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LARGE ATOMS IN LARGE MAGNETIC FIELDS*

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I. INTRODUCTION.

In this talk we shall discuss the effect on matter, specifically atoms, of a very strong magnetic field. We shall present results obtained in collaboration with E. Lieb and J. Yngvason. Details will appear elsewhere [LSY]. The motivation for studying extremely strong magnetic fields of the order of 10^{12} Gauss is that they are supposed to exist on the surface of neutron stars The heuristic argument usually given to explain these strong fields is that in the collapse, resulting in the neutron star, the magnetic field lines follow the collapse and thus become very dense.

The structure of matter in strong magnetic fields is thus a question of considerable interest in astrophysics (see [R], [FGP] and references therein).

II. THE PAULI HAMILTONIAN.

To give the quantum mechanical energy of a charged spin-$\frac{1}{2}$ particle in a magnetic field $\mathbf{B}$, we have to make a choice of vector potential $\mathbf{A}(x)$, $x \in \mathbb{R}^3$ satisfying $\mathbf{B} = \nabla \times \mathbf{A}$.

The energy is then given by the Pauli Hamiltonian

$$H_{\mathbf{A}} = \left((\mathbf{p} - \mathbf{A}(x)) \cdot \boldsymbol{\sigma}\right)^2 . \tag{2.1}$$

Here $\mathbf{p} = -i\nabla$ and $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, where

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

are the Pauli matrices. The Pauli Hamiltonian acts in the space $L^2(\mathbb{R}^3; \mathbb{C}^2)$. We can also write $H_{\mathbf{A}} = (\mathbf{p} - \mathbf{A})^2 - \mathbf{B} \cdot \boldsymbol{\sigma}$. In the case $\mathbf{A} = 0$ we get as usual $H_0 = \mathbf{p}^2 = -\Delta$. We shall here concentrate on the case where $\mathbf{B}$ is constant, say $\mathbf{B} = (0, 0, B)$, with $B \geq 0$. We choose $\mathbf{A} = \frac{1}{2}\mathbf{B} \times x$. In this case the spectrum of $H_{\mathbf{A}}$ is described by the so called Landau bands $\varepsilon_{p\nu} = 2B\nu + p^2$, where p is the momentum along the field and $\nu = 0, \ldots$ is the index of the band. The higher bands $\nu = 1, \ldots$ are twice as degenerate as the lowest band $\nu = 0$.

As usual in the study of fermionic energies we shall be interested in the sum of the negative eigenvalues of operators of the form $H = H_{\mathbf{A}} - V(x)$, where $V(\geq 0$ for simplicity) is an external potential. In this connection there is an important difference between $H_{\mathbf{A}}$ and the operator $(\mathbf{p} - \mathbf{A})^2$ which has no spin dependence. While the spectrum for $(\mathbf{p} - \mathbf{A})^2$ is (B, ∞) the spectrum for $H_{\mathbf{A}}$ is $(0, \infty)$.

Indeed, one can estimate the sum of the negative eigenvalues of the operator $(\mathbf{p}-\mathbf{A})^2$ by $L\int V(x)^{5/2}\,dx$, according to the standard Lieb-Thirring inequality (with a magnetic field the proof of this inequality given in [LT] is still correct if one appeals to the diamagnetic inequality, i.e., that the heat kernel with a magnetic field is pointwise bounded in absolute value by the heat kernel without a magnetic field.) However, in the case of $H_{\mathbf{A}}-V$ the question is somewhat more subtle. In fact, if $V\in L^{3/2}(\mathbb{R}^3)$ the operator $(\mathbf{p}-\mathbf{A})^2-V$ has a finite number of negative eigenvalues, while the operator $H_{\mathbf{A}}-V$ can have infinitely many negative eigenvalues (compare [I]). We can, however, prove [LSY]

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

$$\sum_j |e_j(B,V)| \le L_1 B\int V(x)^{3/2}\,dx + L_2\int V(x)^{5/2}\,dx\,. \tag{2.2}$$

We can choose L_1 as close to $2/3\pi$ as we please, compensating with L_2 large.

The first term on the right side is a contribution from the lowest band $\nu=0$. For large B this is the leading term.

We now ask the question of a semiclassical analog of (2.2). Thus consider the operator

$$\left[(h\mathbf{p}-b\mathbf{a}(x))\cdot\boldsymbol{\sigma}\right]^2 - v(x)\,, \tag{2.3}$$

where $\mathbf{a}(x)=\frac{1}{2}\hat{z}\times x$, $\hat{z}=(0,0,1)$ and $0\le v$.

If one computes the leading term in h^{-1} of the sum of the negative eigenvalues of (2.3) for fixed b one finds as in [HR] that there is no b dependence. In our case, however, we shall not assume b fixed, or more precisely not assume that b is small compared with h^{-1}. The reason for this is that in the application to neutron stars it is not true, as we shall discuss below, that $b\ll h^{-1}$.

The interesting fact is, however, that we can prove ([LSY]) a semiclassical formula for the sum of the negative eigenvalues of the operator (2.3), which holds uniformly in b (even for large b).

THEOREM 2. *Let $e_j(h,b,v)$, $j=1,2,\dots$, denote the negative eigenvalues of the operator (2.3), with $0\le v\in L^{3/2}(\mathbb{R}^3)\cap L^{5/2}(\mathbb{R}^3)$. Then*

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

uniformly in b, where

$$E_{\mathrm{scl}}(h,b,v)=\frac{1}{3\pi^2}h^{-2}b\int\Big(v(x)^{3/2}+2\sum_{\nu=1}^{\infty}[v(x)-2\nu bh]_+^{3/2}\Big)\,dx\,. \tag{2.4}$$

Here $[t]_+=t$ if $t>0$, zero otherwise.

The formula (2.4) was already implicitly noted in [Y].

For $bh \ll 1$, the right side of (2.4) reduces to the standard semiclassical formula from [HR],

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

(Recall that we are counting the spin which accounts for the 2 in front of the sum in (2.4).) For $bh \gg 1$, the sum in (2.4) is negligible, and we are left with the first term.

Formula (2.4) (with h replaced by 1) can be compared with the Lieb-Thirring inequality (2.2), which holds even outside the semiclassical regime. The two terms in (2.2) correspond to respectively the $b \to \infty$ (first term) and $b \to 0$ (last term) asymptotics of (2.4). A natural question, which is similar to the so called Lieb-Thirring conjecture, is whether the semiclassical constant $1/3\pi^2$ is the optimal value for L_1 in (2.2) rather than as proved $2/3\pi$.

III. THE ATOMIC HAMILTONIAN.

The Hamiltonian describing an atom with N electrons and nuclear charge Z in a constant magnetic field $\mathbf{B} = (0, 0, B)$ is

$$H_N = \sum_{i=1}^{N} \left(H_{\mathbf{A}}^{(i)} - Z|x_i|^{-1} \right) + \sum_{1 \le i < j \le N} |x_i - x_j|^{-1} \ , \tag{3.1}$$

acting in $\mathcal{H} = \overset{N}{\wedge} L^2(\mathbb{R}^3; \mathbb{C}^2)$. We shall here give a short sketch of what we call the Thomas-Fermi theory for (3.1). The goal of this theory is to approximate the ground state energy

$$E(N, B, Z) = \inf \operatorname{spec}_{\mathcal{H}} H_N \ . \tag{3.2}$$

Furthermore, in the case where $H(N)$ has a (normalized) ground state $\psi \in \mathcal{H}$, i.e., $H(N)\psi = E(N, B, Z)\psi$, we also want to estimate the density

$$\rho_\psi(x) = N \int \|\psi(x, x_2, \dots, x_N)\|^2_{\wedge \mathbb{C}^2}\, dx_2 \dots dx_N \ . \tag{3.3}$$

The first step in studying (3.1) is to replace the repulsive two-body term, $\sum_{i<j} |x_i - x_j|^{-1}$, by a so called self-consistent mean field potential of the form $\sum_i \rho * |x_i|^{-1}$. (This replacement is as in standard Thomas-Fermi theory (see [L]) and shall not be discussed here.) The question is how to find the appropriate self-consistent density ρ. It must of course be an approximation to ρ_ψ.

It should be noted that as we replace the two-body potential by a self-consistent one-body potential we must also subtract a term $\frac{1}{2} \int \rho(x)|x - y|^{-1}\rho(y)\, dxdy$ from the Hamiltonian. With this term our new Hamiltonian is

$$\sum_{i=1}^{N} \left(H_{\mathbf{A}}^{(i)} - V(x_i) \right) - \frac{1}{2} \int \rho(x)|x - y|^{-1}\rho(y)\, dxdy \ , \tag{3.4}$$

with $V(x) = Z|x|^{-1} - \rho * |x|^{-1}$. The ground state energy of the operator in (3.4) (without the extra term) is the sum of the N first negative eigenvalues of $H_{\mathbf{A}} - V$.

We assume now that V is such that we can estimate the sum of the negative eigenvalues by the semiclassical formula (2.4). We of course have to verify this assumption. Unfortunately, this verification relies on properties of the density ρ, which we shall only know at the end of the analysis. This somewhat backwards reasoning is typical for self-consistent mean field theories like Thomas-Fermi theory (see [L]).

In Thomas-Fermi theory there is a standard way ([L]) of approximating the expectation value of the kinetic energy operator $\sum_{i=1}^{N} H_{\mathbf{A}}^{(i)}$ by a functional of ρ using semiclassical formulas like (2.4). In our case we replace $\sum_{i=1}^{N} H_{\mathbf{A}}^{(i)}$ by $\int w_B\big(\rho(x)\big)\,dx$, where w_B is the Legendre transform of the convex function

$$V \mapsto \frac{1}{3\pi^2} B\Big(V^{3/2} + 2\sum_{\nu=1}^{\infty} [V - 2\nu B]_+^{3/2}\Big) \tag{3.5}$$

which is derived from (2.4) (without h). Here we point out that w_B is convex (by definition) and $w_B(t) \sim \dfrac{t^3}{B^2}$ for small t ($t \lesssim B^{3/2}$), $w_B(t) \sim t^{5/3}$ for large t ($t \gg B^{3/2}$).

The ground state energy of (3.4) should then be well approximated by

$$\begin{aligned} \mathcal{E}_{\mathrm{MTF}}(\rho) &= \int w_B(\rho) - \int V(x)\rho(x)\,dx - \frac{1}{2}\int \rho(x)|x-y|^{-1}\rho(y)\,dxdy \\ &= \int w_B(\rho) - \int Z|x|^{-1}\rho(x)\,dx + \frac{1}{2}\int \rho(x)|x-y|^{-1}\rho(y)\,dxdy\ . \end{aligned} \tag{3.6}$$

We call this functional the **Magnetic Thomas-Fermi Functional**. It is studied in detail in [LSY] (see also [FGP] and [Y]). We now choose our density ρ to be the unique minimizer for $\mathcal{E}_{\mathrm{MTF}}$ constrained to the set $\int \rho \le N$. We denote

$$E_{\mathrm{MTF}}(N,B,Z) = \inf\{\mathcal{E}_{\mathrm{MTF}}(\rho) \mid \int \rho \le N\}\ .$$

Knowing ρ we can now prove that $E_{\mathrm{MTF}}(N,B,Z)$ is really a semiclassical approximation to the true ground state energy for (3.4). To do this one should first realize that it follows from the study of $\mathcal{E}_{\mathrm{MTF}}$ with our choice of ρ that the potential $V(x) = Z|x|^{-1} - \rho * |x|^{-1}$ will have the following behavior in Z and B

$$\begin{aligned} V(x) &= Z^{4/3} v(Z^{1/3}x) \ \text{ if } \ B \le Z^{4/3} \\ V(x) &= Z^{4/5}B^{2/5} v(Z^{-1/5}B^{2/5}x) \ \text{ if } \ B \ge Z^{4/3}\ , \end{aligned} \tag{3.7}$$

where v is a function which does not depend significantly on B and Z.

Concentrating on the case $B \ge Z^{4/3}$ we see by a simple rescaling that the Hamiltonian $H_{\mathbf{A}} - V(x)$ from (3.4) is unitarily equivalent to the operator

$$Z^{4/5}B^{2/5}\left[\big((h\mathbf{p} - b\mathbf{a}(x))\cdot\boldsymbol{\sigma}\big)^2 - v(x)\right]\ , \tag{3.8}$$

where

$$h = \left(B/Z^3\right)^{1/5} \text{ and } b = \left(B^2/Z\right)^{1/5} . \tag{3.9}$$

In the case when $B \leq Z^{4/3}$ we get $Z^{4/3}$ in front of [ ] in (3.8) and

$$h = Z^{-1/3} \text{ and } b = B/Z . \tag{3.10}$$

When h is small we can study (3.8) by semiclassical methods. Indeed, using (2.4) we can now prove that if Z is sufficiently large and B/Z^3 sufficiently small, E_{MTF} approximates the true ground state energy (3.2) as well as we please.

THEOREM 3. *For all sequences N_n, B_n and Z_n such that $Z_n \to \infty$, $B_n/Z_n^3 \to 0$ and N_n/Z_n is bounded away from zero, we have*

$$E(N_n, B_n, Z_n)/E_{\mathrm{MTF}}(N_n, B_n, Z_n) \to 1 \text{ as } n \to \infty . \tag{3.11}$$

Furthermore, if $N_n \leq Z_n$, then $H(N_n)$ has a ground state ψ_n. The corresponding density ρ_{ψ_n} defined by equation (3.3) is well approximated by the unique minimizer ρ_n for $\mathcal{E}_{\mathrm{MTF}}$ in the following sense. If $\chi \in C_0^\infty(\mathbb{R}^3)$ then

$$Z_n^{-1} \int \Big(\rho_{\psi_n}(x) - \rho_n(x)\Big)\chi\big((Z_n^{1/3} + Z_n^{-1/5}B_n^{2/5})x\big)dx \to 0 . \tag{3.12}$$

(The above scaling of χ should be compared to equation (3.7).) We emphasize that from the uniqueness the minimizer ρ is spherically symmetric.

Notice that from equations (3.9) and (3.10), $hb = 1$ if $B = Z^{4/3}$, which when compared to equation (2.4) explains why the behavior in (3.7) changes at this point. Indeed, when $B \gg Z^{4/3}$ all electrons are in a certain sense confined to the lowest Landau band. This result which is given in the next theorem is completely independent of the semiclassical analysis.

THEOREM 4. *If Π_0^N is the projection in $\mathcal{H} = \overset{N}{\wedge} L^2(\mathbb{R}^3; \mathbb{C}^2)$ onto the subspace where all electrons are in the lowest Landau band we define the* **confined energy**

$$E_0(N, B, Z) = \inf \mathrm{spec}_{\mathcal{H}} \Pi_0^N H(N) \Pi_0^N . \tag{3.13}$$

Then if $N < \lambda Z$ for some fixed $\lambda > 0$ we get

$$E_0(N, B, Z)/E(N, B, Z) \to 1 \text{ if } Z^{4/3}/B \to 0 . \tag{3.14}$$

The preceeding analysis gives the following different regimes in B and Z.

1) $B \ll Z^{4/3}$, Z *large (i.e., $hb \ll 1$, h small)*:

The effect of the magnetic field is negligible. We get standard Thomas-Fermi theory with $w_B(\rho) \sim \rho^{5/3}$.

2) $B \sim Z^{4/3}$, *Z large (i.e.,* $hb \sim 1$, *h small):*

The magnetic field becomes important. The function w_B is complicated because we have a finite number of terms in (3.5). The density is still almost spherical and stable atoms are almost neutral (see [Y]).

3) $Z^{4/3} \ll B \ll Z^3$, *Z large (i.e.,* $hb \gg 1$, *h small).*

The magnetic field is increasingly important. Most electrons will be confined to the lowest Landau band. The function w_B is simple since there is only one term in (3.5), $w_B(\rho) \sim \rho^3/B^2$. The density is almost spherical and stable atoms are almost neutral. Furthermore, the atom is getting smaller. The atomic radius behaves like $Z^{1/5}B^{-2/5}$ (compare (3.7) and (3.12)).

4) $B \sim Z^3$ *(i.e.,* $h \sim 1$).

In this regime one can no longer use semiclassics. The functional $\mathcal{E}_{\mathrm{MTF}}$ from (3.6) is not a good approximation to the energy and we have no description of the atom in this case.

5) $B \gg Z^3$.

However, in the case when $B \gg Z^3$ and Z is large we can find a new functional of ρ very different from $\mathcal{E}_{\mathrm{MTF}}$ which approximates the energy. We shall discuss this in the following section. In this super strong case it turns out that the atom becomes very cylindrical in shape.

We end this section by a short discussion of which regime is relevant in the case of neutron stars. Since the natural unit of magnetic field is $(2m)^2e^3c/\hbar^3 = 9.4 \times 10^9$ Gauss. we get in our units where all relevant physical constants have been suppressed that the magnetic field on the surface of a neutron star is in order of magnitude $B \sim 10^2$. Thus for, say, iron with $Z = 26$ we have $bh = (B/Z^{4/3})^{3/5} \sim 1$. To make a quantitative evaluation we would of course have to really estimate error terms in the analysis. Qualitatively, however, (all relevant constants are of order 1) it seems unreasonable to assume $bh \ll 1$ in this case. Thus the magnetic field will almost certainly have a significant effect.

IV. THE SUPER STRONG CASE $B \gg Z^3$.

We shall here present the correct energy functional of the density when $B \gg Z^3$, and very briefly indicate what is involved in proving the correctness of the approximation.

The correct functional is now

$$\mathcal{E}_{\mathrm{SS}}(\rho) = \int \left(\frac{\partial}{\partial x_3}\sqrt{\rho}\right)^2 - \int \frac{Z}{|x|}\rho(x) + \frac{1}{2}\int \rho(x)|x-y|^{-1}\rho(y)\,dx\,dy\,, \tag{4.1}$$

with the condition that

$$\int \rho(x)dx_3 \leq \frac{B}{2\pi} \quad \text{for all} \quad (x_1, x_2)\,. \tag{4.2}$$

The claim is that

$$E_{\rm SS}(N) = \inf\{\mathcal{E}_{\rm SS}(\rho) \mid \int \rho \leq N\,,\ \rho \ \text{satisfies (4.2)}\} \tag{4.3}$$

is a good approximation to the energy in a certain regime of B and Z with $B \gg Z^3$.

In understanding this the first step is to recall that from Theorem 4 all electrons are confined to the lowest Landau band. In the lowest band the degeneracy is such that we have $B/2\pi$ states per area perpendicular to the field $\mathbf{B}$. Thus given any infinite cylinder parallel to the field and of base area $2\pi/B$. If there is more than one electron in such a cylinder, they will have to occupy orthogonal states in the parallel direction, but this one can prove costs too much energy if $B \gg Z^3$. This shows that (4.2) must hold. The functional (4.1) now follows because in each infinite cylinder with only one electron, the electron can be treated as a boson, i.e., we can neglect the exclusion principle and that is why $\mathcal{E}_{\rm SS}$ is reminiscent of (bosonic) Hartree theory. (For details see [LSY]).

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