Relativistic Hydrogen in Strong Magnetic Fields

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Relativistic Hydrogenic Atom (Ion) in Strong Homogeneous Magnetic Field

Constant magnetic field Be_z in z-direction; $e_z = (0,0,1)$; $r = (x,y,z) \in \mathbb{R}^3$

$$D^B = D_0^B - \frac{\gamma}{|r|}, \quad \gamma = \alpha Z$$

$$D_0^B = \alpha \cdot \left(i^{-1}\nabla_r + \mathbb{A}\right) + \beta;$$

$$\mathbb{A} = \frac{1}{2} B e_z \wedge r;$$

$\alpha = (\alpha_x, \alpha_y, \alpha_z), \beta$: Dirac-matrices

[Energy]= mc^2; [Length] $= \frac{\hbar}{mc}$; $[B] = \frac{m^2c^2}{|e|\hbar} \simeq 4.410^9$ tesla

$[D^B, J_z] = 0$, $J_z = L_z + S_z \Rightarrow$ restrict to $J_z = L_z + S_z = -1/2$

Questions, I

- Spectral properties for large B - Stability, non-empty discrete spectrum?
- Existence of effective one-dimensional Hamiltonian(s) approximating D^B in norm-resolvent sense as $B \to \infty$? (Parallel to non-relativistic case where there is a hierarchy effective one-dim potentials including the δ and the regularized 1-dim Coulomb potential)
- *Possible Interest:* singular potentials like δ-potential, 1-dim Coulomb, occur as natural limits of more physical models
- *Mathematically:* defining a Hamiltonian with singular potential amounts to finding self-adjoint extension of the operator defined away of the singularity through appropriate B.C. at the singularity (cf. Kurasov's talk on monday for δ, $\nabla\delta$ in $\mathbb{R}^3$)
- Limiting procedure will single out some natural extension

Questions, II

- Dolbeault, Esteban & Loss (2006): by variational argument show disappearance of lowest eigenvalue in $(-1, 1)$ into negative continuous spectrum for sufficiently large B
- Does the discrete spectrum remain non-empty, or does the atom become unstable?
- Interpretation? QED-effects like pair creation?

Method: essentially perturbative, starting from D_0^B with Coulomb term as perturbation

$$D_0^B = D_{0,tr}^B + D_{0,//}^B$$

transverse resp. parallel Dirac operator (to magnetic field)

"Free" Dirac operator D_0^B:

$$(D_{0,tr}^B)^2 = |i^{-1}\nabla_{x,y} + \mathbb{A}_{x,y}|^2 + \sigma_z B \otimes I_{\mathbb{C}^2}$$

magnetic Pauli in dimension 2 with discrete spectrum: $2nB$, $n = 0, 1, \ldots$ (Landau levels)

$$\begin{aligned} \Pi_{\mathrm{L}} &:= \text{Projection onto Lowest Landau Level} \\ &= |\chi_0^B\rangle\langle\chi_0^B| \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \text{ (recall } J_z = -1/2) \end{aligned}$$

$$\chi_0^B(x,y) = \left(\frac{B}{2\pi}\right)^{1/2} e^{-B\rho^2/4}$$

Fundamental Property: $|D_{0,tr}^B| \geq \sqrt{2B}$ on $\mathrm{Im}(\Pi_L)^{\perp}$

Adiabatic Approximation

Assume: to 1-st approximation. electrons "frozen" in lowest Landau orbits (with $J_z = -1/2$) in directions perpendicular to the field

$$
\begin{aligned}
D^B &\rightsquigarrow \Pi_{\mathrm{L}} D^B \Pi_{\mathrm{L}} =: d_{\mathrm{L}}^B \\
d_{\mathrm{L}}^B &= d_{0,z} + V_{\mathrm{L}}^B(z)
\end{aligned}
$$

Here:

$$d_{0,z} = \sigma_1 p_z + \sigma_3 m = \begin{pmatrix} m & p_z \\ p_z & -m \end{pmatrix} \text{ (free Dirac in dim. 1)}$$

$$V_{\mathrm{L}}^B(z) := -\gamma \langle \chi_0^B(x,y) | \frac{1}{|r|} | \chi_0^B \rangle = \sqrt{B} V_L^1(\sqrt{B} z)$$

where

$$V_L^1(z) = -\gamma \int_0^\infty \frac{e^{-u}}{\sqrt{2u + z^2}} \, du.$$

Effective Adiabatic Hamiltonian: preview

- Eigenvalue problem for d_L^B: not directly analytically solvable $\Rightarrow$ we try to further simplify for large B
- Potential $\sqrt{B}V^1(\sqrt{B}z)$: looks like δ-family, except that $V^1(z) \simeq 1/|z|$ at $\pm\infty$ and therefore not integrable over $\mathbb{R}$
- For $|z| \neq 0$: $\sqrt{B}V^1(\sqrt{B}z) \to 1/|z|$ as $B \to \infty$ Coulomb in dimension 1: needs to be regularized in 0
- Will see:

$$d_{0,z} + \sqrt{B}V^1(\sqrt{B}z) \simeq_{B\to\infty} \begin{cases} d_{0,z} - \frac{\gamma}{|z|} & z \neq 0 \\ \text{B.C. in 0 } (B\text{-dependent}) \end{cases}$$

Adiabatic Hamiltonian: large B asymptotics

$$d_L^B = \begin{pmatrix} m + V_L^B & p_z \\ p_z & -m + V_L \end{pmatrix}$$

$$= U_{\pi/4} \begin{pmatrix} p_z + V_L^B & m \\ m & -p_z + V_L^B \end{pmatrix} U_{\pi/4}^*$$

$U_{\pi/4} := \begin{pmatrix} \frac{1}{2}\sqrt{2} & -\frac{1}{2}\sqrt{2} \\ \frac{1}{2}\sqrt{2} & \frac{1}{2}\sqrt{2} \end{pmatrix}$. Now e.g.

$$p_z + V_L^B = e^{-iF^B} p_z e^{iF^B}$$

$$F^B(z) := \int_0^z V_L^B(y)\, dy = \int_0^{\sqrt{B}z} V_L^1(y)\, dy$$

Large B-asymptotics

$$F^B(x) \simeq \underbrace{-\gamma \mathrm{sgn}(z)(\log(\sqrt{B}\,|z|) + C}_{:=F^{\infty,B}} + O(|z|^{-2}))$$

$C = (\Gamma'(1) + \log 2)/2$, where $\Gamma'(1) =$ Euler's constant.

$$\begin{aligned} p_z + V^B = e^{-iF^B} p_z e^{iF^B} &\simeq e^{-iF^{\infty,B}} p_z e^{iF^{\infty,B}}, \quad B \to \infty \\ &= \begin{cases} p_z - \frac{\gamma}{|z|}, & z \neq 0 \\ \text{B.C. in } 0 \end{cases} \end{aligned}$$

B.C.: $e^{-i\gamma \mathrm{sgn}(z)(\log(\sqrt{B}z)+C)}u(z) \in H^1(\mathbb{R})$ and in particular continuous at 0 $\Rightarrow$ u has jump at 0 (reminiscent of δ-potential):

$$u(-\varepsilon)e^{i\gamma(\log(\varepsilon)+\log\sqrt{B}+C)} \simeq u(\varepsilon)e^{-i\gamma(\log(\varepsilon)+\log\sqrt{B}+C)}, \ \varepsilon \to 0.$$

Effective Adiabatic Hamiltonian

After conjugation by $U_{\pi/4}$, d_L^B is asymptotic, *in norm resolvent convergence sense*, to:

$$d_L^{\infty,B} := \begin{pmatrix} p_z - \gamma/|z| & m \\ m & -p_z - \gamma/|z| \end{pmatrix}, \quad z \neq 0$$

$$u = (u_1, u_2) \in Dom(d_L^{\infty,B}) \Leftrightarrow \begin{cases} u_j \in H^1(\mathbb{R} \setminus 0) \\ u_j \text{ satisfies jump-type B.C. in } 0 \end{cases}$$

B.C.: B-dependent and in fact *periodic* in $\log B$ with period $2\pi/\gamma$
$\Rightarrow$ same true for eigen-values (if exist).

E.v. problem:

$$d_L^{\infty,B} u = Eu, \quad u \in L^2(\pm\infty), \; u \text{ satisfies B.C.}$$

explicitly solvable using Whittaker functions (Coulomb wave functions)

Spectrum of $h_L^{\infty,B}$

- Continuous spectrum : $(-\infty,-1]\cup[1,\infty)$
- $E=E(B)\in(-1,1)$ eigenvalue iff for some $k=0,\pm1,\pm2,\dots$

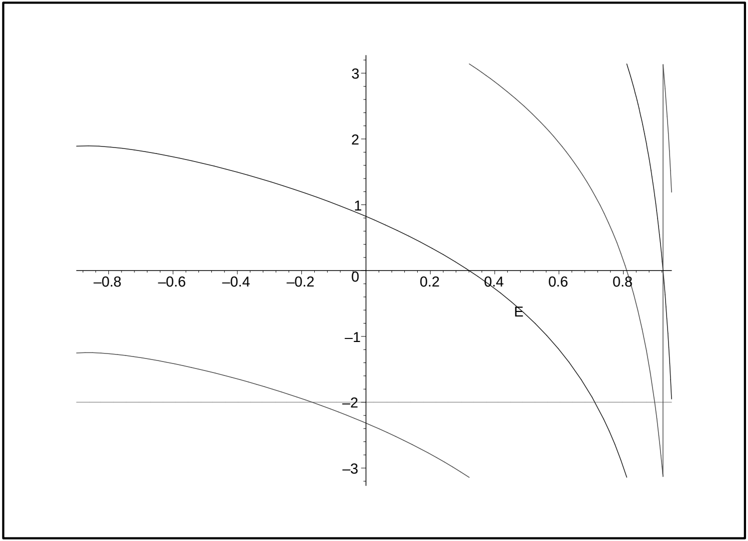
$$A_\pm(E)=\gamma\log B+2k\pi$$

Here:

$$\begin{aligned}A_\pm(E) &:= \mathrm{Arg}(F_\pm(E))\\ F_\pm(E) &:= (\mp)\frac{E+i\tau/2}{|E+i\tau/2|}\cdot\tau^{2i\gamma}\cdot\frac{\Gamma(1-2i\gamma)}{\Gamma(1+2i\gamma)}\cdot\frac{\Gamma(1+i\gamma-\kappa)}{\Gamma(1-i\gamma-\kappa)}\\ &\quad\cdot e^{-i\gamma(\log(2)+\Gamma'(1))}\end{aligned}$$

$\tau:=\tau(E):=2\sqrt{1-E^2}$, $\kappa:=\kappa(E):=2\gamma E/\tau$
$\mathrm{Arg}(w):=$ princ. value of argument of $w\in\mathbb{C}$; $\in(-\pi,\pi]$)

Graphical Analysis



Large B-behavior of eigen-values

- Infinitely many e.v. $E_0(B) < E_1(B) < \cdots$ accumulating at 1 : $E_n(B) \uparrow 1$, $n \to \infty$
  $E_n(B)$: decreasing in B

- Stability for all B in sense that $\sigma_{\mathrm{discr}} \neq \emptyset$ for all B (both for $d_L^{\infty,B}$ and for d_B^L for B suff. large)
- $E_0(B) \to -1$ if $B \uparrow B_c$, where

$$\gamma \log B_c = \pi + 2\gamma(\log \gamma + 1) - i\gamma\Gamma'(1) + \mathrm{Arg}\left(\frac{\Gamma(1-2i\gamma)}{\Gamma(1+2i\gamma)}\right)$$

  In particular: $\gamma \log B_c \to \pi$ as $\gamma \to 0$ (Dolbeault, Esteban, Loss)
- $E_2(B)$ becomes the new lowest e.v., which decreases further with increasing B, etc. Whole phenomenon periodic in $\log B$, period $2\pi/\gamma$

Problems

- What about D^B? OK if $\gamma^2\sqrt{B} \ll 1$;
  Otherwise: Coulomb interaction between lowest and higher Landau-levels needs somehow to be taken into account - not yet clear how
- Physical interpretation of bound electron-state in $(-1, 1)$ with negative energy?
- Physical interpretation of bound electron disappearing into negative sea?