Characterization of the critical magnetic field in the Dirac-Coulomb equation

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Outline of the talk

- 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 $\frac{m^2c^2}{|q|\hbar} \approx 4.4 \times 10^9$ 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	4.5×10^5 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 magneticfields]

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 1. *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 2. *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 $\nu/|x|$

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

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

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

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

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

Consider the functional

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

on the set of admissible functions

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

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

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

The critical magnetic field is defined by

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

Auxiliary functional

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

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

Scaling invariance

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

We define

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

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 3. *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,

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

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

Proof of the main result

- Preliminary results
- Proof

Preliminary results

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

is a concave, bounded function of $\nu \in (0,1)$, for any $\phi \in C_0^\infty(\mathbb{R}^3)$, and so is its infimum with respect to ϕ

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

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

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

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

Lemma 4. *On the interval $(0,1)$, the function $\nu \mapsto \mu(\nu)$ is continuous, monotone decreasing and takes only negative real values*

Proofs

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

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

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

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 $\chi_n(x) := \chi(|x|/R_n)$, $\lim_{n\to\infty} R_n = \infty$, $\tilde{\phi}_n := \phi_n\, \chi_n$

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

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

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

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

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

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

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

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

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

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

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

$$\tilde B(\nu') \leq B = B(\nu) \quad \forall\, \nu' > \nu$$

By continuity, $\tilde B(\nu) \leq B(\nu)$ $\square$

A Landau level ansatz

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

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

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

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

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

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

then

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

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

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

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

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

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

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

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

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

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

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

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

$$\mu(\nu) \leq \mu_{\mathcal{L}}(\nu)$$

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

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

and

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

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

Lemma 5. *For any* $\nu \in (0,1)$,

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

Lemma 6. *With the above notations,* $\lim_{\nu \to 0_+} \nu \, \log |\mu_{\mathcal{L}}(\nu)| = -\frac{\pi}{2}$

$\Longrightarrow \log B_{\mathcal{L}}(\nu) \sim \frac{\pi}{\nu}$ as $\nu \to 0_+$

Comparison of the critical magnetic fields

Theorem 7. *With the above notations,* $\lim_{\nu\to 0_+} \dfrac{\log B(\nu)}{\log B_{\mathcal{L}}(\nu)} = 1$

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,

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

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

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

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

(estimate of the interaction term and Cauchy-Schwartz)

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

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

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

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

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

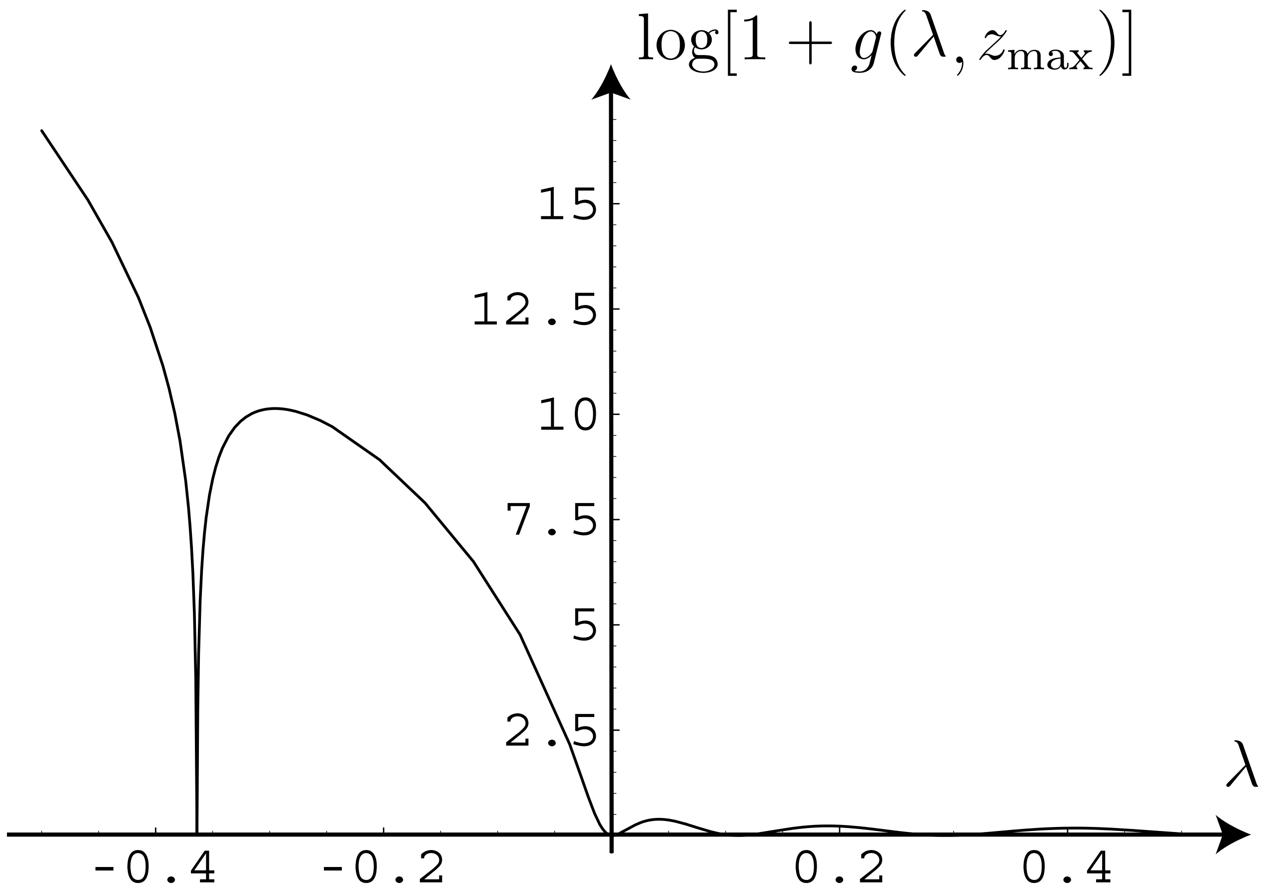
We notice that $b'(z) = z\,a(z)$, and, for any $z > 0$,

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

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)



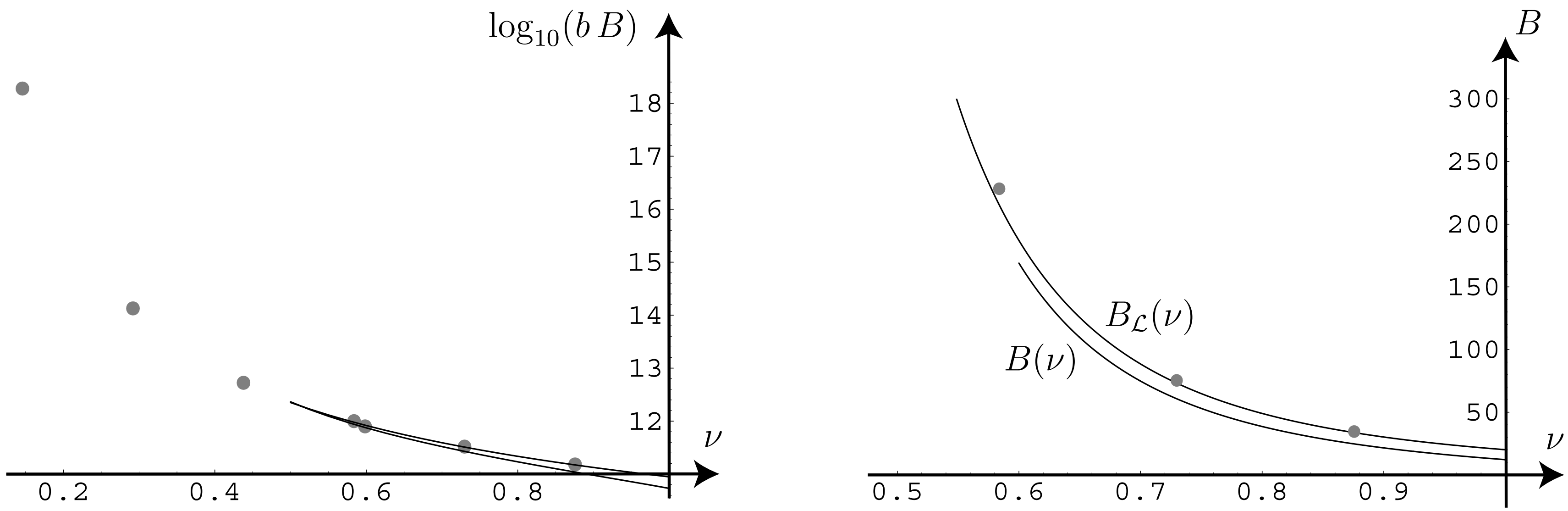
Plot of $\lambda \mapsto \log[1 + g(\lambda, z_{\max})]$ with $z_{\max} = 100$, for $\nu = 0.9$

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)



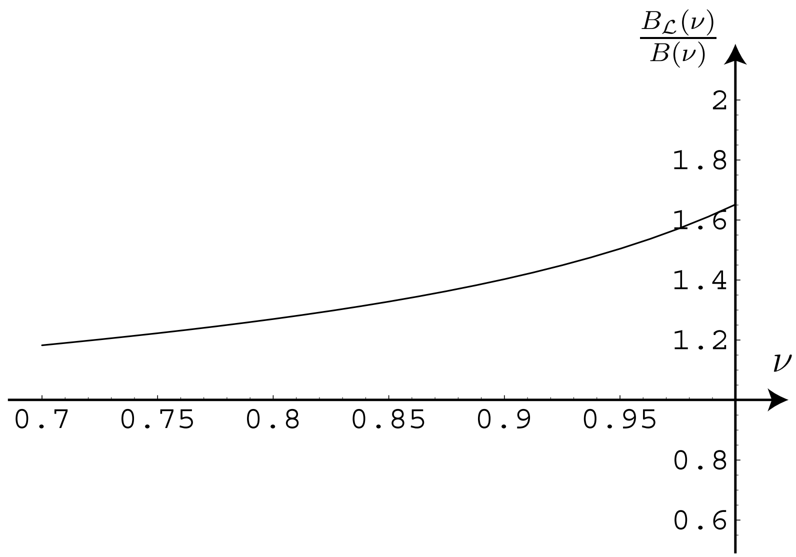
Left: values of the critical magnetic field in Tesla ($\log_{10}$ scale)
Right: values in dimensionless units
Ground state levels in the Landau level ansatz: upper curve
Levels obtained by a direct computation: lower curve
Dots correspond to the values computed by [Schlüter, Wietschorke, Greiner] in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

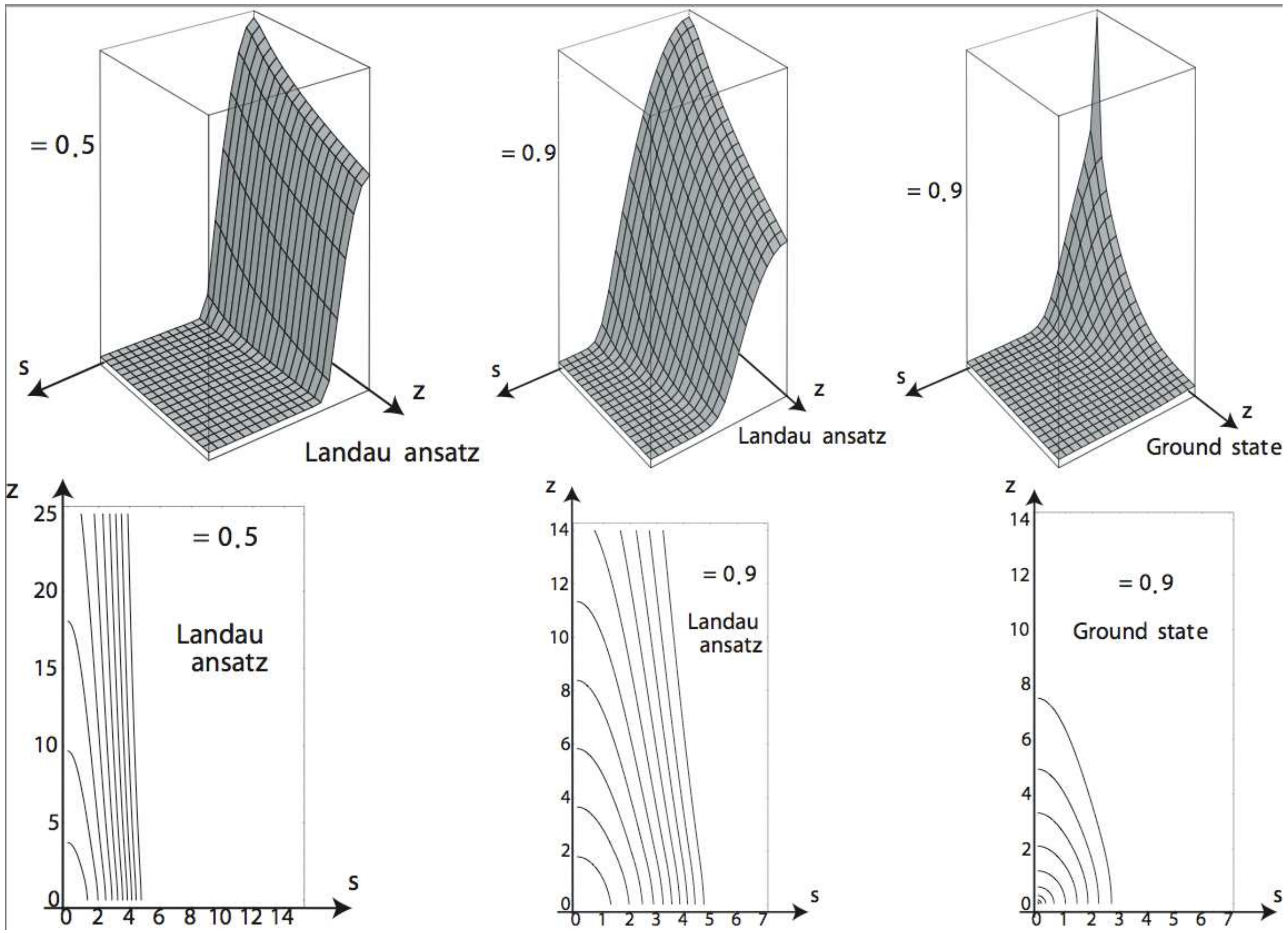
General case (2)



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.