MATTER UNDER THE INFLUENCE OF EXTREMELY STRONG MAGNETIC FIELDS

(with E.H. Lieb and J. Yngvason)

There are huge magnetic fields at the surface of a neutron star - as large as 10^{13} Gauss, as measured spectroscopically. The atoms there are *iron* with nuclear charge $Z = 26$. The natural unit of magnetic field is

$$B^* = m^2 e^3 c/\hbar^3 = 2.35 \times 10^9 \text{ Gauss},$$

so we are talking about large fields.

The cyclotron radius $= a_0(B^*/B)^{1/2}$, $a_0 =$ Bohr radius.

These large fields are trapped by collapsing current loops when the neutron star is born from a collapsing star.

HAMILTONIAN (non-relativistic)

$$H_N = \sum_{i=1}^{N} (H_{\mathbf{A}}^{(i)} - Z|x(i)|^{-1}) + \sum_{1 \le i < j \le N} |x(i) - x(j)|^{-1}$$

$$H_{\mathbf{A}} = \Big((\boldsymbol{p} - \boldsymbol{A}(x)) \cdot \boldsymbol{\sigma}\Big)^2 = (\boldsymbol{p} - \boldsymbol{A}(x))^2 - \boldsymbol{\sigma} \cdot \boldsymbol{B}$$

$$\boldsymbol{B} = (0, 0, B) = \text{ constant}, \quad \boldsymbol{A} = \tfrac{1}{2}\mathbf{B} \times x$$

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

We want the ground state energy, E_N of H_N for N (e.g. $N = Z$) fermions with spin, i.e. $\psi \in \bigwedge^N L^2(\boldsymbol{R}^3; \boldsymbol{C}^2)$.

THOMAS-FERMI THEORY

As usual, we hope that we can replace the N-body problem by a functional of the electron density ρ.

$$E_N^{\mathrm{TF}} = \inf\{\mathcal{E}^{\mathrm{MTF}}(\rho) | \rho : \boldsymbol{R}^3 \to \boldsymbol{R}^+, \int \rho = N\}$$

$$\mathcal{E}^{\mathrm{MTF}}(\rho) = \int \tau_B(\rho) dx - \int \frac{Z}{|x|} \rho(x) dx + \frac{1}{2} \int \rho(x) |x-y|^{-1} \rho(y) dx dy$$

What is $\tau_B(\rho)$? $(= \rho^{5/3}$ when $B = 0)$. We first study the one-body problem with Hamiltonian

$$H = H_{\mathbf{A}} - V(x).$$

Generalized Lieb-Thirring inequality:

Theorem 1. *There exist universal constants* $L_1, L_2 > 0$ *such that if we let* $e_j(B,V)$, $j = 1, 2, \ldots$ *denote the negative eigenvalues of* $H_{\mathbf{A}} - V$ *with* $0 \le V \in L^{3/2}(\boldsymbol{R}^3) \cap L^{5/2}(\boldsymbol{R}^3)$ *then*

$$\sum_j |e_j(B,V)| \le L_1 B \int V(x)^{3/2} dx + L_2 \int V(x)^{5/2} dx.$$

We can choose L_1 *as close to 2/3π as we please, compensating with* L_2 *large.*

Note: $\boldsymbol{\sigma} \cdot \boldsymbol{B}$ is a constant. What we are really estimating is the sum of the eigenvalues of $(\boldsymbol{p} - \boldsymbol{A})^2 - V(x)$. below $+B$ (the bottom of the continuous spectrum).

SCALING AND SEMI-CLASSICAL LIMIT

$$H = [(h\boldsymbol{p} - b\boldsymbol{a}(x)) \cdot \boldsymbol{\sigma}]^2 - v(x),$$

$a(x) = \frac{1}{2}(0,0,1) \times x$ and $v \geq 0$.

Theorem 2. *Let $e_j(h,b,v), j = 1,2,\ldots,$ denote the negative eigenvalues of H, with $0 \leq v \in L^{3/2}(\boldsymbol{R}^3) \cap L^{5/2}(\boldsymbol{R}^3)$. Then*

$$\lim_{h\to 0} \sum_j |e_j(h,b,v)| \Big/ E_{\mathrm{scl}}(h,b,v) = 1$$

uniformly in b, where

$$E_{\mathrm{scl}}(h,b,v) = \frac{1}{3\pi^2} h^{-2} b \int \left(v(x)^{3/2} + 2\sum_{\nu=1}^{\infty} [v(x) - 2\nu bh]_+^{3/2} \right) dx.$$

The effective parameter is bh. For $bh \ll 1$, the right side reduces to the standard semiclassical formula

$$\frac{2}{15\pi^2} h^{-3} \int v(x)^{5/2} dx.$$

We take $\tau_B(\rho)$ to be the Legendre transform of the semi-classical function

$$V \mapsto \frac{1}{3\pi^2} B \left(V^{3/2} + 2 \sum_{\nu=1}^{\infty} [V - 2\nu B]_+^{3/2} \right). \qquad (*)$$

Thus, $\tau_B(\rho)$ = energy/unit volume of free particles in box with magnetic field B.

The many-body Hamiltonian H_N can be reduced to a one-body operator with the mean field potential:

$$V = Z|x|^{-1} - |x|^{-1} * \rho^{\mathrm{MTF}}.$$

From the scaling of the minimizer ρ^{MTF} of $\mathcal{E}^{\mathrm{MTF}}$ we find that the effective parameters are

$$h = (B/Z^3)^{1/5} \quad \text{and} \quad b = (B^2/Z)^{1/5}.$$

Thus when $B \ll Z^3$ the semiclassical approach is appropriate and our analysis is consistent.

1) $B \ll Z^{4/3}$, *(i.e., $hb \ll 1, h$ small):*
The effect of the magnetic field is negligible. We get standard Thomas-Fermi theory with $\tau_B(\rho) = \rho^{5/3}$.

2) $B \sim Z^{4/3}$ *(i.e., $hb \sim 1, h$ small):*
J. Yngvason, Lett. Math. Phys. *22*, 107 (1991).
The magnetic field becomes important. The function τ_B is complicated because we have a finite number of terms in $(*)$. The density is still spherical.

3) $Z^{4/3} \ll B \ll Z^3$ *(i.e., $hb \gg 1, h$ small):*
The magnetic field is increasingly important. (Most electrons will, in a certain sense, be confined to the lowest Landau band.) The function τ_B is simple since the sum is not present in $(*)$ and therefore $\tau_B(\rho) \sim \rho^3/B^2$. The density is spherical and furthermore the atom is getting smaller. The atomic radius behaves as $Z^{1/5}B^{-2/5}$.

4) $B \sim Z^3$ *(i.e., $h \gtrsim 1$):*
In this regime one can no longer use semiclassics. The functional $\mathcal{E}^{\mathrm{MTF}}$ is not a good approximation to the energy for any $\tau_B(\rho)$. *The atom is no longer spherical.* A *density matrix* functional works, however.

5) $B \gg Z^3$, *(i.e., $h \gg 1$):*
This is the hyper-strong regime. Atoms are highly cylindrical, almost one-dimensional.

THE NON-SEMICLASSICAL CASE $B \geq Z^3$

The following result is important in the study of the non-semiclassical case

Theorem 3. *Let* $B/Z^{4/3} \to \infty$ *as* $Z \to \infty$. *Let* Π_0 *denote the projection in* $\bigwedge^N L^2(\boldsymbol{R}^3; \boldsymbol{C}^2)$ *onto states in which all* N *electrons are in the lowest Landau band. Consider*

$$\Pi_0 H_N \Pi_0 = \Pi_0 \left(\sum_i p_3(i)^2 - Z|x(i)|^{-1} + \sum_{i<j} |x(i) - x(j)|^{-1} \right) \Pi_0,$$

(using $\Pi_0 H_{\mathbf{A}} \Pi_0 = \Pi_0((\boldsymbol{p} - \boldsymbol{A}(x)) \cdot \boldsymbol{\sigma})^2 \Pi_0 = \Pi_0 p_3^2 \Pi_0$*) and let* $E_N^{(0)}$ *be the corresponding ground state energy. Then, as* $Z \to \infty$*,*

$$E_N^{(0)}/E_N \to 1.$$

We again reduce to a mean-field Hamiltonian:

$$\Pi_0 \sum_i \left(p_3(i)^2 - Z|x(i)|^{-1} + \rho * |x(i)|^{-1} \right) \Pi_0 = \Pi_0 \sum_i h_i(x_\perp(i)) \Pi_0,$$

where $h_i(x_\perp(i))$ is a one-dimensional Schrödinger operator depending on the two-dimensional parameter $x_\perp(i) = (x_1(i), x_2(i))$.

Our problem is to find the infimum

$$\inf\langle\Psi, \sum_i h_i(x_\perp(i))\Psi\rangle$$

over all Ψ satisfying

$$\Psi \in \bigwedge^N L^2(\boldsymbol{R}^3;\boldsymbol{C}^2), \qquad \|\Psi\| = 1, \qquad \Pi_0\Psi = \Psi. \qquad (**)$$

Define

$$\boxed{\begin{gathered}\gamma_{x_\perp}(x_3, y_3) = \\ N\int \Psi^*\Big((x_\perp, y_3), x(2), \dots\Big)\Psi\Big((x_\perp, x_3), x(2), \dots\Big)dx(2)\dots dx(N).\end{gathered}}$$

We can consider $\gamma_{x_\perp}$ as a trace class operator on $L^2(\mathbf{R})$. Then because of the density of states in the lowest Landau band

$$\|\Psi\| = 1 \Longrightarrow \int \mathrm{Tr}_{L^2(\mathbf{R})}[\gamma_{x_\perp}]dx_\perp = N$$

$$\Psi \in \bigwedge^N L^2(\boldsymbol{R}^3;\boldsymbol{C}^2), \quad \Pi_0\Psi = \Psi \Longrightarrow 0 \le \gamma_{x_\perp} \le \frac{B}{2\pi}\mathbf{1}. \ (***)$$

We avoid Π_0 by relaxing $(**)$ to the right side of $(***)$.

The operator $h(x_\perp)$ depends on the unknown density $\rho(x)$. We get around this problem again by defining a *functional*:

$$\mathcal{E}^{\mathrm{DM}}(\gamma) = \int \mathrm{Tr}_{L^2(\mathbf{R})}[(p_3^2 - Z|x|^{-1})\gamma_{x_\perp}]dx_\perp + \tfrac{1}{2}\int\int \rho_\gamma(x)\rho_\gamma(y)|x-y|^{-1}dxdy$$

where $\rho_\gamma(x) = \gamma_{x_\perp}(x_3, x_3)$.

We define the energy

$$E^{\rm DM}(N,Z,B) = \inf\{\mathcal{E}^{\rm DM}(\gamma) | \int {\rm Tr}_{L^2(\mathbf{R})}[\gamma_{x_\perp}]dx_\perp = N,\ \ 0 \le \gamma_{x_\perp} \le \frac{B}{2\pi}\mathbf{1}\}.$$

The scaling is

$$E^{\rm DM}(N,Z,B) = Z^3 E^{\rm DM}(\frac{N}{Z},1,\frac{B}{Z^3}).$$

This is the second time that we see the ratio B/Z^3 as a non-trivial parameter in the theory, it also played the role of an effective Planck's constant.

Theorem 1. (Energy) *Let $E^{\rm Q}(N,Z,B)$ denote the quantum energy. If N/Z is fixed and $B/Z^{4/3} \to \infty$ (to ensure confinement in the lowest Landau band) as $Z \to \infty$ then*

$$E^{\rm Q}(N,Z,B)/E^{\rm DM}(N,Z,B) \to 1$$

Theorem 2. (Regions)
Region 4: *If B/Z^3 is fixed then $\gamma_{x_\perp}$ has finite rank (depending on B/Z^3) for almost all $x_\perp$.*
Region 3: *As $B/Z^3 \to 0$ the rank of $\gamma_{x_\perp}$ tends to infinity allowing for the semiclassical treatment.*

Region 5: *There is a critical* η_c *such that for* $B/Z^3 \geq \eta_c$ *the rank of* $\gamma_{x_\perp}$ *is one. Then*

$$\gamma_{x_\perp}(x_3, y_3) = \sqrt{\rho_\gamma(x_\perp, x_3)}\sqrt{\rho_\gamma(x_\perp, y_3)}.$$

Thus the energy is in this case again a functional only of the density

$$\mathcal{E}^{\mathrm{DM}}(\gamma) = \mathcal{E}^{\mathrm{SS}}(\rho_\gamma).$$

In the limit $B/Z^3 \to \infty$, the functional $\mathcal{E}^{\mathrm{SS}}$ reduces after an appropriate rescaling to a functional of a one-dimensional density which can be minimized in closed form. Examples of the conclusions we can draw from this explicit minimization:

As $Z \to \infty$ and $B/Z^3 \to \infty$ we get

- Maximal number of electrons in atom:

$$\liminf N_c(Z)/Z \geq 2 \quad \text{(non-neutrality)}$$

- Energy:

$$E^{\mathrm{Q}}(N, Z, B) \approx \left(-\tfrac{1}{48}\left(\frac{N}{Z}\right)^3 + \tfrac{1}{8}\left(\frac{N}{Z}\right)^2 - \tfrac{1}{4}\left(\frac{N}{Z}\right)\right) Z^3 \left[\ln(B/Z^3)\right]^2$$

- Binding energy of neutral diatomic molecule $(Z + Z)$:
  (a) Energy of molecule $\approx -\frac{7}{6} Z^3 \left[\ln(B/Z^3)\right]^2$
  (b) Energy of two atoms $\approx -\frac{7}{24} Z^3 \left[\ln(B/Z^3)\right]^2$
  (b) Binding energy $\approx \frac{7}{8} Z^3 \left[\ln(B/Z^3)\right]^2$