B := -\,i\,\sigma\cdot(\nabla - i\,A_B(x))$

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

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

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

Theorem 1. *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, $(-1, 1)$

Scalings

Lemma 2. *Let $B \geq 0$, $\lambda \geq -1$, $\theta > 0$ and $\phi_\theta(x) := \theta^{3/2}\phi(\theta\, x)$. Then*

$$\nabla_{A_{\theta^2 B}}\phi_\theta(x) = \theta^{5/2}\left[\nabla\phi(\theta\, x) - i\, A_B(\theta\, x)\, \phi(\theta\, x)\right]$$

and for any $a \in \mathbb{R}$, $\nu \in (0,1)$,

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

Proposition 3. *For all $\nu \in (0,1)$, $B \mapsto \lambda_1(\nu, B)$ is Lipschitz continuous as long as it takes its values in $(-1, +\infty)$ and*

$$\frac{\lambda_1(\nu, \theta^2 B)}{\theta} - \frac{\theta - 1}{\theta} \leq \lambda_1(\nu, B) \leq \frac{\lambda_1(\nu, \theta^2 B)}{\theta} + \frac{\theta - 1}{\theta}$$

if $\lambda_1(\nu, B) \in (-1, +\infty)$ and $\theta \in (1, 2/(1 - \lambda_1(\nu, B)))$

Proposition 4. *Let* $\nu \in (0,1)$*. Then for* B *large enough,* $\lambda_1(\nu, B) \leq 0$ *and there exists* $B^* > 0$ *such that* $\lambda_1(\nu, B) = -1$ *for any* $B \geq B^*$

Proof. Consider

$$\phi = \sqrt{\frac{B}{2\,\pi}}\, e^{-B(|x_1|^2+|x_2|^2)/4} \begin{pmatrix} f(x_3) \\ 0 \end{pmatrix}, \quad \chi \equiv 0$$

and $f \in C_0^\infty(\mathbb{R}, \mathbb{R})$ is such that $f \equiv 1$ for $|x| \leq \delta$, δ small but fixed, and $\|f\|_{L^2(\mathbb{R})} = 1$

$$G_B[\phi] := \int_{\mathbb{R}^3} \left(\frac{r}{\nu}\, |P_B \phi|^2 - \frac{\nu}{r}\, |\phi|^2 \right) d^3x \leq \frac{C_1}{\nu} + C_2\, \nu - C_3\, \nu \log B$$

For B large enough, $G_B[\phi] + 2\, \|\phi\|^2 \leq 0$, $J[\phi, -1, \nu, B] \leq 0$ and $\lambda_1(\nu, B) = -1$

□

Critical magnetic field

The critical magnetic field

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

Corollary 5. *For all* $\nu \in (0,1)$, $\lambda_1(\nu, B) \le \frac{\theta - 1}{\theta} < 1$ *for any* $B \in (0, B(\nu))$

The previous computations show that $B(\nu) \le e^{\,C/\nu^2}$, for all $\nu \in (0,1)$

Theorem 6. *For all* $\nu \in (0,1)$, *there exists a constant* $C > 0$ *such that*

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

Proof. Consider the trial function $\psi = \binom{\phi}{0}$, $\phi = \left(\frac{B}{2\pi}\right)^{3/4} e^{-B\,|x|^2/4} \binom{1}{0}$

Proof (1/2)

$$G_B[\phi] = B^2 \int \frac{r\,|x_3|^2}{4\,\nu}\,|\phi|^2\,d^3x - \int \frac{\nu}{r}\,|\phi|^2\,d^3x$$

$$= \quad (2\pi)^{-\frac{3}{2}}\,B^{\frac{1}{2}}\left[\frac{\pi}{2\,\nu}\int_0^\infty e^{-r^2/2}\,r^5\,dr\int_0^\pi \cos^2\theta\,\sin\theta\,d\theta - 4\,\pi\,\nu\int_0^\infty e^{-r^2/2}\,r\,dr\right]$$

$$= \quad (2\pi)^{-\frac{3}{2}}\,B^{\frac{1}{2}}\left[\frac{\pi}{3\,\nu}\int_0^\infty e^{-r^2/2}r^5dr - 4\,\pi\,\nu\int_0^\infty e^{-r^2/2}\,r\,dr\right]$$

$$= \quad (2\pi)^{-\frac{3}{2}}\,B^{\frac{1}{2}}\left[\frac{8\,\pi}{3\,\nu} - 4\,\pi\,\nu\right]$$

If $\nu^2 \in (2/3, 1)$ and $\sqrt{B} \geq \frac{3\,\sqrt{2\,\pi}\,\nu}{3\,\nu^2-2}$, then $G_B[\phi] \leq -2 = -||\phi||_2$ and so $\lambda_1(\nu, B) = -1$, which proves the first estimate

Proof (2/2)

For all $\nu \in (0,1)$, $B(\nu) \geq \frac{4}{5\,\nu^2}$ and

$$G_B[\phi] = \int_{\mathbb{R}^3} \frac{|x|}{\nu}\,|P_B\phi|^2\,d^3x - \int_{\mathbb{R}^3} \frac{\nu}{|x|}\,|\phi|^2\,d^3x \geq -\nu\,\sqrt{5B}\int_{\mathbb{R}^3} |\phi|^2\,d^3x$$

1. Scale the function ϕ according to $\phi_B := B^{3/4}\,\phi\left(B^{1/2}\,x\right)$ so that $G_B[\phi_B] = \sqrt{B}\,G_1[\phi]$
2. Use the truncation function

$$t(r) = \begin{cases} 1 & \text{if } r \leq R \\ R/r & \text{if } r \geq R \end{cases}$$

3. Use spectral information on $\sigma \cdot L$

Asymptotics for the critical magnetic field

For small values of ν, $B(\nu) \sim$?

Landau levels

Lowest energy level in the gap is expected to behave as $B \to \infty$ like the eigenfunctions associated to the lowest levels of the Landau operator

$$L_B := -\, i\, \sigma_1\, \partial_{x_1} - \, i\, \sigma_2\, \partial_{x_2} - \sigma \cdot A_B(x)$$

Goal: small coupling limit $\nu \to 0^+$ and $B \to \infty$

Lemma 7. *The operator L_B in $L^2(\mathbb{R}^2, \mathbb{C}^2)$ has discrete spectrum $\{2nB \,:\, n \in \mathbb{N}\}$, each eigenvalue being infinitely degenerate*

Ker(L_B) *is generated by*

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

Diagonalization of the free magnetic Dirac Hamiltonian

$$K_B = \begin{pmatrix} \mathbb{I} & P_B \\ P_B & -\mathbb{I} \end{pmatrix} = \sqrt{\mathbb{I} + P_B^2} \begin{pmatrix} R & Q \\ Q & -R \end{pmatrix} ,$$

where R and Q are operators acting on 2 spinors, given by

$$R = \frac{1}{\sqrt{\mathbb{I} + P_B^2}} , \quad Q = \frac{P_B}{\sqrt{\mathbb{I} + P_B^2}}$$

$$U = \frac{1}{\sqrt{2\,(\mathbb{I} - R)}} \begin{pmatrix} Q & R - \mathbb{I} \\ \mathbb{I} - R & Q \end{pmatrix} , \qquad U^* K_B\, U = \begin{pmatrix} \sqrt{\mathbb{I} + P_B^2} & 0 \\ 0 & -\sqrt{\mathbb{I} + P_B^2} \end{pmatrix}$$

Price to pay: $P := U^* V U = \begin{pmatrix} p & q \\ q^* & t \end{pmatrix}$, R, Q, U... depend on B

The Dirac energy for an electronic wave function $Z = \binom{X}{Y}$

$$\mathcal{E}_\nu[Z] := \mathcal{K}[Z] - \nu\,(Z, P\,Z)$$

$$\mathcal{K}[Z] := (Z, U^* K_B\, U Z) = \Big(X, \sqrt{\mathbb{I} + P_B^2}\, X\Big) - \Big(Y, \sqrt{\mathbb{I} + P_B^2}\, Y\Big)$$

Full magnetic Dirac Hamiltonian

$$U^* H_B\, U = U^* K_B\, U - \nu\, P = \begin{pmatrix} \sqrt{\mathbb{I} + P_B^2} & 0 \\ 0 & -\sqrt{\mathbb{I} + P_B^2} \end{pmatrix} - \nu\, \begin{pmatrix} p & q \\ q^* & t \end{pmatrix}$$

This formulation allows to decompose upper and lower components of the wave function on Landau levels...

Denote by $\Pi_{\mathcal{L}}$ the projector on the lowest Landau level

$$(x_1, x_2, x_3) \mapsto \phi_\ell(x_1, x_2)\, f(x_3) \quad \forall\, \ell \in \mathbb{N}\,, \quad \forall\, f \in L^2(\mathbb{R})$$

$\Pi_{\mathcal{L}}$, $\Pi_{\mathcal{L}}^c := \mathbb{I} - \Pi_{\mathcal{L}}$ commute with L_B. For all $\xi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$,

$$\left(\xi, \sqrt{\mathbb{I} + P_B^2}\, \xi\right) = \left(\Pi_{\mathcal{L}}\xi, \sqrt{\mathbb{I} + P_B^2}\, \Pi_{\mathcal{L}}\xi\right) + \left(\Pi_{\mathcal{L}}^c\xi, \sqrt{\mathbb{I} + P_B^2}\, \Pi_{\mathcal{L}}^c\xi\right)$$

At the level of the 4-components spinor

$$Z \in (L^2(\mathbb{R}^3, \mathbb{C}))^4\,, \quad Z = \Pi\, Z + \Pi^c\, Z\ ,$$

where

$$\Pi := \begin{pmatrix} \Pi_{\mathcal{L}} & 0 \\ 0 & \Pi_{\mathcal{L}} \end{pmatrix}\ , \quad \Pi^c := \begin{pmatrix} \Pi_{\mathcal{L}}^c & 0 \\ 0 & \Pi_{\mathcal{L}}^c \end{pmatrix}$$

Main estimates

Using

$$(a+b)^2 \le a^2+b^2+2\,|a\,b| = \inf_{\nu>0}\left[\left(1+\sqrt{\nu}\right)\,a^2+\left(1+\frac{1}{\sqrt{\nu}}\right)\,b^2\right]$$

$$(a+b)^2 \ge a^2+b^2-2\,|a\,b| = \sup_{\nu>0}\left[\left(1-\sqrt{\nu}\right)\,a^2+\left(1-\frac{1}{\sqrt{\nu}}\right)\,b^2\right]$$

we get

$$(Z,P\,Z) \le \left(1+\sqrt{\nu}\right)\,(\Pi_{\mathcal{L}}\,Z,P\,\Pi\,Z)+\left(1+\frac{1}{\sqrt{\nu}}\right)\,(\Pi^c\,Z,P\,\Pi^c\,Z)$$

$$(Z,P\,Z) \ge \left(1-\sqrt{\nu}\right)\,(\Pi_{\mathcal{L}}\,Z,P\,\Pi\,Z)+\left(1-\frac{1}{\sqrt{\nu}}\right)\,(\Pi^c\,Z,P\,\Pi^c\,Z)$$

Proposition 8. *For all* $Z\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^4]$

$$\mathcal{E}_{\nu+\nu^{3/2}}[\Pi\,Z]+\mathcal{E}_{\nu+\sqrt{\nu}}\,[\Pi^c\,Z]\;\le\;\mathcal{E}_\nu[Z]\;\le\;\mathcal{E}_{\nu-\nu^{3/2}}[\Pi\,Z]+\mathcal{E}_{\nu-\sqrt{\nu}}\,[\Pi^c\,Z]$$

$$P_B^2 + (1+B)\,\mathbb{I} = (\nabla - iA_B)^2\,\mathbb{I} + \sigma\cdot\mathbf{B} + (1+B) \geq \left(\frac{1}{4}\,\frac{1}{|x|^2} + 1\right)$$

follows from $P_B^2 = (\nabla - iA_B)^2\,\mathbb{I} + \sigma\cdot\mathbf{B}$, the diamagnetic inequality

$$\int_{\mathbb{R}^3} \Big|\,(\nabla - iA_B)\,\psi\,\Big|^2\,d^3x \geq \int_{\mathbb{R}^3} \Big|\,\nabla|\psi|\,\Big|^2\,d^3x$$

and Hardy's inequality. The square root is operator monotone

$$\sqrt{B} + \sqrt{\mathbb{I} + P_B^2} \geq \sqrt{P_B^2 + (1+B)\,\mathbb{I}} \geq \sqrt{\frac{1}{4}\,\frac{1}{|x|^2} + 1}$$

Consider $\bar\nu \approx 0.056$ such that $2\,(\bar\nu + \sqrt{\bar\nu}\,) = 2 - \sqrt{2}$ and define

$$d(\delta) := (1-2\delta)\sqrt{2} - 2\delta\ , \quad d_\pm(\nu) := d(\delta_\pm(\nu)) \quad \text{with} \quad \delta_\pm(\nu) := \sqrt{\nu} \pm \nu$$

We have

$$d(\delta) > 0 \quad \Longleftrightarrow \quad \delta < 1 - \sqrt{2}/2$$

$$d_\pm(\nu) > 0 \quad \text{if} \quad \nu < \bar\nu$$

Proposition 9. *Let $B > 0$ and $\delta \in (1 - \sqrt{2}/2)$. For any $\tilde Z = \binom{X}{0}$, $\bar Z = \binom{0}{Y}$, $X, Y \in L^2(\mathbb{R}^3, \mathbb{C}^2)$*

$$\mathcal{E}_\delta\,[\Pi^c\,\tilde Z] \geq d(\delta)\,\sqrt{B}\ \|\,\Pi^c_{\mathcal{L}}\,X\,\|^2_{L^2(\mathbb{R}^3)}$$

$$\mathcal{E}_{-\delta}\,[\Pi^c\,\bar Z] \leq -d(\delta)\,\sqrt{B}\ \|\,\Pi^c_{\mathcal{L}}\,Y\,\|^2_{L^2(\mathbb{R}^3)}$$

The restricted problem

The goal is to compare

$$\lambda_1(\nu, B) = \inf_{\substack{X \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ X \neq 0}} \sup_{\substack{Y \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \|Z\|_{L^2(\mathbb{R}^3)}=1 \,,\ Z=\binom{X}{Y}}} \mathcal{E}_\nu[Z]$$

with

$$\lambda_1^{\mathcal{L}}(\nu, B) := \inf_{\substack{X \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \\ \Pi_{\mathcal{L}}^c X = 0 \,,\ 0 < \|X\|^2_{L^2(\mathbb{R}^3)} < 1}} \sup_{\substack{Y \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^2) \,,\ Z=\binom{X}{Y} \\ \Pi_{\mathcal{L}}^c Y = 0 \,,\ \|Y\|_{L^2(\mathbb{R}^3)} = 1 - \|X\|^2_{L^2(\mathbb{R}^3)}}} \mathcal{E}_\nu[Z]$$

which can be reduced to a one-dimensional problem

A one-dimensional problem

Define the function $a_0^B : \mathbb{R} \times \mathbb{R}^+ \longrightarrow \mathbb{R}$ by

$$a_0^B(z) := B \int_0^{+\infty} \frac{s\, e^{-Bs^2/2}}{\sqrt{s^2 + z^2}}\, ds$$

and implicitly define $\mu_{\mathcal{L}}$ by

$$\mu_{\mathcal{L}}[f, \nu, B] = \frac{\displaystyle\int_{\mathbb{R}} \frac{|f'(z)|^2}{1 + \mu_{\mathcal{L}}[f, \nu, B] + \nu\, a_0^B(z)}\, dz + \int_{\mathbb{R}} (1 - \nu\, a_0^B(z))\, |f(z)|^2\, dz}{\displaystyle\int_{\mathbb{R}} |f(z)|^2\, dz}$$

Theorem 10. *For all* $B > 0$ *and* $\nu \in (0, 1)$*,*

$$\lambda_1^{\mathcal{L}}(\nu, B) = \inf_{f \in C_0^\infty(\mathbb{R}, \mathbb{C}) \setminus \{0\}} \mu_{\mathcal{L}}[f, \nu, B]$$

Asymptotic results

Theorem 11. *Let* $\nu \in (0, \bar{\nu})$. *For any*
$B \in \big(1/d_+(\nu)^2, \min\big\{B(\nu), B_{\mathcal{L}}(\nu+\nu^{3/2})\big\}\big)$,

$$\lambda_1^{\mathcal{L}}\Big(\nu+\nu^{3/2}, B\Big) \;\leq\; \lambda_1(\nu, B) \;\leq\; \lambda_1^{\mathcal{L}}(\nu-\nu^{3/2}, B)$$

Proof. The upper bound

$$\begin{aligned}
\lambda_1(\nu,B) \quad &\leq \quad \inf_{\substack{X\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \Pi_{\mathcal{L}}^c X=0,\Pi_{\mathcal{L}}X\neq 0}} \; \sup_{Y\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)} \mathcal{E}_{\nu-\nu^{3/2}}[\Pi\, Z] + \mathcal{E}_{\nu-\sqrt{\nu}}[\Pi^c\, Z] \\
&\leq \quad \inf_{\substack{X\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \Pi_{\mathcal{L}}^c X=0,\Pi_{\mathcal{L}}X\neq 0}} \; \sup_{Y\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)} \frac{\mathcal{E}_{\nu-\nu^{3/2}}[\Pi\, Z] - d_-(\nu)\,\sqrt{B}\,\|\Pi_{\mathcal{L}}^c Y\|^2_{L^2(\mathbb{R}^3)}}{\|\Pi\, Z\|^2_{L^2(\mathbb{R}^3)} + \|\Pi_{\mathcal{L}}^c Y\|^2_{L^2(\mathbb{R}^3)}} \\
&\leq \quad \inf_{\substack{X\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)\\ \Pi_{\mathcal{L}}^c X=0,\Pi_{\mathcal{L}}X\neq 0}} \; \sup_{Y\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^2)} \frac{\mathcal{E}_{\nu-\nu^{3/2}}[\Pi\, Z]}{\|\Pi\, Z\|^2_{L^2(\mathbb{R}^3)}} = \lambda_1^{\mathcal{L}}(\nu-\nu^{3/2}, B)
\end{aligned}$$

Asymptotics of the critical magnetic field

Define $B_{\mathcal{L}}(\nu) := \inf\{B > 0 \ : \ \lambda_1^{\mathcal{L}}(\nu, B) = -1\}$

Corollary 12. *If* $\nu \in (0, \bar{\nu})$,

$$B_{\mathcal{L}}(\nu + \nu^{3/2}) \ \leq \ B(\nu) \ \leq \ B_{\mathcal{L}}(\nu - \nu^{3/2})$$

Asymptotic behavior of the critical magnetic field $B(\nu)$

Theorem 13.

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

Proof. Use: $a_0^B(z) = \sqrt{B}\, a_0^1\left(\sqrt{B}\, z\right)$ and the changes of variables

$$y(z) := \int_0^z a_0^1(t)\, dt\,, \quad f\left(\frac{z}{\sqrt{B}}\right) = B^{1/4}\, g(y)$$

to get

$$\lambda_{\mathcal{L}}(\delta, B) = 1 + \sqrt{B}\,(\lambda_{\mathcal{L}}(\delta,1) - 1)$$
$$\lambda_{\mathcal{L}}(\delta,1) = 1 + \inf_{\substack{g \in C_0^\infty(\mathbb{R},\mathbb{C})\setminus\{0\} \\ \int_{\mathbb{R}} g(y)^2\, d\mu(y)=1}} \int_{\mathbb{R}} \left(\frac{1}{\delta}\,|g'(y)|^2 - \delta\,|g(y)|^2\right)\, dy$$

Let $\kappa = \kappa(\delta) := \delta\left(1 - \lambda_{\mathcal{L}}(\delta,1)\right)$, $\mu(y) := 1/a_0^1(z(y))$ and look for the first eigenvalue $E_1 = E_1(\delta)$ of the operator $-\partial_y^2 + \kappa(\delta)\,\mu(y)$ such that

$$\delta^2 = E_1(\delta)$$

The function a_0^1 satisfies

$$a_0^1(z) \leq a_0^1(0) = \sqrt{\frac{\pi}{2}} \quad \forall\, z \in \mathbb{R}\,, \quad a_0^1(z) \sim \frac{1}{|z|} \text{ as } |z| \to \infty$$

To get an upper estimate of E_1, consider $g_\sigma(y) := \sigma^{-1/2} \cos(\pi\, y/2\,\sigma)$

$$E_1(\delta) \leq \frac{\pi^2}{4\,\sigma^2} + \kappa \int_{-1}^{1} |g_1|^2\, \mu(\sigma\, y)\, dy \quad \leq \quad \frac{\pi^2}{4\,\sigma^2} + \kappa\, c \int_{-1}^{1} e^{\sigma |y|} |g_1|^2\, dy$$
$$\leq \frac{\pi^2}{4\,\sigma^2} + 2\,\kappa\, c\, (e^{\sigma} - 1)$$

and optimize w.r.t. σ : $\pi^2 = 4\,\kappa\, c\, \sigma^3\, e^\sigma$, $E_1(\delta) \leq \frac{\pi^2}{4\,\sigma_\delta^2}\,(1 + o(1))$
Lower estimate: use a step potential

Numerical computations

Numerical scheme

(i) Consider the solutions of the ODE

$$-g'' + \kappa\,\mu\,g = E\,g \quad g(0) = 1 \quad g'(0) = 0$$

Adjust $E = E_1(\kappa)$ to be the lowest $E > 0$ such that $\lim_{y\to\infty}\left[g(y)^2 + g'(y)^2\right] = 0$

(ii) By definition of the critical magnetic field, $B_{\mathcal{L}}(\delta)$ is such that

$$-2 = -1 + \lambda_{\mathcal{L}}(\delta, B_{\mathcal{L}}(\delta)) = -\sqrt{B_{\mathcal{L}}(\delta)}\,\frac{\kappa(\delta)}{\delta}$$

(iii) Parametrize the problem by κ, define $\delta = \delta(\kappa) = \sqrt{E_1(\kappa)}$

$$B_{\mathcal{L}}(\delta(\kappa)) = 4\,\frac{E_1(\kappa)}{\kappa^2}$$

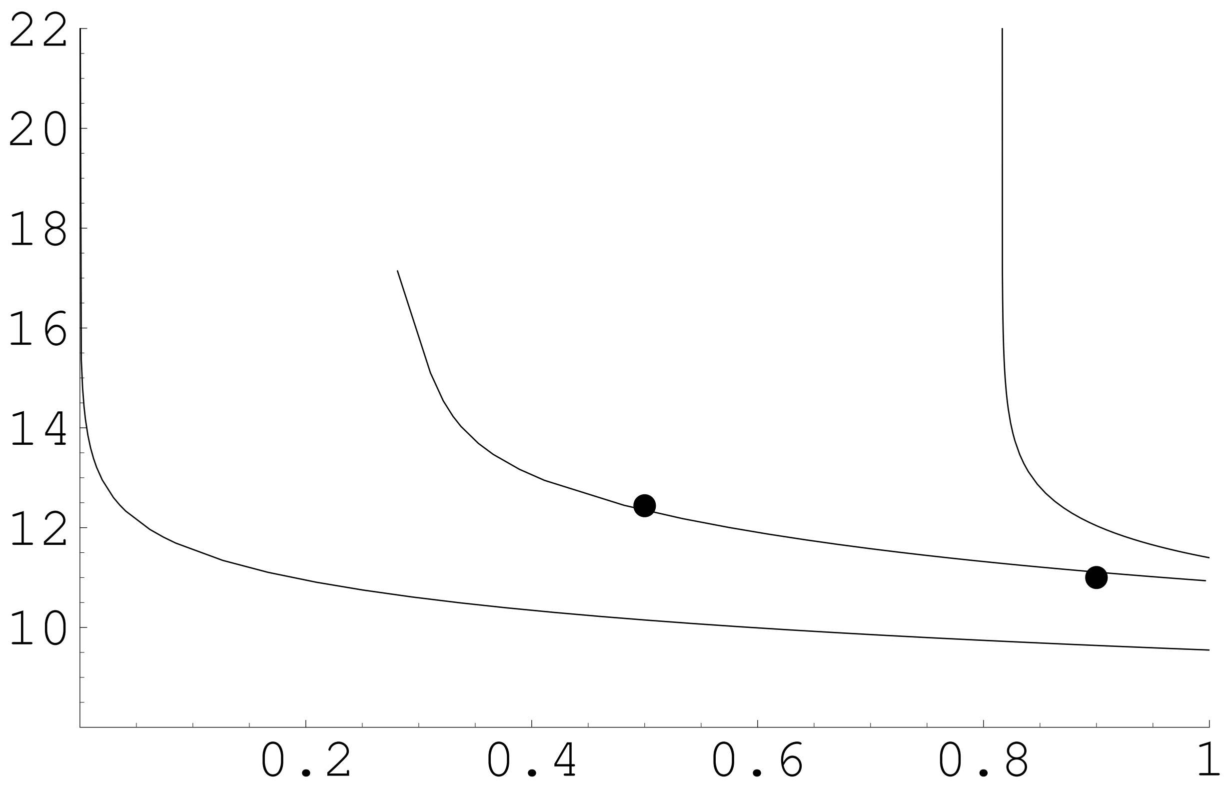
$\mu(y) \sim e^y$ as $y \to \infty$, new variables to $x = e^{y/2} - 1 \Leftrightarrow y = 2\log(1+x)$

Numerical results

	Z	ν	$B_{\mathcal{L}}(\nu)$	b (Tesla)	$\log(b)/\log(10)$
Zr_{40}^{39+}	40	0.292...	$5.7...\times 10^6$	$2.5...\times 10^{16}$	16.4...
Ba_{56}^{55+}	56	0.409...	$2.1...\times 10^3$	$9.4...\times 10^{12}$	13.0...
Magnetars			$2.3...–2.3...\times 10^2$	$10^{10}–10^{12}$	10–12
Pb_{82}^{81+}	82	0.598...	$1.8...\times 10^2$	$8.1...\times 10^{11}$	11.9...
U_{92}^{91+}	92	0.671...	$1.0...\times 10^2$	$4.6...\times 10^{11}$	11.6...
	137.037...	1.0	$1.9...\times 10^1$	$8.5...\times 10^{10}$	10.9...
$\frac{m^2c^2}{\lvert q\rvert\,\hbar}$			1	$4.4...\times 10^9$	9.6...
Radio pulsars			$2.3...\times 10^{-2}–2.3...\times 10^{-1}$	$10^8–10^9$	8–9

Summary

Upper bound, lower bound, estimates based on Landau levels and direct estimates



Ongoing research project [A. Decoene, J.D., M. Esteban, M. Loss]