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LARGE ATOMS IN LARGE MAGNETIC FIELDS

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I. INTRODUCTION.

In this talk I shall discuss the effect on matter, specifically atoms, of a very strong magnetic field. This turns out to be an interesting exercise in semiclassical analysis. Results obtained in collaboration with J.P. Solovej and J. Yngvason will be summarized and details will appear elsewhere [LSY I, II, III]. 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 (cf. [FGP]). 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.

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

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

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

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

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 socalled 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 H 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 I,III]

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 $0 \leq V \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$ then*

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

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 $0 \leq v$.

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 III]) 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 $e_j(h,b,v)$, $j = 1,2,\ldots$, denote the negative eigenvalues of the operator (2.3), with $0 \leq v \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$. 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

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

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 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

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

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 socalled 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

$$\frac{1}{2} \int \rho(x) |x - y|^{-1} \rho(y) \, dx dy$$