Atoms in strong magnetic fields: The high field limit at fixed nuclear charge

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Abstract

Let $E(B, Z, N)$ denote the ground state energy of an atom with N electrons and nuclear charge Z in a homogeneous magnetic field B. We study the asymptotics of $E(B, Z, N)$ as $B \to \infty$ with N and Z fixed but arbitrary. It is shown that the leading term has the form $(\ln B)^2 e(Z, N)$, where $e(Z, N)$ is the ground state energy of a system of N *bosons* with delta interactions in *one* dimension. This extends and refines previously known results for $N = 1$ on the one hand, and $N, Z \to \infty$ with $B/Z^3 \to \infty$ on the other hand.

1 Introduction

The effects of extremely strong magnetic fields (order of 10^9 Gauss and higher) on atoms and molecules are of considerable astrophysical as well as mathematical interest and are far from being completely understood in spite of many theoretical studies since the early seventies. We refer to [LSYa] and [RWHG] for a general discussion of this subject and extensive lists of references. An atom (ion) with N electrons and nuclear charge Z in a homogeneous magnetic field $\mathbf{B} = (0, 0, B)$ is (in appropriate units) usually modeled by the nonrelativistic many-body Hamiltonian

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

Here $x_i \in \mathbb{R}^3$ are the postitions of the electrons, $i = 1, \ldots, N$, $\mathbf{A}(x) = \frac{1}{2}\mathbf{B} \times x$ is the vector potential, and

$$H_{\mathbf{A}} = [(\mathrm{i}\nabla + \mathbf{A}(x)) \cdot \boldsymbol{\sigma}]^2 \tag{2}$$

with $\boldsymbol{\sigma}$ the vector of Pauli spin matrices. The Hamiltonian $H_{B,Z,N}$ operates on the Hilbert space $\mathcal{H}_N = \bigwedge^N L^2(\mathbb{R}^3; \mathbb{C}^2)$ appropriate for Fermions of spin 1/2. In this paper we are concerned with the ground state energy

$$\begin{aligned} E(B, Z, N) &= \inf \operatorname{spec} H_{B,Z,N} \\ &= \inf\{\langle \Psi, H_{B,Z,N}\Psi\rangle \,:\, \Psi \in C_0^\infty\left(\mathbb{R}^{3N}; \mathbb{C}^{2^N}\right) \cap \mathcal{H}_N, \|\Psi\|_2 = 1\} \end{aligned} \tag{3}$$

more precisely the $B \to \infty$ asymptotics of this quantity. Such an asymptotic study is relevant at the field strengths prevailing on white dwarfs and neutron stars.

Previous investigations of the asymptotics of $E(B, Z, N)$ have either dealt with the case $N = 1$, i.e., hydrogen-like atoms [AHS], or the case when Z and N tend to ∞ together with B [LSYa], [LSYb], [I]. The most complete rigorous treatment of the $N = 1$ case so far is [AHS] where the following $B \to \infty$ asymptotics was derived:

$$\begin{aligned} E(B, Z, 1)/Z^2 = &- \tfrac{1}{4}[\ln(B/2)]^2 + [\ln(B/2) \ln\ln(B/2)] \\ &- [(C + \ln 2)\ln(B/2)] - [\ln\ln(B/2)]^2 \\ &+ 2(C - 1 + \ln 2)\ln\ln(B/2) + O(1), \end{aligned} \tag{4}$$

with a constant C (Euler's constant/2). The basic results on the $N, Z \to \infty$ case were obtained in [LSYa] and [LSYb]. In particular, in [LSYa] it was shown that if $N, Z \to \infty$ with $\lambda = N/Z$ fixed, and $B/Z^3 \to \infty$, then

$$E(B, Z, N)/(Z^3[\ln(B/Z^3)]^2) \to \begin{cases} -\frac{1}{4}\lambda + \frac{1}{8}\lambda^2 - \frac{1}{48}\lambda^3 & \text{if} \quad \lambda < 2 \\ -\frac{1}{6} & \text{if} \quad \lambda \geq 2. \end{cases} \tag{5}$$

The fact that the right side of (5) decreases with increasing N/Z as long as $N/Z < 2$ shows that in the limit $Z \to \infty$, $B/Z^3 \to \infty$ an atom can bind at least $2Z$ electrons. In [I] some higher order corrections to the leading asymptotics for the energy are discussed.

The main result of the present paper is a derivation of the leading term in the $B \to \infty$ asymptotics of $E(B, Z, N)$ where Z and N are *fixed*, but arbitrary. The precise statement is as follows:

1.1. THEOREM (High field limit of the energy). *For each fixed Z and N*

$$\lim_{B\to\infty} \frac{E(B, Z, N)}{(\ln B)^2} = e(Z, N) \tag{6}$$

where $e(Z,N)$ is the ground state energy of the Hamiltonian

$$h_{Z,N} = \sum_{i=1}^{N} \left(-\partial^2/\partial z_i^2 - Z\delta(z_i)\right) + \sum_{i<j}^{N} \delta(z_i - z_j) \tag{7}$$

of N bosons *with δ-interaction in one dimension, defined in the sense of quadratic forms as*

$$e(Z,N) = \inf\{\langle \Psi, h_{Z,N}\Psi\rangle \, : \, \Psi \in C_0^\infty(\mathbb{R}^N), \|\Psi\|_2 = 1\}. \tag{8}$$

It is trivial to compute $e(Z,1) = -Z^2/4$. Thus (6) generalizes the first term in the expansion (4) to the case $N > 1$. The relevance of the δ-function model for the ground state of hydrogen in strong magnetic fields was noted already in [S].

We also verify that the mean field limit of $e(Z,N)$ agrees with (5):

1.2. THEOREM (Mean field limit). *If $Z, N \to \infty$ with $\lambda = N/Z$ fixed, then*

$$e(Z,N)/Z^3 \to \begin{cases} -\frac{1}{4}\lambda + \frac{1}{8}\lambda^2 - \frac{1}{48}\lambda^3 & \text{if} \quad \lambda < 2 \\ \\ -\frac{1}{6} & \text{if} \quad \lambda \geq 2 \end{cases} \tag{9}$$

Taken together, Theorems 1.1 and 1.2 lead to the same high B, high Z limit as Theorem 1.4 in [LSYa], where $Z \to \infty$ and $B/Z^3 \to \infty$ simultaneously (the “hyper-strong” limit.)

We now describe briefly the strategy for the proof of these results and introduce some notation that will be used throughout. The first step in the proof of Theorem 1.1 is a reduction to the subspace $\mathcal{H}_N^0 \subset \mathcal{H}_N$ generated by wave functions in the lowest Landau band. Let Π_N^0 denote the projector on $\mathcal{H}_N^0$. (Its integral kernel is given by Eqs. (52)–(53) in Section 5. Note that Π_N^0 and $\mathcal{H}_N^0$ depend on B.) Let $E^{\mathrm{conf}}(B,Z,N)$ denote the ground state energy of $\Pi_N^0 H_{B,Z,N} \Pi_N^0$. It is clear that

$$E(B,Z,N) \leq E^{\mathrm{conf}}(B,Z,N), \tag{10}$$

and by Theorem 1.2 in [LSYa],

$$E^{\mathrm{conf}}(B,Z,N) \leq E(B,Z,N)(1 - \delta(B,Z,N)) \tag{11}$$

where $\delta(B,Z,N) \to 0$ for $B \to \infty$ with Z, N fixed. Hence it suffices to prove (6) with $E(B,Z,N)$ replaced by $E^{\mathrm{conf}}(B,Z,N)$. We note in passing that (11) also holds for bosons. In fact, it will become evident in the sequel that Theorem 1.1 is independent of the statistics of the particles.

To study $E^{\mathrm{conf}}(B,Z,N)$ the next step is to introduce a Hamiltonian for the motion parallel to the magnetic field with the coordinates perpendicular to the magnetic field as parameters. We write the variables $x_i \in \mathbb{R}^3$ as $x_i = (x_i^\perp, z_i)$, where $x_i^\perp \in \mathbb{R}^2$ and $z_i \in \mathbb{R}$ are respectively the components perpendicular and parallel to the field. Moreover, we write $(x_1,\ldots,x_N) = (\underline{x}^\perp,\underline{z})$ with $\underline{x}^\perp = (x_1^\perp,\ldots,x_N^\perp)\in\mathbb{R}^{2N}$ and $\underline{z}=(z_1,\ldots,z_N)\in\mathbb{R}^N$.

In the lowest Landau band the part of (2) associated with the motion perpendicular to the field is exactly canceled by the spin contribution and only the part corresponding to the motion along the field remains. Hence

$$\Pi_N^0 H_{B,Z,N}\Pi_N^0 = \Pi_N^0 H_{Z,N}\Pi_N^0 \tag{12}$$

with

$$H_{Z,N} = \sum_{i=1}^N \left(-\partial^2/\partial z_i^2 - \frac{Z}{|x_i|}\right) + \sum_{i<j}^N \frac{1}{|x_i - x_j|}. \tag{13}$$

The operator (13) contains no derivatives perpendicular to the field and hence the variables $\underline{x}^\perp$ can be regarded as parameters for a differential operator in the variables parallel to the field. For each $\underline{x}^\perp$ such that $x_1^\perp,\ldots,x_N^\perp$ are all different from zero, we consider the one-dimensional Hamiltonian

$$H_{Z,N}(\underline{x}^\perp) = \sum_{i=1}^N\left(-\partial_{z_i}{}^2 - \frac{Z}{\sqrt{z_i^2+(x_i^\perp)^2}}\right) + \sum_{i<j}^N \frac{1}{\sqrt{(z_i-z_j)^2+(x_i^\perp-x_j^\perp)^2}} \tag{14}$$

acting on $\bigotimes^N L^2(\mathbb{R}) = L^2(\mathbb{R}^N)$. The expectation values of $H_{Z,N}$ can be written as

$$\langle\Psi, H_{Z,N}\Psi\rangle = \int \langle\Psi(\underline{x}^\perp,\cdot), H_{Z,N}(\underline{x}^\perp)\Psi(\underline{x}^\perp,\cdot)\rangle_{L^2(\mathbb{R}^N)}\, d\underline{x}^\perp. \tag{15}$$

The next step is a scaling of the variables. In the lowest Landau level the characteristic length in the directions perpendicular to the field is $B^{-1/2}$. One can therefore expect that for the computation of $E^{\rm conf}(B,Z,N)$, i.e., the infimum of (15) over (normalized) $\Psi\in\mathcal{H}_N^0$, the properties of $H_{Z,N}(\underline{x}^\perp)$ for $|x_i^\perp|\sim B^{-1/2}$ are decisive. Anticipating this, it is natural to make a transformation of variables, $(\underline{x}^\perp,\underline{z})\to(B^{1/2}\underline{x}^\perp, L(B)\underline{z})$ where the scale factor $L(B)$ in the direction of the field has still to be specified. The corresponding unitary operator on $L^2(\mathbb{R}^N)$ is

$$U\Psi(\underline{z}) = L(B)^{1/2}\Psi(L(B)\underline{z}), \tag{16}$$

and the Hamiltonian transforms in the following way:

$$U^{-1}H_{Z,N}(\underline{x}^\perp)U = L(B)^2 h_{Z,N}^B(B^{1/2}\underline{x}^\perp) \tag{17}$$

where

$$h_{Z,N}^B(\underline{y}^\perp) = \sum_{i=1}^N\left(-\partial_{z_i}^2 - ZV_{B,|y_i^\perp|}(z_i)\right) + \sum_{i<j} V_{B,|y_i^\perp-y_j^\perp|}(z_i-z_j) \tag{18}$$

and the potential $V_{B,r}(z)$ is (for $r > 0$) defined as

$$V_{B,r}(z) = L(B)^{-1}(B^{-1}L(B)^2r^2 + z^2)^{-1/2}. \tag{19}$$

Let $E_{Z,N}(\underline{x}^\perp)$ and $e^B_{Z,N}(\underline{y}^\perp)$ denote the ground state energies of $H_{Z,N}(\underline{x}^\perp)$ and $h^B_{Z,N}(\underline{y}^\perp)$ respectively. In order to avoid discussions about the domains of the Hamiltonians, which in fact depend on whether some of the parameters $x_i^\perp$ (resp. $y_i^\perp$) coincide, we define the ground state energies in terms of quadratic forms in the same way as (8):

$$\begin{aligned} E_{Z,N}(\underline{x}^\perp) &= \inf\{\langle\Psi, H_{Z,N}(\underline{x}^\perp)\Psi\rangle \,:\, \Psi \in C_0^\infty(\mathbb{R}^N),\ \|\Psi\|_2 = 1\}, &(20)\\ e^B_{Z,N}(\underline{y}^\perp) &= \inf\{\langle\Psi, h^B_{Z,N}(\underline{y}^\perp)\Psi\rangle \,:\, \Psi \in C_0^\infty(\mathbb{R}^N),\ \|\Psi\|_2 = 1\}. &(21)\end{aligned}$$

These energies are connected by the scaling relation

$$E_{Z,N}(B^{-1/2}\underline{y}^\perp)/L(B)^2 = e^B_{Z,N}(\underline{y}^\perp). \tag{22}$$

In the next section we show that with the choice $L(B) \sim \ln B$ the potential $V_{B,r}(z)$ converges for each $r > 0$ in the sense of distributions to the delta function as $B \to 0$. This is the heuristic basis of Theorem 1.1. Since the convergence is not uniform in r, however, more is needed for a rigorous proof. In particular, one needs estimates on the r-dependence of the convergence $V_{B,r}(z) \to \delta(z)$. These estimates, stated in Lemmas 2.1 and 2.2 in the next section, can be regarded as variants of Propositions 3.3 and 3.4 in [LSYa] and the Appendix in [JY], adapted to the problem at hand. They are included here for completeness.

The upper bound on the energy, given in Section 3, is a straight-forward variational calculation. The lower bound is more subtle. An important ingredient needed is the superharmonicity of the energy $E_{Z,N}(\underline{x}^\perp)$ in the variables $x_i^\perp$. This result, established in Theorem 4.3, generalizes a corresponding result (Proposition 2.3) in [LSYa]. Superharmonicity implies that the lowest value of $E_{Z,N}(B^{-1/2}\underline{y}^\perp)$ for $|y_i^\perp| \geq \varepsilon$ with $\varepsilon > 0$ is obtained at the boundary of the variable range, i.e., when either $|y_i^\perp| = \varepsilon$ or $|y_i^\perp| \to \infty$. Variables tending to infinity can be ignored, since $V_{B,r}(z) \to 0$ for $r \to \infty$, so by this result one may in (15) restrict the attention to wave functions localized where $|x_i^\perp| \leq (\text{const.})B^{-1/2}$. On the other hand, the requirement that only wave functions in the lowest Landau band are taken into account in (15) plays the role of a 'hard core condition' that prevents collapse, since such wave functions cannot be concentrated on shorter scales than $O(B^{-1/2})$. This statement is made precise in Lemma 5.3.

The lower bound is obtained in Section 5 by combining Theorem 4.3, Lemma 5.3 and the convergence of the potentials $V_{B,r}$ discussed in Section 2. It is noteworthy that this lower bound holds also for bosonic statistics while the upper bound holds for fermionic statistics, so that altogether the convergence of $E(Z,N,B)/(\ln B)^2$ to $e(Z,N)$ is independent of the statistics.

In section 6 we discuss the delta-function model (7) and in particular prove Theorem 1.2. In the course of the proof we compare (7) with another model, whose ground state energy can be explicitly calculated. This model provides an upper bound for the ground state energy of (7) and has the same mean field limit. The Hamiltonian for this model is

$$\widetilde{h}_{Z,N} = \sum_{i=1}^{N} \left(p_i^2 - \delta(z_i)\right) + \frac{1}{2Z} \sum_{i<j} \delta(|z_i| - |z_j|). \tag{23}$$

An interesting feature of this model is the fact that the maximal number $N_{\rm c}$ of electrons that a nucleus of charge Z can bind is exactly the largest integer satisfying

$$N_{\rm c} < 2Z + 1. \tag{24}$$

(This fact is unrelated to Lieb's upper bound [L] for the maximal negative ionization of atoms that does not apply to the Pauli Hamiltonian with a homogeneous magnetic field.) A corresponding statement for the Hamiltonian (7) is not known, except in the mean field limit, cf. Theorem 1.2. In this connection it should be mentioned that an estimate of the form form $N_{\rm c} < 2Z + 1 + (\text{const.})\, B^{1/2}$ has been derived in [BR] for a Hamiltonian of a similar type as (18).

2 The high B limit of the Coulomb interaction

We define the scaling factor $L(B)$ in the potential (19) as the solution of the equation

$$B^{1/2} = L(B) \sinh[L(B)/2]. \tag{25}$$

Since $\int_0^1 (a^2 + z^2)^{-1/2} dz = \sinh^{-1}(1/a)$, we have with this choice

$$\int_{|z| \le r} V_{B,r}(z) dz = 1. \tag{26}$$

for all B. Note also that

$$L(B) = \ln B + O(\ln \ln B) \tag{27}$$

as $B \to \infty$.

Let $\psi \in H^1(\mathbf{R}) = \{\psi : \int |\psi|^2 + \int |d\psi/dz|^2 < \infty\}$. Every such ψ is a continuous function on $\mathbb{R}$.

2.1. LEMMA (Delta approximation, part 1).

$$\left| |\psi(0)|^2 - \int V_{B,r}(z) |\psi(z)|^2 dz \right| \le L(B)^{-1} \left[\lambda r^{-1} + 8 \lambda^{1/4} T^{3/4} r^{1/2} \right] \tag{28}$$

with $\lambda = \int |\psi|^2$, $T = \int |d\psi/dz|^2$.

Proof. It suffices to take $r = 1$, for the general case follows by scaling $z \to rz$. Write the difference on the left side of (28) as $A_1 + A_2$ with

$$\begin{aligned} A_1 &= -\int_{|z|\geq 1} V_{B,1}(z)|\psi(z)|^2 dz, & (29)\\ A_2 &= \int_{|z|\leq 1} V_{B,1}(z)\left[|\psi(0)|^2 - |\psi(z)|^2\right] dz. & (30)\end{aligned}$$

The missing term

$$A_3 = \left[1 - \int_{|z|\leq 1} V_{B,1}(z)dz\right] |\psi(0)|^2 \tag{31}$$

is zero because of (26). Since $|V_{B,1}(z)| \leq L(B)^{-1}$ for $|z| \geq 1$, we have

$$|A_1| \leq \lambda L(B)^{-1}. \tag{32}$$

For $|z| \leq 1$ we have in any case

$$|V_{B,1}(z)| \leq L(B)^{-1}|z|^{-1}. \tag{33}$$

Moreover,

$$\begin{aligned} \left||\psi(z)|^2 - |\psi(0)|^2\right| &\leq |\psi(z) - \psi(0)|\,[|\psi(z)| + |\psi(0)|] \\ &\leq \left|\int_0^z \frac{d\psi}{dz'}dz'\right| \cdot 2\left[\int_{-\infty}^{\infty} \frac{d|\psi(z')|^2}{dz'}dz'\right]^{1/2} \\ &\leq |z|^{1/2}T^{1/2}2\lambda^{1/4}T^{1/4} = 2\lambda^{1/4}T^{3/4}|z|^{1/2}. & (34)\end{aligned}$$

Hence

$$|A_2| \leq 2L(B)^{-1}\left(\int_{|z|\leq 1} |z|^{-1/2}dz\right)\lambda^{1/4}T^{3/4} = 8L(B)^{-1}\lambda^{1/4}T^{3/4}. \tag{35}$$

Combining the estimates for A_1 and A_2 gives (28). □

2.2. LEMMA (Delta approximation, part 2). *Let* $\Psi \in H^1(\mathbb{R}^2)$ *and put*

$$\lambda = \int\int |\Psi(z,z')|^2 dzdz', \qquad T = \int\int |\partial_{z'}\Psi(z,z')|^2 dzdz'. \tag{36}$$

Then

$$\begin{aligned} &\left|\int |\psi(z,z)|^2 dz - \int\int V_{B,r}(z-z')|\psi(z,z')|^2 dzdz'\right| \\ &\qquad\qquad \leq L(B)^{-1}[\lambda r^{-1} + 8\lambda^{1/4}T^{3/4}r^{1/2}]. & (37)\end{aligned}$$

Proof. Put $\lambda(z) = \int |\Psi(z,z')|^2 dz'$, $T(z) = \int |\partial_{z'}\Psi(z,z')|^2 dz'$. By (28) we have

$$\begin{aligned} &\left||\Psi(z,z)|^2 - \int V_{B,r}(z-z')|\Psi(z,z')|^2 dz'\right| \\ &\leq L(B)^{-1}[\lambda(z)r^{-1} + 8\lambda(z)^{1/4}T(z)^{3/4}r^{1/2}]. & (38)\end{aligned}$$

Integration over z, using the Hölder inequality to estimate $\int \lambda(z)^{1/4}T(z)^{3/4}dz$, gives (37). □

3 Upper Bound

Let $\psi \in \mathcal{S}(\mathbb{R}^{2N})$ be a smooth and rapidly decreasing wave function in the lowest Landau level at field strength 1, and let $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^N)$. If ψ and ϕ are normalized, i.e., $\int_{\mathbb{R}^{2N}} |\psi|^2 = \int_{\mathbb{R}^N} |\phi|^2 = 1$, then

$$\Psi_B(\underline{x}^\perp, \underline{z}) = (BL(B))^{N/2}\psi(B^{1/2}\underline{x}^\perp)\phi(L(B)\underline{z}) \tag{39}$$

is a normalized wave function in the lowest Landau band at field strength B. Moreover, using (15) and (17) we have

$$\begin{aligned} E(B,Z,N) &\leq \langle \Psi_B, H_{Z,N}\Psi_B\rangle \\ &= L(B)^2 \int |\psi(\underline{y}^\perp)|^2 \langle \phi, h^B_{Z,N}(\underline{y}^\perp)\phi\rangle d^{2N}\underline{y}^\perp \end{aligned}$$

where $h^B_{Z,N}(\underline{y}^\perp)$ is given by (18). Since $L(B)^2/(\ln B)^2 \to 1$ as $B \to \infty$ and ψ is normalized, one has for the upper bound in Theorem 1.1 only to check that

$$\begin{aligned} &\int |\psi(\underline{y}^\perp)|^2 V_{B,|y_i^\perp|}(z_i)|\phi(\underline{z})|^2 d^{2N}\underline{y}^\perp d^N\underline{z} \\ &\qquad \to \int \delta(z_i)|\phi(\underline{z})|^2 d^N\underline{z} \end{aligned}$$

and

$$\begin{aligned} &\int |\psi(\underline{y}^\perp)|^2 V_{B,|y_i^\perp - y_j^\perp|}(z_i - z_j)|\phi(\underline{z})|^2 d^{2N}\underline{y}^\perp d^N\underline{z} \\ &\qquad \to \int \delta(z_i - z_j)|\phi(\underline{z})|^2 d^N\underline{z} \end{aligned}$$

as $B \to \infty$. But this is taken care of by Lemmas 2.1 and 2.2. (That $V_{B,r}(z)$ is not defined for $r = 0$ is of no consequence here, because the error terms in (28) and (37) are integrable all the way to $r = 0$.) We therefore have

3.1. PROPOSITION (Upper bound).

$$\liminf_{B\to\infty} \frac{E(B,Z,N)}{(\ln B)^2} \leq e(Z,N). \tag{40}$$

Remark. It is clear that our upper bound holds for fermions, although $e(Z,N)$ is the bosonic ground state energy of (7). In fact, in the ansatz (39) above we may choose ψ to be antisymmetric and ϕ to be symmetric; then Ψ_B is antisymmetric. Note also that for the Hamiltonian (7) the bosonic ground state energy is the same as its ground state energy without symmetry restriction.

4 Superharmonicity

In this section we take a closer look at the dependence of the ground state energy $E_{Z,N}(\underline{x}^\perp)$ of the Hamiltonian (14) on the parameter $\underline{x}^\perp$. We start with a simple estimate:

4.1. LEMMA (Simple bounds). *The function $\underline{x}^\perp \mapsto E_{Z,N}(\underline{x}^\perp)$ satisfies the bounds*

$$-\sum_{i=1}^{N} Z^2 \left(1 + \left[\sinh^{-1}((Z|x_i^\perp|)^{-1})\right]^2\right) \leq E_{Z,N}(\underline{x}^\perp) \leq 0 \tag{41}$$

on the set

$$\mathcal{A} = \{\underline{x}^\perp \in \mathbb{R}^{2N} \ : \ x_i^\perp \neq 0, \ \textit{for all } i = 1, \ldots, N\}. \tag{42}$$

Proof. The non-positivity of E is straightforward from the definition by an appropriate choice of Ψ. Note that this also holds in the case where some of the $x_i^\perp$ variables coincide. The lower bound on $E_{Z,N}(\underline{x}^\perp)$ follows from Lemma 2.1 in [LSYa] together with the operator inequality

$$H_{Z,N}(\underline{x}^\perp) \geq \sum_{i=1}^{N} \left(-\partial_{z_i}^2 - \frac{Z}{\sqrt{z_i^2 + (x_i^\perp)^2}} \right)$$

which is obtained by ignoring the positive two-body interactions. □

Next we turn to the superharmonicity properties of $E_{Z,N}(\underline{x}^\perp)$. We shall need the following general result.

4.2. LEMMA (Inherited superharmonicity). *Let U be an open set in $\mathbb{R}^d$ and assume that $f : U \times \mathbb{R} \to (-\infty, \infty]$ is a superharmonic function with the property that*

$$b = \min\{\liminf_{t\to\infty} f(x,t), \liminf_{t\to-\infty} f(x,t)\}$$

is independent of x for all $x \in U$. Then $g(x) = \inf_t f(x,t)$ is a superharmonic function on U.

Proof. We shall prove this by showing that $\Delta g \leq 0$ as a distribution. We shall use that f is a lower semicontinuous function satisfying the mean value inequality

$$\int_{|(x,t)-(y,s)|\leq r} f(y,s)dyds \leq f(x,t)c_{d+1}r^{d+1},$$

for all $(x,t) \in U \times \mathbb{R}$ if $r > 0$ is small enough, where c_{d+1} is the volume of the unit ball in $\mathbb{R}^{d+1}$.

For $x \in U$ it follows from the lower semicontinuity of f that we have either $g(x) = b$ or there exists $t \in \mathbb{R}$ such that $g(x) = f(x,t)$. In the first case we obviously have

$$c_{d+1} r^{d+1} g(x) \geq 2 \int_{|x-y|\leq r} g(y)\sqrt{r^2 - (x-y)^2}\,dy \tag{43}$$

since $g(y) \leq b$ for all y. If $g(x) < b$ we also conclude the above inequality since

$$\begin{aligned} g(x) c_{d+1} r^{d+1} &= f(x,t) c_{d+1} r^{d+1} \geq \int_{|(x,t)-(y,s)|\leq r} f(y,s)\,dy\,ds \\ &\geq \int_{|(x,t)-(y,s)|\leq r} g(y)\,dy\,ds = 2\int_{|x-y|\leq r} g(y)\sqrt{r^2-(x-y)^2}\,dy. \end{aligned}$$

Note now that for any $\phi \in C_0^\infty(U)$ we have for any $x \in U$ that

$$\lim_{r\to 0} r^{-(d+3)} \int_{|x-y|\leq r} [\phi(y) - \phi(x)]\sqrt{r^2-(x-y)^2}\,dy = C\Delta\phi(x)$$

for some constant $C > 0$ and in fact this limit holds in the topology of $C_0^\infty(U)$. Thus if $\phi \geq 0$ we have

$$\int_U g(x)\Delta\phi(x)\,dx = C^{-1}\lim_{r\to 0} r^{-(d+3)} \int_{|x-y|\leq r} g(x)(\phi(y)-\phi(x))\sqrt{r^2-(x-y)^2}\,dy\,dx \leq 0$$

by the inequality (43). Hence $\Delta g \leq 0$. $\square$

4.3. THEOREM (Superharmonicity of the energy). *On the set $\mathcal{A}$ defined in (42) the function $\underline{x}^\perp \mapsto E_{Z,N}(\underline{x}^\perp)$ is superharmonic in each of the variables $x_i^\perp$, $i = 1, \ldots, N$ independently.*

Proof. We follow closely the proof of Prop. 2.3 in [LSYa], which stated the superharmonicity of the ground state energy of a one-body operator which can be considered as a mean field approximation of $H_{Z,N}(\underline{x}^\perp)$.

It is clearly enough to prove that $E_{Z,N}(\underline{x}^\perp)$ is superharmonic in $x_1^\perp$ (on the region $x_1^\perp \neq 0$) for $x_2^\perp, \ldots, x_N^\perp$ fixed. We shall prove this by showing that $x_1^\perp \mapsto E_{Z,N}(\underline{x}^\perp)$ satisfies the mean value inequality around any given point $x_{1,0}^\perp$. Let $\underline{x}_0^\perp = (x_{1,0}^\perp, x_2^\perp, \ldots, x_N^\perp)$. Choose a sequence of L^2 normalized functions $\Psi_n \in C_0^\infty(\mathbb{R}^N)$ such that $\langle \Psi_n, H_{Z,N}(\underline{x}_0^\perp)\Psi_n\rangle \to E_{Z,N}(\underline{x}_0^\perp)$ as $n \to \infty$.

For $w \in \mathbb{R}$ denote by $\Psi_n^{(w)}$ the function

$$\Psi_n^{(w)}(z_1, \ldots, z_N) = \Psi_n(z_1 - w, z_2, \ldots, z_N).$$

We clearly have

$$\inf_{w\in\mathbb{R}} \langle \Psi_n^{(w)}, H_{Z,N}(\underline{x}_0^\perp)\Psi_n^{(w)}\rangle \to E_{Z,N}(\underline{x}_0^\perp) \quad \text{as } n \to \infty.$$

If $x_1^\perp$ is close to $x_{1,0}^\perp$ we shall use $\Psi_n^{(w)}$ as a trial function for $H(\underline{x}^\perp)$. We then obtain

$$E_{Z,N}(\underline{x}^\perp) \le \liminf_n \inf_{w\in\mathbb{R}} \langle \Psi_n^{(w)}, H_{Z,N}(\underline{x}^\perp)\Psi_n^{(w)}\rangle.$$

Hence

$$E_{Z,N}(\underline{x}^\perp)-E_{Z,N}(\underline{x}_0^\perp) \le \liminf_n \left[\inf_{w\in\mathbb{R}} \langle \Psi_n^{(w)}, H_{Z,N}(\underline{x}^\perp)\Psi_n^{(w)}\rangle - \inf_{v\in\mathbb{R}} \langle \Psi_n^{(v)}, H_{Z,N}(\underline{x}_0^\perp)\Psi_n^{(v)}\rangle\right]. \tag{44}$$

The potential appearing in $H_{Z,N}(\underline{x}^\perp)$, i.e.,

$$W_{Z,N,\underline{x}^\perp}(z_1,\ldots,z_N) = -\sum_{i=1}^N \frac{Z}{\sqrt{z_i^2+(x_i^\perp)^2}} + \sum_{i<j}^N \frac{1}{\sqrt{(z_i-z_j)^2+(x_i^\perp-x_j^\perp)^2}}.$$

is a superharmonic function of $(z_1, x_1^\perp) \in \mathbb{R}^3 \setminus \{0\}$. Writing

$$\langle \Psi_n^{(w)}, W_{Z,N,\underline{x}^\perp}\Psi_n^{(w)}\rangle = \int W_{Z,N,\underline{x}^\perp}(z_1+w, z_2,\ldots,z_N)|\Psi_n(z_1,\ldots,z_N)|^2 dz_1\cdots dz_N$$

we see that $\langle \Psi_n^{(w)}, W_{Z,N,\underline{x}^\perp}\Psi_n^{(w)}\rangle$ is superharmonic in $(w, x_1^\perp)$ away from the line $x_1^\perp = 0$. Since $\langle \Psi_n^{(w)}, \partial_{z_i}^2\Psi_n^{(w)}\rangle$ is independent of w and $x_1^\perp$ for all $i = 1,\ldots,N$ we have that $\langle \Psi_n^{(w)}, H_{Z,N}(\underline{x}^\perp)\Psi_n^{(w)}\rangle$ is superharmonic in $(w, x_1^\perp)$ away from the line $x_1^\perp = 0$.

Moreover, we also have that the two limits

$$\liminf_{w\to\pm\infty} \langle \Psi_n^{(w)}, H_{Z,N}(\underline{x}^\perp)\Psi_n^{(w)}\rangle$$

are independent of $x_1^\perp$. This is true simply because the contribution from the terms in the Hamiltonian depending on $x_1^\perp$ tend to zero as $w \to \pm\infty$. We may therefore apply the above lemma to the function $f(w, x_1^\perp) = \langle \Psi_n^{(w)}, H_{Z,N}(\underline{x}^\perp)\Psi_n^{(w)}\rangle$. We conclude that the function

$$x_1^\perp \mapsto \inf_{w\in\mathbb{R}} \langle \Psi_n^{(w)}, H_{Z,N}(\underline{x}^\perp)\Psi_n^{(w)}\rangle$$

is superharmonic for $x_1^\perp \neq 0$. Moreover by the inequality (41) this function is bounded below if $|x_1^\perp|$ is bounded away from 0.

Now using Fatou's Lemma we see from (44) that the average of $E_{Z,N}(\underline{x}^\perp) - E_N(\underline{x}_0^\perp)$ over the set $\{x_1^\perp \;:\; |x_1^\perp - x_{1,0}^\perp| < r\}$ is non-positive for all $r > 0$ small enough. □

5 Lower Bound

The first lemma in this section concerns the ground state energy $e_{Z,N}^B(\underline{y}^\perp)$ of $h_{Z,N}^B(\underline{y}^\perp)$ and does not use superharmonicity.

5.1. LEMMA (Lower bound on $e^B_{Z,N}(\underline{y}^\perp)$). *Let $\mathcal{K}$ be a compact subset of the set $\mathcal{A}$ given in (42). Then*

$$\liminf_{B\to\infty} \inf_{\underline{y}^\perp\in\mathcal{K}} e^B_{Z,N}(\underline{y}^\perp) \geq e(Z,N). \tag{45}$$

Proof. To avoid problems at points $\underline{y}^\perp$ with $y_i^\perp - y_j^\perp = 0$ for some i,j, we replace the repulsive potential $V_{B,|y_i^\perp-y_j^\perp|}(z_i-z_j)$ by the smaller potential $V_{B,|y_i^\perp-y_j^\perp|+1}(z_i-z_j)$. We denote the corresponding Hamiltonian by $\tilde{h}^B_{Z,N}(\underline{y}^\perp)$ and its ground state energy by $\tilde{e}^B_{Z,N}(\underline{y}^\perp)$. It is obvious that $e^B_{Z,N}(\underline{y}^\perp) \geq \tilde{e}^B_{Z,N}(\underline{y}^\perp)$, so a lower bound on $\tilde{e}^B_{Z,N}(\underline{y}^\perp)$ gives a lower bound on $e^B_{Z,N}(\underline{y}^\perp)$.

Let Ψ be a normalized, symmetric wavefunction in $C_0^\infty(\mathbb{R}^N)$. Since $\langle\Psi, h_{Z,N}\Psi\rangle \geq e(Z,N)$ we have to estimate the matrix elements of the difference $\tilde{h}^B_{Z,N}(\underline{y}^\perp) - h_{Z,N}$. Using Lemmas 2.1 and 2.2, together with the Hölder inequality for the integration over $z_2,\ldots,z_N$ and $z_3,\ldots,z_N$ respectively, we obtain

$$\begin{aligned}\left|\langle\Psi,\tilde{h}^B_{Z,N}\Psi\rangle - \langle\Psi,h_{Z,N}\Psi\rangle\right| &\leq L(B)^{-1}(ZN+N(N-1)) \\ &\quad\times\left[r_{\min}^{-1} + 8T_\Psi^{3/4}(2r_{\max}+1)^{1/2}\right]\end{aligned} \tag{46}$$

where $r_{\min}$ and $r_{\max}$ are respectively the minimum and the maximum value of $|y_i^\perp|$, $i=1,\ldots,N$, with $\underline{y}^\perp\in\mathcal{K}$, and

$$T_\Psi = N\int |\partial_z\Psi(z,z_2,\ldots,z_N)|^2 dz dz_2\cdots dz_N \tag{47}$$

is the kinetic energy of Ψ. Now if $\Psi^B_{\underline{y}^\perp,n}$, $n=1,2,\ldots$ is a minimizing sequence of normalized wave functions for $\tilde{h}^B_{Z,N}(\underline{y}^\perp)$, then we may assume that the corresponding kinetic energy is uniformly bounded in n, B and $\underline{y}^\perp\in\mathcal{K}$. In fact, we may assume that $\langle\Psi^B_{\underline{y}^\perp,n}, \tilde{h}^B_{Z,N}(\underline{y}^\perp)\Psi^B_{\underline{y}^\perp,n}\rangle$ is a bounded sequence. If we use the bound from Lemma 2.1 in [LSYa], we obtain

$$\langle\Psi^B_{\underline{y}^\perp,n}, \tilde{h}^B_{Z,N}(\underline{y}^\perp)\Psi^B_{\underline{y}^\perp,n}\rangle \geq \frac{T_n}{2} - \frac{1}{2}\left(\frac{2Z}{L(B)}\right)^2\left(1+\left[\sinh^{-1}\{(2Z)^{-1}B^{1/2}\}\right]^2\right), \tag{48}$$

where we have saved half of the the kinetic energy T_n of $\Psi^B_{\underline{y}^\perp,n}$. For large B, $L(B)^{-1}\left[\sinh^{-1}\{(2Z)^{-1}B^{1/2}\}\right]$ is bounded and hence we see that T_n is bounded. The error term (46) with $\Psi = \Psi^B_{\underline{y}^\perp,n}$ thus tends to zero as $B\to\infty$, uniformly in n, and the lemma is established. □

5.2. LEMMA (Uniform bounds on $E_{Z,N}(\underline{x}^\perp)$). *Let $\varepsilon>0$. Consider the set*

$$\mathcal{C}^{B,\varepsilon} = \{\underline{x}^\perp \;:\; \varepsilon B^{-1/2} \leq\; |x_i^\perp|, \textit{ for all } i=1,\ldots,N\}. \tag{49}$$

Then

$$\liminf_{B\to\infty}(\ln B)^{-2}\inf\{E_{Z,N}(\underline{x}^\perp) \;:\; \underline{x}^\perp\in\mathcal{C}^{B,\varepsilon}\} \geq e(Z,N). \tag{50}$$

where $e(Z,N)$ as before denotes the 1-dimensional delta function atom energy.

Proof. Define the sets

$$\mathcal{C}_n^{B,\varepsilon} = \{\underline{x}^\perp \ : \ \varepsilon B^{-1/2} \le \ |x_i^\perp| \le n, \text{ for all } i = 1, \dots, N\}.$$

Since $\mathcal{C}_n^{B,\varepsilon}$ is compact and $E_{Z,N}$ is lower semicontinuous (being superharmonic, in fact, superharmonic in each variable) we may find $\underline{x}_n^\perp \in \mathcal{C}_n^{B,\varepsilon}$ such that

$$E_{Z,N}(\underline{x}_n^\perp) = \min\{E_{Z,N}(\underline{x}^\perp) \ : \ \underline{x}^\perp \in \mathcal{C}_n^{B,\varepsilon}\}.$$

Clearly,

$$\lim_{n\to\infty} E_{Z,N}(\underline{x}_n^\perp) \to \inf\{E_{Z,N}(\underline{x}^\perp) \ : \ \underline{x}^\perp \in \mathcal{C}^{B,\varepsilon}\}.$$

By the superharmonicity of $E_{Z,N}(\underline{x}^\perp)$ in each variable $x_i^\perp$ we know that each coordinate $x_{i,n}^\perp$ of the point $\underline{x}_n^\perp$ satisfies either $|x_{i,n}^\perp| = \varepsilon B^{-1/2}$ or $|x_{i,n}^\perp| = n$. Moreover, since $E_{Z,N}(\underline{x}^\perp)$ is invariant under permutations of the coordinates of $\underline{x}^\perp$ we may assume that $|x_{1,n}^\perp| \le |x_{2,n}^\perp| \le \ldots \le |x_{N,n}^\perp|$ for all n. By possibly going to a subsequence we may assume that there exists an integer $0 \le K \le N$ such that for n large enough

$$|x_{i,n}^\perp| = \begin{cases} \varepsilon B^{-1/2}, & \text{for } i = 1, \dots, K \\ n, & \text{for } i > K \end{cases} .$$

Moreover, we may assume that $x_{i,n}^\perp$ converges as $n \to \infty$ for $i = 1, \dots, K$.

Since we may ignore the variables $x_{i,n}^\perp$, $i = K+1, \dots, N$, which tend to infinity we have

$$\lim_{n\to\infty} E_{Z,N}(\underline{x}_n^\perp)/E_{Z,K}(x_{1,n}^\perp, \dots, x_{K,n}^\perp) = 1$$

Since $E_{Z,K}(\underline{x}^\perp)$ is lower semicontinuous we conclude that there exists a point $(x_{1,\infty}^\perp, \dots, x_{K,\infty}^\perp) \in \mathbb{R}^{2K}$ with $|x_{i,\infty}^\perp| = \varepsilon B^{-1/2}$ for all $i = 1, \dots, K$ such that

$$\inf\{E_{Z,N}(\underline{x}^\perp) \ : \ \underline{x}^\perp \in \mathcal{C}^{B,\varepsilon}\} = E_{Z,K}(x_{1,\infty}^\perp, \dots, x_{K,\infty}^\perp).$$

By Lemma 5.1 we have that

$$\liminf_{B\to\infty} \inf\{L(B)^{-2} E_{Z,K}(B^{-1/2}y_1^\perp, \dots, B^{-1/2}y_K^\perp) \ : \ |y_i^\perp| = \varepsilon, \text{ for all } i\} \ge e(Z,K).$$

Since $K \le N$ and hence $e(Z,K) \ge e(Z,N)$ we have proved the lemma. ☐

5.3. LEMMA (Wave functions in the lowest Landau band). *If $\Psi \in \mathcal{H}_N^0$ belongs to the lowest Landau band at field strength B, then $\int |\Psi(\underline{x}^\perp, \underline{z})|^2 d\underline{z}$ is a bounded function of $\underline{x}^\perp$ (possibly after a modification on a null set) and for all $1 \le n \le N$*

$$\sup_{x_1^\perp, \dots, x_n^\perp} \left| \int \int |\Psi(\underline{x}^\perp, \underline{z})|^2 d\underline{z} dx_{n+1}^\perp \cdots dx_N^\perp \right| \le \frac{B^n}{(2\pi)^n} \|\Psi\|^2 \tag{51}$$

Proof. The projector Π^0_N on the lowest Landau band is the N-th tensorial power of the projector Π^0 that operates on $L^2(\mathbb{R}^3;\mathbb{C}^2)$ and is given by the integral kernel

$$\Pi^0(x,x') = \Pi^0_\perp(x^\perp, x'^\perp)\delta(z-z')P^\downarrow, \tag{52}$$

where

$$\Pi^0_\perp(x^\perp, x'^\perp) = \frac{B}{2\pi}\exp\left\{\tfrac{\mathrm{i}}{2}(x^\perp \times x'^\perp)\cdot\mathbf{B} - \tfrac{1}{4}(x^\perp - x'^\perp)^2 B\right\} \tag{53}$$

and $P^\downarrow$ is the the projector on vectors in $\mathbb{C}^2$ with spin component $-1/2$. The kernel $\Pi^0_\perp(x^\perp, x'^\perp)$ is a continuous function with

$$\int \Pi^0(x^\perp, u^\perp)\Pi^0(u^\perp, y^\perp)du^\perp = \Pi^0(x^\perp, y^\perp) \tag{54}$$

and

$$\Pi^0(x^\perp, x^\perp) = \frac{B}{2\pi} \tag{55}$$

for all $x^\perp$. A wave function in the lowest Landau band has the representation $\Psi = \Pi^0_N\Psi$. After writing Π^0_N as an integral operator (51) follows from the Cauchy-Schwarz inequality, using (54) and (55). □

5.4. PROPOSITION (Lower bound).

$$\liminf_{B\to\infty} \frac{E(B,Z,N)}{(\ln B)^2} \geq e(Z,N). \tag{56}$$

Proof. For fixed B let Ψ be a normalized wave function in the lowest Landau band. By (15) we have

$$\langle\Psi, H_{Z,N}\Psi\rangle \geq \int E_{Z,N}(\underline{x}^\perp)\left(\int |\Psi(\underline{x}^\perp, \underline{z})|^2 d\underline{z}\right) d\underline{x}^\perp. \tag{57}$$

We split the integral over $\underline{x}^\perp$ into an integral over $\mathcal{C}^{B,\varepsilon}$ (defined in (49)) and its complement in $\mathbb{R}^{2N}$. By Lemma 5.2 we have only to consider the latter. Using the estimate (41) the task is to bound terms of the form

$$\int_{|x_i^\perp|\leq\varepsilon B^{-1/2}} (1 + [\sinh^{-1}(Z|x_j^\perp|^{-1})]^2)\left(\int |\Psi(\underline{x}^\perp, \underline{z})|^2 d\underline{z}\right) d\underline{x}^\perp \tag{58}$$

from above. If $i = j$ we carry out the integration over all $x_k^\perp$ with $k \neq i$ and use Lemma 5.3 for the remaining variable $x_i^\perp$. For small r, $|\sinh^{-1} r^{-1}| \leq$ (const.)$|\ln r|$ and the term can be estimated by

$$(\text{const.})\int_{|x^\perp|\leq\varepsilon B^{-1/2}} (\ln|x^\perp|)^2 B dx^\perp \leq (\text{const.})\varepsilon^2(\ln B)^2. \tag{59}$$

For $i \neq j$ we split the integration over $x_j^\perp$ into two parts, namely $|x_j^\perp| \leq B^{-1/2}$ and $|x_j^\perp| \geq B^{-1/2}$. For the first part we obtain the following bound, after transforming variables and using Lemma 5.3, this time for $n = 2$,

$$(\text{const.})\varepsilon^2 \int_{|y_i^\perp|\leq 1, |y_j^\perp|\leq 1} (\ln B^{-1/2}|y_j^\perp|)^2 dy_i^\perp dy_j^\perp \leq (\text{const.})\varepsilon^2(\ln B)^2. \tag{60}$$

For the integral over $|x_j^\perp| \geq B^{-1/2}$ we estimate $|\sinh^{-1}(Z|x_j^\perp|^{-1})|^2$ by its maximum value, $\leq$ (const.)$(\ln B)^2$ and obtain for this part of the integral the upper bound

$$\begin{aligned}&\int_{|x_i^\perp|<\varepsilon B^{-1/2}} (1 + (\text{const.})(\ln B)^2) \left(\int |\Psi(\underline{x}^\perp, \underline{z})|^2 d\underline{z} \right) d\underline{x}^\perp \\ \leq &\int_{|x_i^\perp|<\varepsilon B^{-1/2}} (1 + (\text{const.})(\ln B)^2) B dx_i^\perp \leq \varepsilon^2(1 + c(\ln B)^2), \end{aligned} \tag{61}$$

where we have used Lemma 5.3 again. We see that (55) is bounded above by (const.)$(\varepsilon \ln B)^2$, for B large enough. Since $\varepsilon > 0$ is arbitrary this completes the proof. □

6 The one-dimensional delta-function model

We now want to study the the delta-function Hamiltonian (7), in particular its mean field limit, $N \to \infty$, $Z \to \infty$, with $\lambda = N/Z$ fixed.

For this it is convenient to make a scale transformation $z \to z/Z$, which implies a unitary equivalence

$$h_{Z,N} \cong Z^2 \widehat{h}_{Z,N} \tag{62}$$

with

$$\widehat{h}_{Z,N} = \sum_{i=1}^{N} \left(p_i^2 - \delta(z_i)\right) + \frac{1}{Z} \sum_{i<j} \delta(z_i - z_j). \tag{63}$$

We denote its ground state energy (again in the sense of quadratic forms) by $\widehat{e}(Z,N)$. The formal mean field theory of this system is identical to the so called hyper-strong theory discussed in [LSYa], Section 3. The energy of a (one dimensional) electron density $Z\rho$ in this theory is $Z\mathcal{E}^{\text{HS}}[\rho]$ with

$$\mathcal{E}^{\text{HS}}[\rho] = \int_{\mathbb{R}} \left(\frac{d}{dz} \sqrt{\rho(z)} \right)^2 - \rho(0) + \int \rho^2 dz \tag{64}$$

The infimum over densities with fixed normalization $\int \rho = \lambda$ leads to the hyper-strong energy $E^{\text{HS}}(\lambda)$ given by the right side of (5).

We shall now establish this mean field limit rigorously and prove Theorem 1.2.

6.1 A comparison model

An upper bound to the Hamiltonian (7) can be obtained from another model whose ground state can be computed explicitly. The corresponding Hamiltonian is completely symmetric with regard to each single reflection $z_i \to -z_i$, and the electronic repulsions are equally distributed between the sites z_i and $-z_i$:

$$\widetilde{h}_{Z,N} = \sum_{i=1}^{N} \left(p_i^2 - \delta(z_i)\right) + \frac{1}{2Z} \sum_{i<j} \left[\delta(z_i - z_j) + \delta(z_i + z_j)\right]. \tag{65}$$

Its ground state energy is denoted by $\widetilde{e}(Z, N)$.

The replacement of $1/Z$ by $1/(2Z)$ is important, because it compensates to a certain extent the doubling of the interaction sites. In particular it leads to the *same* formal mean field theory as (63) for symmetric electron densities ρ. This observation will be substantiated by the mathematical treatment in the sequel.

The model (65) was used in [WS] for $N = 2$ as a starting point for a perturbational calculation. It was also considered in [Ro] (for $N = 2$) as an upper bound to the model (7), but with the coupling $1/Z$ instead of $1/(2Z)$. The present considerations and extensions to $N \geq 3$ appear to be new.

The ground state wave function $\widetilde{\psi}$, if it exists, is completely symmetric under permutations of $\{z_1 ... z_N\}$ and reflections $z_i \to -z_i$. Such a highly symmetric function $\widetilde{\psi}$ is determined by its restriction to the cone

$$\mathcal{M} = \{\underline{z} : 0 \leq z_1 \leq z_2 \leq \ldots \leq z_N\} \tag{66}$$

In $\mathcal{M}$ we make the ansatz

$$\widetilde{\psi}(z_1 \ldots z_N) = c \prod_{i=1}^{N} e^{-\kappa_i z_i}, \tag{67}$$

with c a normalization constant and let $\widetilde{h}_{Z,N}$ act on the symmetrically extended $\widetilde{\psi}$.

The delta-function interactions dictate the jumps in the partial logarithmic derivatives of $\widetilde{\psi}$ at the boundary of $\mathcal{M}$ and we find

$$\kappa_1 = \frac{1}{2}, \qquad \kappa_i - \kappa_{i-1} = -\frac{1}{4Z},$$

which implies

$$\kappa_n = \frac{1}{2} - \frac{n-1}{4Z}. \tag{68}$$

The function (67) is square integrable if and only if all κ_n are strictly positive, which is equivalent to

$$N < 2Z + 1. \tag{69}$$

The corresponding eigenfunction $\widetilde{\psi}$, is everywhere positive, and it is easy to see that it is, indeed, a ground state for (65): Define the operators A_n on $L^2(\mathbb{R}^N)$ by

$$A_n = \partial_{z_n} - \partial_{z_n}(\ln\widetilde{\psi})\,, \tag{70}$$

with obvious domains of definition. Denoting by $\widetilde{e}(\widetilde{\psi})$ the eigenvalue of $\widetilde{h}_{Z,N}$ corresponding to $\widetilde{\psi}$ we can write the quadratic form $\widetilde{h}_{Z,N}$ as

$$\widetilde{h}_{Z,N} = \sum_{i=1}^{N} A_n^* A_n + \widetilde{e}(\widetilde{\psi}). \tag{71}$$

The equation

$$\langle\psi, \widetilde{h}_{Z,N}\psi\rangle = \sum_{i=1}^{N} \parallel A_n\psi \parallel^2 + \widetilde{e}(\widetilde{\psi}) \parallel \psi \parallel^2 \geq \ \widetilde{e}(\widetilde{\psi}) \parallel \psi \parallel^2, \tag{72}$$

which holds for each ψ in the form domain of $\widetilde{h}_{Z,N}$, shows that $\widetilde{e}(Z,N) = \widetilde{e}(\widetilde{\psi})$.

If $N \geq 2Z+1$, the simple inequality $\widetilde{e}(Z,N) \leq \widetilde{e}(Z,N-1)$ is sufficient for our purposes. To prove it, one may use trial-wave-functions of the form $\psi(z_1 \dots z_{N-1})\varepsilon\varphi(\varepsilon^2 z_N)$ whith a smooth φ, and take ε to zero. This inequality for the energies can be iterated to

$$\widetilde{e}(Z,N) \leq \widetilde{e}(Z,N_\mathrm{o}), \tag{73}$$

where N_o is the largest integer satisfying (69).

For $N < 2Z+1$ the *ground state energy* is the eigenvalue corresponding to (67):

$$\begin{aligned} \widetilde{e}(Z,N) &= \widetilde{e}(\widetilde{\psi}) = -\sum_{n=1}^{N}\kappa_n^2 = \\ &= -\frac{1}{4}\left\{N\left(1-\frac{\lambda}{2}+\frac{\lambda^2}{12}\right)+\left(\frac{\lambda}{2}-\frac{\lambda^2}{8}\right)+\frac{\lambda^2}{24N}\right\}. \end{aligned} \tag{74}$$

If $N \geq N_\mathrm{o}$ we may use (73), i.e., $\widetilde{e}(Z,N)$ is bounded from above by (74) with λ replaced by $\lambda_\mathrm{o} = N_\mathrm{o}/Z$. Dividing by Z and keeping λ fixed, the leading term for $N \to \infty$ is identical to $E^{\mathrm{HS}}(\lambda)$. By the next proposition this is sufficient for the upper bound in Theorem 1.2. But one can in fact show that $\widetilde{e}(Z,N_\mathrm{o})$ is *equal* to $\widetilde{e}(Z,N)$ for $N \geq 2Z+1$ and not only an upper bound to it. Hence N_o is equal to N_c, the maximal number of electrons that can be bound in the model (65). We give the proof of this result in the appendix.

6.1. PROPOSITION (The comparison model gives upper bounds). *The ground state energy of the symmetrized model $\widetilde{h}_{Z,N}$ is an upper bound to the ground state energy of $\widehat{h}_{Z,N}$:*

$$\widehat{e}(Z,N) \leq \widetilde{e}(Z,N). \tag{75}$$

This inequality is strict, if $N \geq 2$ and $N < 2Z+1$.

Proof. The Hamiltonian $\widetilde{h}_{Z,N}$ is the symmetrization of $\widehat{h}_{Z,N}$ with respect to the group $\mathcal{R}$ with 2^N elements, generated by the reflections $z_i \to -z_i$, $i = 1, \ldots, N$. For $R \in \mathcal{R}$ let U_R denote the corresponding unitary operators on $L^2(\mathbb{R}^N)$. Then

$$\frac{1}{2^N} \sum_{R \in \mathcal{R}} \langle U_R \psi, \widehat{h}_{Z,N} U_R \psi \rangle = \langle \psi, \widetilde{h}_{Z,N} \psi \rangle$$

for any ψ, so

$$\widehat{e}(Z,N) \leq \widetilde{e}(Z,N).$$

If $N < 2Z+1$ we may take the square integrable ground state wave function of $\widetilde{h}_{Z,N}$, given by (67), as a test state for $\widehat{h}_{Z,N}$. It satisfies $U_R \widetilde{\psi} = \widetilde{\psi}$ for all R, so

$$\langle \widetilde{\psi}, \widehat{h}_{Z,N} \widetilde{\psi} \rangle = \widetilde{e}(Z,N).$$

But $\widetilde{\psi}$ is not an eigenfunction of $\widehat{h}_{Z,N}$ if $N \geq 2$, so $\widehat{e}(Z,N)$ is strictly below $\widetilde{e}(Z,N)$. □

Combining the last proposition with Eq. (74), recalling that $e(Z,N) = Z^2 \widehat{e}(Z,N)$, we obtain

6.2. PROPOSITION (Upper bound in the mean field limit). *If $N, Z \to \infty$ with $\lambda = N/Z$ fixed, then*

$$\limsup e(Z,N)/Z^3 \leq E^{\mathrm{HS}}(\lambda) \tag{76}$$

where $E^{\mathrm{HS}}(\lambda)$ is given by (5).

6.2 Lower bounds to the delta-function Hamiltonian

An elegant way to obtain lower bounds for Hamiltonians with repulsive pair interactions is the use of positive definite functions. This was probably done for the first time in [HLT]. In this method, the positive definite functions have to be finite at the origin, however, and hence it is impossible to bound the δ-function interaction in this way without additional help. Our way out is to borrow a bit of kinetic energy (this was also done in Theorem 7.1 in [LSYa]). So we search for *operator inequalities*

$$a\, p^2 + \frac{1}{Z} \delta(z) \geq w_{Z,a,b}(z) \tag{77}$$

with appropriate functions $w_{Z,a,b}(z)$, depending on a parameter b in addition to a and Z to allow convergence to a delta function.

6.3. LEMMA (An operator inequality). *The inequality (77) holds for*

$$w_{Z,a,b}(z) = \frac{1}{Z^2 a} \frac{b^2}{(2b+1)} e^{-b|z|/Za} \tag{78}$$

Proof. With the simple reformulation to

$$a\,p^2 + \frac{1}{Z}\delta(z) - w_{Z,a,b}(z) \geq 0 \tag{79}$$

we are on well known territory: The Hamiltonian on the left side shall have no negative eigenvalue. By the scale transformation $z \to Zaz$, this inequality is transformed to

$$p^2 + \delta(z) - W_b(z) \geq 0, \qquad W_b(z) = Z^2\, a\, w_{Z,a,b}(Zaz). \tag{80}$$

This inequality will hold for

$$W_b(z) = \frac{b^2}{2b+1} e^{-b|z|} \tag{81}$$

if it is true for the larger potential

$$\widetilde{W}_b(z) = \frac{b^2}{(2b+1)} \frac{e^{-b|z|}}{(1-e^{-b|z|})},$$

because the Hamiltonian in (80) is bounded from below by

$$p^2 + \delta(z) - \widetilde{W}_b(z). \tag{82}$$

This Hamiltonian has

$$f(z) = 1 - \frac{1}{2b+1} e^{-b|z|} \tag{83}$$

as a positive symmetric solution to the Schrödinger equation - as a differential equation - with zero energy.

Now, if (82) would have a square integrable ground state wave function $g(z)$, this wave function would also be symmetric under reflection $z \to -z$, and the delta-function would dictate the same value for $g'(z)/g(z)$ as it does for $f'(z)/f(z)$ at $z = 0_+$. So the question of the existence of $g(z)$ can be dealt with by the methods which are used for proving Sturm's comparison theorem: We assume that $g(z)$ exists, with negative energy E. The Wronskian $W(z) := f'(z)g(z) - g'(z)f(z)$ is zero at $z = 0_+$. Its derivative is determined as $W'(z) = Ef(z)g(z)$. If $g(z)$ is chosen positive, then $W'(z)$ is negative, which implies that $W(z)$ is negative for $z \geq 0$, and $g'(z)/g(z) > f'(z)/f(z)$. This inequality can be integrated to give $g(z)/g(0) > f(z)/f(0)$, a contradiction to the assumption of the square-integrability of g(z).

Therefore we know that the Hamiltonian (82) has no negative eigenvalue. And so the operator inequality holds. $\square$

The $\{W_b(z)\}$ and hence $\{Zw_{Z,a,b}(z)\}$ are δ-sequences in the limit $b \to \infty$. All these functions are positive definite, and finite at the origin:

$$w_{Z,a,b}(0) < \frac{b}{2Z^2\, a}. \tag{84}$$

With this tool we can now deduce the lower bound for the many body Hamiltonian:

6.4. PROPOSITION (Lower bound in the mean field limit). *If* $N, Z \to \infty$ *with* $\lambda = N/Z$ *fixed, then*

$$\liminf e(Z,N)/Z^3 \geq E^{\mathrm{HS}}(\lambda). \tag{85}$$

Proof. We use the operator inequality (77) with $w_Z(z) := w_{Z,a,b}(z)$, (a and b will finally be chosen as appropriate powers of N) to bound $\widehat{h}_{Z,N}$ from below. For each $\delta(z_i - z_j)$ we use it twice; one time with ap_i^2, and a second time with ap_j^2. Then we add these inequalities and divide by two:

$$\begin{aligned} \widehat{h}_{Z,N} &= \sum_{i=1}^{N} \left[\left(1 - a\frac{N-1}{2}\right) p_i^2 - \delta(z_i) \right] + \sum_{i<j} \left[a\frac{p_i^2 + p_j^2}{2} + \frac{1}{Z}\delta(z_i - z_j) \right] \\ &\geq \sum_{i=1}^{N} [\ldots] + \sum_{i<j} w_Z(z_i - z_j). \end{aligned} \tag{86}$$

At this point the positive definiteness of $w_Z(z)$ becomes essential. It implies, that for any real valued integrable function $\sigma(z)$:

$$\frac{1}{2} \iint dz dy \left(N\sigma(z) - \sum_{i=1}^{N} \delta(z - z_i) \right) w_Z(z-y) \left(N\sigma(y) - \sum_{i=1}^{N} \delta(y - z_j) \right) \geq 0 \tag{87}$$

Expanding this expression and integrating the delta-functions we get

$$\begin{aligned} \sum_{i<j} w_Z(z_i - z_j) \geq \sum_i N \int w_Z(z_i - z)\sigma(z) dz - \frac{N}{2} w_Z(0) \\ -\frac{N^2}{2} \iint \sigma(z) w_Z(z-y) \sigma(y) dz dy. \end{aligned} \tag{88}$$

Combining this with (86) gives

$$\widehat{h}_{Z,N} \geq \sum_{i=1}^{N} h_i(Z,N,\sigma) - \frac{N^2}{2} \iint \sigma(z) w_Z(z-y) \sigma(y) dz dy \tag{89}$$

with the one-particle operators

$$h_i(Z,N,\sigma) = \left(1 - a\frac{N-1}{2}\right) p_i^2 - \delta(z_i) + N(\sigma * w_Z)(z_i) - \frac{1}{2} w_Z(0). \tag{90}$$

The parameters are now chosen as

$$a = N^{-1-\varepsilon}, \qquad b = N^{\varepsilon}, \qquad \text{with } 0 < \varepsilon < 1/2.$$

The fraction of kinetic energy per particle that we borrowed in (86) then decreases as $N^{-\varepsilon}$, and the functions $w_Z(z)$ become

$$w_Z(z) = \frac{N^{1+\varepsilon}}{Z^2}\frac{N^{2\varepsilon}}{(2N^\varepsilon+1)}e^{-z\cdot N^{1+2\varepsilon}/Z}. \tag{91}$$

In the mean field limit $N, Z \to \infty$ with $N/Z = \lambda > 0$ fixed the sequence $Zw_Z(z)$ is a δ-sequence, and $w_Z(0) \sim \lambda N^{2\varepsilon}/Z \to 0$. If $\sigma(z)$ is smooth with $|\sigma'(z)| \leq \gamma$, then $|N(\sigma * w_Z)(z) - \sigma(z)| \leq 2\gamma\lambda^2 N^{-\varepsilon}$. The one particle Hamiltonians $h(Z, N, \sigma)$, with smooth $\sigma(z)$, converge as quadratic forms pointwise (i.e., for each test function) to

$$h_{\lambda\sigma} = p^2 - \delta(z) + \lambda\sigma(z). \tag{92}$$

Moreover

$$h(Z, N, \sigma) \geq h_{\lambda\sigma} - (N^{-\varepsilon}/2)p^2 - 2\delta\lambda^2 N^{-\varepsilon} - (\lambda^2/2)N^{2\varepsilon-1}. \tag{93}$$

Since the ground state energies of operators of the type $\alpha p^2 + V$ are concave functions of α and hence continuous in α, the ground state energies of the right side of (93) converge in the limit $N \to \infty$.

The ground state energy of $h_{\lambda\sigma}$ is a concave functional $e[\lambda\sigma]$, and the lower bound (89), when divided by the number of electrons N, gives

$$\liminf_{\substack{N,Z\to\infty \\ N/Z=\lambda}} \frac{1}{N}\widehat{e}(Z, N) \geq e[\lambda\sigma] - \frac{\lambda}{2}\int \sigma^2(z)dz =: \mathcal{I}_\lambda[\sigma]. \tag{94}$$

Inserting the mean field density ρ for $\lambda\sigma$ (i.e., the minimizer of (64) which satisfies Eq. (3.8) of [LSYa]) gives the mean field energy, divided by λ, as a lower bound to the limit of the energy per electron. □

We remark that searching for the supremum of $\mathcal{I}_\lambda[\sigma]$ in (94) also leads to the mean field equation of [LSYa]: Assuming $e(\lambda\sigma) = \langle\psi, h_{\lambda\sigma}\psi\rangle$ with a normalized ψ the variational condition on $\sigma(z)$ for maximizing $\mathcal{I}_\lambda[\sigma]$ is

$$\sigma(z) = \psi^2(z). \tag{95}$$

Inserting this into the Schrödinger equation $h_{\lambda\sigma}\psi = \mu_\lambda\psi$ for ψ gives

$$-\psi''(z) - \delta(z)\psi(0) + \lambda\psi^3(z) = -\mu_\lambda\psi(z), \tag{96}$$

i.e., Equation (3.8) in [LSYa].

Finally we remark that the energy per electron, $\widehat{e}(Z, N)/N$, approaches the mean field limit monotonously. There is also a subadditivity property, which in the limit becomes concavity of $E^{\mathrm{HS}}(\lambda)/\lambda$. These properties of the approach to a mean field hold in some other cases too, as will be shown elsewhere [B99].

7 Conclusions

We have shown that the energy of an atom in a strong magnetic field B approaches, after division by $(\ln B)^2$, the energy of a many body Hamiltonian with delta interactions in one dimension as $B \to \infty$. This delta function model is not explicitly solvable, but an upper bound to the energy can be given in terms of another model with the same mean field limit and where we can explicitly calculate the ground state energy. In the latter model an atom with nuclear charge Z can bind up to $2Z$ electrons. Whether this represents the true state of affairs for the atomic Hamiltonian in the $B \to \infty$ limit is an open problem.

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Appendix

We prove here that the ground state energy $\widetilde{e}(Z,N)$ of the Hamiltonian (65) is independent of N if $N \geq 2Z+1$.

PROPOSITION (Maximal negative ionization for the comparison model). *If $N \geq 2Z+1$, then*

$$\widetilde{e}(Z,N) = \widetilde{e}(Z,N_{\rm o}) \tag{97}$$

where $N_{\rm o}$ is the largest integer strictly smaller than $2Z+1$. Moreover, there is then no L^2-function with $\widetilde{e}(Z,N)$ as an eigenvalue.

Proof. In the cone $\mathcal{M}$ defined by (66) we consider the wave function

$$\check{\psi}(z_1,\ldots,z_N) = \prod_{i=1}^{N_{\rm o}} e^{-\kappa_i z_i} \prod_{j=N_{\rm o}+1}^{N} (1-\kappa_j z_j), \tag{98}$$

with κ_n defined by (68). Since $\kappa_j \leq 0$ for $j \geq N_{\rm o}+1$, the function $\check{\psi}$ is strictly positive. We extend $\check{\psi}$ symmetrically from $\mathcal{M}$ to all of $\mathbb{R}^N$ as a continuous function.

The jumps in the logarithmic derivatives of $\check{\psi}$ at the boundary of $\mathcal{M}$ are not of the right size required for an eigenfunction of $\widetilde{h}_{Z,N}$. But $\check{\psi}$ is an eigenfunction of a slightly different operator:

$$\check{h}_{Z,N}\check{\psi} = \check{e}(Z,N)\check{\psi} \tag{99}$$

with

$$\check{e}(Z,N) = -\sum_{i=1}^{N_o} \kappa_i^2 = \widetilde{e}(Z,N_o) \tag{100}$$

and

$$\check{h}_{Z,N} = \sum_{i=1}^{N} \left(p_i^2 - \delta(z_i)\right) + \frac{1}{2Z}\sum_{i<j} \gamma_{i,j}(z_1,\ldots,z_N)\left[\delta(z_i - z_j) + \delta(z_i + z_j)\right]. \tag{101}$$

with certain functions $\gamma_{i,j}$. It is sufficient to specify $\gamma_{i,i+1}(z_1,\ldots,z_N)$ on the boundary of $\mathcal{M}$ (other cases follow by permutation and/or reflection of the variables) and one finds for $0 \le z_1 \le z_2 \le \ldots \le z_N$:

$$\gamma_{i,i+1} = \begin{cases} 1 & \text{if} \quad 1 \le i \le N_o - 1 \\ 4Z\left(\kappa_{N_o} + |\kappa_{N_o+1}|(1+|\kappa_{N_o+1}|z_{N_o})^{-1}\right) & \text{if} \quad i = N_o \\ (1+|\kappa_i|z_i)^{-1}(1+|\kappa_{i+1}|z_{i+1})^{-1} & \text{if} \quad N_o + 1 \le i \le N \end{cases}. \tag{102}$$

Since $\gamma_{i,i+1} \le 1$ for all i one has

$$\check{h}_{Z,N} \le \widetilde{h}_{Z,N}. \tag{103}$$

Since $\check{\psi}$ is stricly positive we can in the same way as in (71) write

$$\check{h}_{Z,N} = \sum_{n}^{N} \check{A}_n^* \check{A}_n + \check{e}(Z,N) \tag{104}$$

with

$$\check{A}_n = \partial_{z_n} - \partial_{z_n}(\ln\check{\psi}), \tag{105}$$

and conclude that $\check{e}(Z,N) = \widetilde{e}(Z,N_o)$ is, indeed, the ground state energy of $\check{h}_{Z,N}$. Hence, $\widetilde{e}(Z,N) = \widetilde{e}(Z,N_o)$ for $N \ge 2Z+1$.

To see that there are no bound states at the bottom of the spectrum of $\widetilde{h}_{Z,N}$ assume ψ is an eigenfunction to eigenvalue $\widetilde{e}(Z,N)$, so that

$$\langle\psi, \widetilde{h}_{Z,N}\psi\rangle = \widetilde{e}(Z,N) \parallel \psi \parallel^2 . \tag{106}$$

By (103) and the equality of the ground state energies this implies

$$\langle\psi, \check{h}_{Z,N}\psi\rangle = \check{e}(Z,N) \parallel \psi \parallel^2, \tag{107}$$

which, because of (104), is equivalent to the set of differential equations

$$\check{A}_n\psi = 0. \tag{108}$$

These equations have no other solutions than $c\check{\psi}$, and $\check{\psi}$ is not an L^2 function. $\square$

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