Atoms with bosonic "electrons" in strong magnetic fields

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Abstract

We study the ground state properties of an atom with nuclear charge Z and N bosonic "electrons" in the presence of a homogeneous magnetic field B. We investigate the mean field limit $N \to \infty$ with N/Z fixed, and identify three different asymptotic regions, according to $B \ll Z^2$, $B \sim Z^2$, and $B \gg Z^2$. In Region 1 standard Hartree theory is applicable. Region 3 is described by a one-dimensional functional, which is identical to the so-called Hyper-Strong functional introduced by Lieb, Solovej and Yngvason for atoms with fermionic electrons in the region $B \gg Z^3$; i.e., for very strong magnetic fields the ground state properties of atoms are independent of statistics. For Region 2 we introduce a general *magnetic Hartree functional*, which is studied in detail. It is shown that in the special case of an atom it can be restricted to the subspace of zero angular momentum parallel to the magnetic field, which simplifies the theory considerably. The functional reproduces the energy and the one-particle reduced density matrix for the full N-particle ground state to leading order in N, and it implies the description of the other regions as limiting cases.

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1 Introduction

The ground states of atoms with many electrons in magnetic fields have been studied in [LSY94a, LSY94b, BSY00], and their energies have been evaluated, exactly to leading order, as some of the physical parameters tend to infinity. The atoms have been modeled by the nonrelativistic quantum mechanics of N fermionic electrons, with an unmovable pointlike nucleus of charge Z in a homogeneous magnetic field of strength B. In order to shed some more light onto the interplay of the involved laws of physics, we investigate the effects of changing one of them: What would happen, if the electrons were bosons?

So we study the ground state of the Hamiltonian - written in appropriate units -

$$\underline{H}_{N,Z,B} = \sum_{i=1}^{N} \left(H_{B,i} - B - \frac{Z}{|\mathbf{x}_i|} \right) + \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}, \tag{1.1}$$

where we set

$$H_{B,j} = \left(-i\nabla_j + B\mathbf{a}(\mathbf{x}_j)\right)^2 . \tag{1.2}$$

The vector potential is given by $\mathbf{a}(\mathbf{x}) = \mathbf{e}^{\|} \times \mathbf{x}/2$, where $\mathbf{x} \in \mathbb{R}^3$, $\mathbf{e}^{\|}$ is the unit vector parallel to the magnetic field in z-direction. This Hamiltonian acts on the *symmetric* subspace of $\mathcal{L}^2(\mathbb{R}^{3N}, d^{3N}\mathbf{x})$. We subtract B for every particle because we are interested in the binding energy, which is now equal to the ground state energy $\underline{E}(N,Z,B) = \inf \mathrm{spec}\ \underline{H}_{N,Z,B}$.

In the **study of asymptotics**, as B and Z tend to infinity, we find a division into *three different regions*. They are - always in appropriate units - characterized by: $B \ll Z^2$, $B \sim Z^2$, $B \gg Z^2$. This is in contrast to atoms with fermionic electrons, where five different regions have been identified: $B \ll Z^{4/3}$, $B \sim Z^{4/3}$, $Z^{4/3} \ll B \ll Z^3$, $B \sim Z^3$, $B \gg Z^3$. See [LSY94a] and references therein.

A simple heuristic argument: The length scale, which is typical for the quantum effects of a *single* particle in the magnetic field, is $\sim B^{-1/2}$. Typical energies are the differences of the Landau levels, $2B$. On the other hand, the length scale typical for a particle in the Coulomb potential only is $\sim Z^{-1}$ and hence the typical energy range is $\sim Z^2$. In Region 2, where $B \sim Z^2$, the magnetic and the Coulombic effects are therefore of the same order of magnitude. In Region 1, where $B \ll Z^2$, the Coulomb effects dominate in all directions. Magnetic effects will not contribute in leading order. In Region 3, where $B \gg Z^2$, the magnetic effects dominate the dynamics perpendicular to the magnetic field. The electron with low energy is confined to the lowest Landau band, the typical wave functions are squeezed to needles with diameter $\sim B^{-1/2}$. (See [AHS81, FW94] for a detailed rigorous treatment and for citations concerning the history of this problem.) Turning from the one-body system to the N-body problem, we remark that Bose statistics has no effect on the size of the ground states, if the pair interactions are ignored. Moreover, the repulsion of the particles is of the same order of magnitude as the attraction of the nucleus, if $N \sim Z$. So the scaling properties of the lengths and energies per particle remain the same, and the distinction of the three regions for many bosons is the same as for a single electron.

We remark, that we can moreover identify a Region 4 with strong magnetic field, where the nuclear charge Z is fixed. In this region the asymptotics is, in leading order, independent of the statistics, as has been noted in its evaluation in [BSY00]. It is to be described by the model of one-dimensional atoms with delta-function interactions.

Scaling: In the following we will use the parameters $\lambda = N/Z$, $\beta = B/Z^2$ besides N. By scaling $\mathbf{x} \to \mathbf{x}/Z$ the operator $Z^{-2}\underline{H}_{N,Z,B}$ is unitarily equivalent to

$$H_{N,\lambda,\beta} = \sum_{i=1}^{N} \left(H_{\beta,i} - \beta - \frac{1}{|\mathbf{x}_i|} \right) + \frac{\lambda}{N} \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|}, \tag{1.3}$$

with ground state energy $E(N,\lambda,\beta) = Z^{-2}\underline{E}(N,Z,B)$. We are interested in the limit $N \to \infty$ of $N^{-1}E(N, \lambda, \beta)$ with λ fixed. In Region 1 this limit is coupled with $\beta \to 0$, and in Region 3 with $\beta \to \infty$, while β is fixed in Region 2. The asymptotics of the atomic structure and of its energy for large N in the three regions is modeled by energy functionals in generalized Hartree theory.

In **Region 1** standard Hartree theory is applicable. The energy functional, a functional of the density ρ, is

$$\mathcal{E}^{\mathrm{H}}[\rho] = \int |\nabla \rho^{1/2}(\mathbf{x})|^2 d^3\mathbf{x} - \int \frac{1}{|\mathbf{x}|}\rho(\mathbf{x})d^3\mathbf{x} + D[\rho, \rho], \tag{1.4}$$

where

$$D[\rho, \rho] = \frac{1}{2}\int \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}d^3\mathbf{x}d^3\mathbf{y}. \tag{1.5}$$

Its ground state energy is

$$E^{\mathrm{H}}(\lambda) = \inf_{\rho,\ \int\rho=\lambda} \mathcal{E}^{\mathrm{H}}[\rho]. \tag{1.6}$$

It is known, [BL83], that

$$\lim_{N\to\infty} \frac{1}{N}E(N, \lambda, 0) = \frac{1}{\lambda}E^{\mathrm{H}}(\lambda). \tag{1.7}$$

We will extend this result to

1.1. THEOREM (Energy asymptotics for Region 1). *If $N \to \infty$ and $\beta = \beta(N) \to 0$ with λ fixed, then*

$$\lim_{N\to\infty} \frac{1}{N}E(N, \lambda, \beta) = \frac{1}{\lambda}E^{\mathrm{H}}(\lambda). \tag{1.8}$$

In **Region 2** Hartree theory has to be generalized. The basic idea remains: the electrons occupy the ground states of an effective one-particle Hamiltonian with a mean field potential which has to be determined by self-consistency. Now in the presence of a magnetic field, the ground state of the effective Hamiltonian may a priori be degenerate, so that the electrons can be distributed over a larger set of states. To take this into account, one has to consider in general one-particle *density matrices* Γ in this *Magnetic Hartree Theory.* The energy functional is

$$\mathcal{E}^{\mathrm{MH}}_\beta[\Gamma] = \mathrm{Tr}[(H_\beta - \beta)\Gamma] - \int \frac{1}{|\mathbf{x}|}\rho_\Gamma(\mathbf{x})d^3\mathbf{x} + D[\rho_\Gamma, \rho_\Gamma], \tag{1.9}$$

where $\rho_\Gamma(\mathbf{x})$ is the density defined by Γ, with $\int \rho_\Gamma = \mathrm{Tr}[\Gamma]$. We define the Hartree energy $E^{\mathrm{MH}}(\lambda, \beta)$ as

$$E^{\mathrm{MH}}(\lambda, \beta) = \inf_{\Gamma,\ \mathrm{Tr}[\Gamma]=\lambda} \mathcal{E}^{\mathrm{MH}}_\beta[\Gamma]. \tag{1.10}$$

This general form of magnetic Hartree theory is necessary, if some extra external potential is added, or if one considers, e.g., molecules. For, in the presence of magnetic fields, some well known facts of ordinary quantum mechanics are no longer true: the ground state may be degenerate, and, in the case of an axially symmetric system, it can happen that the energy is not minimized by states with zero angular momentum [LO77, AHS78]. But for the atom without perturbing forces, it turns out that the theory can be reduced to the consideration of pure states, rank one density matrices, with a zero angular momentum component parallel to the magnetic field. In this case (1.9) simplifies to the *Magnetic Hartree density functional*

$$\hat{\mathcal{E}}_{\beta}^{\mathrm{MH}}[\rho] = \int \left(|\nabla\sqrt{\rho}|^2 + \frac{\beta^2}{4} r^2 \rho - \beta\rho - \frac{1}{|\mathbf{x}|}\rho \right) d^3\mathbf{x} + D[\rho,\rho], \tag{1.11}$$

where r is the radial coordinate perpendicular to the magnetic field. This functional is the restriction of (1.9) to density matrices of the form $|\sqrt{\rho}\rangle\langle\sqrt{\rho}|$. We will show in the next section that both $\mathcal{E}^{\mathrm{MH}}$ and $\hat{\mathcal{E}}^{\mathrm{MH}}$ have the same ground state energy and density, so one could alternatively define E^{MH} as the infimum of $\hat{\mathcal{E}}^{\mathrm{MH}}$.

The energy asymptotics for Region 2 are stated in the following theorem:

1.2. THEOREM (Energy asymptotics for Region 2). *If $N \to \infty$ with λ and β fixed, then*

$$\lim_{N\to\infty} \frac{1}{N} E(N,\lambda,\beta) = \frac{1}{\lambda} E^{\mathrm{MH}}(\lambda,\beta). \tag{1.12}$$

In **Region 3** the ground state of the atom is squeezed into a needle with diameter - in the scaled coordinates - $\sim \beta^{-1/2}$. The Coulomb interaction of the confined particles acts along the needle effectively like a one dimensional delta function, with coupling constant $\sim \ln\beta$. It thus dictates the typical extension $\sim (\ln\beta)^{-1}$ of the ground state wave function in the direction of the field, and the typical energies as $\sim (\ln\beta)^2$. This effective reduction to a one dimensional system has been discussed in [LSY94a, JY96, BSY00]; see also [BRW99] for related studies. In the appropriate scaling, $z \sim (\ln\beta)x^{\parallel}$, with $x^{\parallel}$ the coordinate in the direction parallel to the magnetic field, the theory is a Hartree theory for a one dimensional model. It is identical to the theory for Region 5 of fermionic electrons, which has been studied in [LSY94a], including an exact solution of the ground state problem. Its energy functional has been called the *Hyper Strong* Functional; it is

$$\mathcal{E}^{\mathrm{HS}}[\rho] = \int (\frac{d}{dz}\rho^{1/2}(z))^2 dz - \rho(0) + \frac{1}{2}\int \rho(z)^2 dz, \tag{1.13}$$

with its ground state energy defined as

$$E^{\mathrm{HS}}(\lambda) = \inf_{\rho,\ \int\rho=\lambda} \mathcal{E}^{\mathrm{HS}}[\rho]. \tag{1.14}$$

We will prove

1.3. THEOREM (Energy asymptotics for Region 3). *If $N \to \infty$ and $\beta = \beta(N) \to \infty$ with λ fixed, then*

$$\lim_{N\to\infty} \frac{E(N,\lambda,\beta)}{N(\ln\beta)^2} = \frac{1}{\lambda} E^{\mathrm{HS}}(\lambda). \tag{1.15}$$

The difference between bosonic atoms in our Region 3 to fermionic atoms in the fermion-Region 5 is in the condition of applicability of HS-theory. The Pauli principle demands one needle for each electron, electrostatics makes them lying side by side. The fermionic atom is thus a bundle of N needles, with total diameter - in unscaled coordinates and with unscaled parameters - $\sim N^{1/2}B^{-1/2}$. The condition for validity of HS-Theory is that the diameter of the atom, in the directions of $\mathbf{x}^\perp$, perpendicular to the field, is much smaller than the characteristic length of Coulombic quantum effects, $\sim Z^{-1}$. This condition is therefore $B \gg NZ^2$ for fermionic atoms. Bosonic electrons may all occupy the same needle. For them, the particle number does therefore not appear in the condition, which is now $B \gg Z^2$.

In the investigation of the limits we exploit four **principles**:

(i) Restriction to independent particles,

(ii) Spatial concentration near the center,

(iii) Concentration in the lowest Landau band, and

(iv) High field limit of the Coulomb-interaction.

The principle (i) is fundamental for the validity of the Hartree theories: The atom with many interacting particles will be compared to models with independent particles in an effective mean field.
The spatial concentration (ii) had not to be stressed in systems without magnetic fields. In the studies of fermionic electrons, [LSY94a, BSY00], it has been proven as a consequence of the superharmonicity of the repulsive interactions. We will also use this superharmonicity, but in a different way: It implies the vanishing of the parallel component of the angular momentum in the state which minimizes the Hartree energy. Since one of the consequences is the absence of an "angular momentum barrier", it can also be viewed as a spatial concentration of the bound electrons.
The principles (iii) and (iv) are effective in Region 3, in the limit $\beta \to \infty$.

In the investigations of bosonic "electrons" we could probably have mimicked the procedure of [LSY94a], with some changes due to the Bose statistics. Our procedure relies in fact heavily on the same methods, but we combine them in a new way: The principles (ii), (iii) and (iv) mentioned above are studied for single particles in effective mean fields. In the study of many particle systems, we begin with the reduction to independent particles. But this has to be done in a subtle way, anticipating the limits which have to follow. We do this by extending the method of [BSY00].

The Hartree theories will be discussed in Sect. 2, including the restriction to zero angular momentum in Sect. 2.5. The confinement to the lowest Landau band, relevant for Region 3, is treated in Sect. 3.2 and the following subsection. In Sect. 4 Hartree theory is proven to be the limit of many particle quantum mechanics, as it is formulated in the Theorems 1.1, 1.2 and 1.3. Subsection 4.3 treats the restriction to the independent particle model. Finally, some results on the states and on "Bose condensation" are presented in Subsections 4.6 and 4.7.

In the investigations of the limiting procedures, we are interested in the physical dimensions of estimates and bounds, not about numerics. We use "C" or "*const.*" for all the numerical constants.

2 Hartree theory

2.1 Definitions and basic properties

Definitions: The Hartree functional without a magnetic field, $\mathcal{E}^{\mathrm{H}}[\rho]$ in (1.4), is defined for non-negative densities $\rho(\mathbf{x}) \in \mathcal{L}^1(\mathbb{R}^3, d^3\mathbf{x})$ with the restriction that every component of $\nabla\rho^{1/2}(\mathbf{x})$ is an element of $\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{x})$. Analogously, the functional for Region 3, $\mathcal{E}^{\mathrm{HS}}[\rho]$ in (1.13), is defined for non-negative densities $\rho(z) \in \mathcal{L}^1(\mathbb{R}, dz)$ with the restriction $d(\rho^{1/2}(z))/dz \in \mathcal{L}^2(\mathbb{R}, dz)$. The functional for Region 2, $\mathcal{E}^{\mathrm{MH}}[\Gamma]$ in (1.9), is defined for density-matrices, non-negative trace class operators Γ acting on $\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{x})$, with the restriction of a finite magnetic-kinetic energy:

$$\mathrm{Tr}[H_\beta \Gamma] < \infty \tag{2.1}$$

The associated density $\rho_\Gamma(\mathbf{x})$ can be defined in $\mathcal{L}^1(\mathbb{R}^3, d^3\mathbf{x})$ as a norm convergent sum of integrable densities $\sum_k w_k \rho_k$, by diagonalizing the density matrix as

$$\Gamma = \sum_k w_k |\psi_k\rangle\langle\psi_k|, \tag{2.2}$$

with normalized ψ_k, and $\rho_k(\mathbf{x}) = |\psi_k(\mathbf{x})|^2$.

The conditions of finiteness of the kinetic energies imply the finiteness of potential energies, in all three regions: the attraction is bounded by the kinetic energy, because of the boundedness of the Coulomb potential (delta function potential in Region 3) relative to the operator of kinetic energy, which is proven with the stability of the hydrogen atom. Moreover, the repulsion is bounded by attraction, because for $\sigma(\mathbf{x})$ and $\rho(\mathbf{x})$ both non-negative elements of $\mathcal{L}^1(\mathbb{R}^3, d^3\mathbf{x})$,

$$2D[\sigma, \rho] < \lambda \sup_{\mathbf{y}} A_{\mathbf{y}}[\rho], \tag{2.3}$$

with $\lambda = \int \sigma(\mathbf{x})d^3\mathbf{x}$ and $A_{\mathbf{y}}[\rho] = \int \frac{1}{|\mathbf{x}-\mathbf{y}|}\rho(\mathbf{x})d^3\mathbf{x}$. The analogous inequality for the HS theory is

$$\int \sigma(z)\rho(z)dz < \lambda \sup_y \rho(y), \tag{2.4}$$

for $\sigma(z)$ and $\rho(z)$ both non-negative elements of $\mathcal{L}^1(\mathbb{R}, dz)$ and $\lambda = \int \sigma(z)dz$.

In the **variational principles** which define the Hartree energies, the restrictions $\|\rho\|_1 = \lambda$ and $\mathrm{Tr}[\Gamma] = \lambda$ can be weakened to $\|\rho\|_1 \leq \lambda$ and $\mathrm{Tr}[\Gamma] \leq \lambda$, because one can always "move some charge to infinity". This will be used for the proof of the existence of a minimizer for the energy, and this in return means that "inf" can be replaced by "min".

In the following discussion we will explicitly study the magnetic Hartree theory. All the results which do not refer to the dependence on β are also valid - in their essence of physical meaning, with some changes in the mathematics - for the standard and the HS theory. The proofs can be transfered, keeping their structure, but changing the mathematical expressions. This is an indication, that the physics behind the arguments is often the same. We point out, in particular, that the delta potential has the same scaling properties as the Coulomb potential.

Introducing more non-negative parameters, we will study the *extended energy functional*

$$\mathcal{E}^{\mathrm{MH}}_{\lambda,\beta,\zeta,\alpha}[\Gamma] = \lambda \mathrm{Tr}[(H_\beta - \beta)\Gamma] - \lambda \int \frac{\zeta}{|\mathbf{x}|}\rho_\Gamma(\mathbf{x})d^3\mathbf{x} + \alpha\lambda^2 D[\rho_\Gamma, \rho_\Gamma], \tag{2.5}$$

and its ground state energy

$$E^{\mathrm{MH}}_{\mathrm{ext}}(\lambda, \beta, \zeta, \alpha) = \inf_{\Gamma,\ \mathrm{Tr}[\Gamma]\leq 1} \mathcal{E}^{\mathrm{MH}}_{\lambda,\beta,\zeta,\alpha}[\Gamma]. \tag{2.6}$$

By scaling one verifies that the energies are related through

$$E^{\mathrm{MH}}_{\mathrm{ext}}(\lambda, \beta, \zeta, \alpha) = \frac{\zeta^3}{\alpha} E^{\mathrm{MH}}(\frac{\alpha}{\zeta}\lambda, \frac{1}{\zeta^2}\beta). \tag{2.7}$$

Monotonicity, convexity and concavity properties.

(i) Since the functional $\mathcal{E}^{\mathrm{MH}}_{\lambda,\beta,\zeta,\alpha}[\Gamma]$ is decreasing in ζ, increasing in α and jointly linear in (ζ, α), the Hartree energy $E^{\mathrm{MH}}_{\mathrm{ext}}$ is decreasing in ζ, increasing in α and jointly concave in (ζ, α).

(ii) Since the functional $\mathcal{E}^{\mathrm{MH}}_{\lambda,\beta,\zeta,\alpha}[\Gamma]/\lambda$ is increasing in λ and jointly linear in (ζ, λ), the **energy per unit charge** of the electron cloud, $E^{\mathrm{MH}}_{\mathrm{ext}}/\lambda$, is increasing in λ and jointly concave in (ζ, λ).
Because of (2.7), these properties are actually equivalent to (i).

(iii) Since moreover the functional $\mathcal{E}_\beta^{\mathrm{MH}}[\Gamma]$ is convex in Γ (it is even strictly convex in ρ_Γ, since $D[\rho,\rho]$ is strictly convex in ρ), and since the sets $\{\mathrm{Tr}[\Gamma] \leq \lambda\}$ are ordered by inclusion, the Hartree energy $E^{\mathrm{MH}}(\lambda,\beta)$ is decreasing and convex in λ. For, if Γ_n with $\mathrm{Tr}[\Gamma_n] = \lambda$ and Υ_n with $\mathrm{Tr}[\Upsilon_n] = \bar{\lambda}$ are minimizing sequences, it follows, that $E^{\mathrm{MH}}((\lambda+\bar{\lambda})/2,\beta) \leq \inf_n \mathcal{E}_\beta^{\mathrm{MH}}[(\Gamma_n + \Upsilon_n)/2]$.

The convexity property justifies the definition of a **critical charge** λ_c, which a priori might be infinity, indicating the maximal charge which the nucleus can bind: E^{MH} is strictly decreasing for $\lambda \leq \lambda_c$, and constant for $\lambda \geq \lambda_c$.

Moreover, the convexity of E^{MH} in λ and the concavity of E^{MH}/λ give upper and lower bounds on $\partial^2 E^{\mathrm{MH}}/\partial\lambda^2$, guaranteeing the existence of the **chemical potential**

$$\mu = \frac{\partial E^{\mathrm{MH}}}{\partial \lambda} \tag{2.8}$$

as a continuous function of λ.

Comparison with the hydrogen atom:
The extended functional (2.5) with $\alpha = 0$ is obviously related to the energy of the hydrogen atom described with the Pauli Hamiltonian, where the magnetic moment of the electron serves for the subtraction of β in the ground state energy:

$$E_{\mathrm{ext}}^{\mathrm{MH}}(\lambda,\beta,\zeta,0) = \lambda E^{\mathrm{hyd}}(\beta,\zeta). \tag{2.9}$$

We have the following bounds:

2.1. PROPOSITION (Energies of hydrogen as bounds). *For* $\lambda > 0$ *and* $\alpha > 0$

$$E_{\mathrm{ext}}^{\mathrm{MH}}(\lambda,\beta,\zeta,\alpha) \;>\; \lambda E^{\mathrm{hyd}}(\beta,\zeta) \tag{2.10}$$
$$E_{\mathrm{ext}}^{\mathrm{MH}}(\lambda,\beta,\zeta,\alpha) \;<\; \lambda E^{\mathrm{hyd}}(\beta,\zeta-\lambda\alpha/2). \tag{2.11}$$

Proof. The first inequality follows from the strict positivity of $D[\rho,\rho]$. The upper bound can be given by choosing the projection onto the ground state of the Hamiltonian $H_\beta - (\zeta - \lambda\alpha/2)/|\mathbf{x}|$, as a test density matrix Γ. Then we apply the bound to the repulsion by attraction (2.3), together with the observation, that the nucleus has to be at the point of the maximum of the potential $A_y[\rho]$. (Otherwise the energy could be lowered by shifting ρ). □

We remark that the bound (2.11) is of no use for $\lambda\alpha \sim 2\zeta$ or larger. In this case one can use the monotone decrease of the energy $E_{\mathrm{ext}}^{\mathrm{MH}}$ in λ, and bound $E_{\mathrm{ext}}^{\mathrm{MH}}$ by $\min_\lambda\{\lambda E^{\mathrm{hyd}}(\beta,\zeta-\lambda\alpha/2)\}$. We will use these bounds in Subsection 3.2.

As an obvious consequence of these bounds, using also the continuity of the hydrogen energy in ζ, we add

2.2. Remark (The limit $\lambda \to 0$). In the limit $\lambda \to 0$ the energy per unit charge, $E^{\rm MH}_{\rm ext}(\lambda,\beta,\zeta,\alpha)/\lambda$, converges to the energy of the hydrogen atom, $E^{\rm hyd}(\beta,\zeta)$.

The bounds of Proposition 2.1 will actually be used in a simplified form:

2.3. LEMMA (Simple bounds).

$$\begin{aligned} E^{\rm MH}(\lambda,\beta) &\geq -(1/4+\beta)\lambda, && (2.12)\\ E^{\rm MH}(\lambda,\beta) &\leq -(1/4)\lambda(1-\lambda/2)^2, \qquad \text{for} \quad \lambda \leq 2. && (2.13) \end{aligned}$$

Proof. Applying the diamagnetic inequality [S76] to the lower bound in proposition (2.1), we get

$$H_\beta - \beta - \frac{1}{|\mathbf{x}|} \geq \text{inf spec } (H_0 - \beta - \frac{1}{|\mathbf{x}|}) = -\frac{1}{4} - \beta. \tag{2.14}$$

To get the upper bound, we apply Lieb's inequality (Theorem A.1. in [AHS78])

$$\text{inf spec } (H_\beta - \beta + V) \leq \text{inf spec } (H_0 + V) \tag{2.15}$$

to the upper bound in proposition (2.1). □

2.2 Minimizers

2.4. THEOREM (Existence of a minimizer). *For each $\beta \geq 0$ and $\lambda > 0$ there is a minimizer $\Gamma^{\rm H}$ for $\mathcal{E}^{\rm MH}_\beta$ under the condition $\mathrm{Tr}[\Gamma^{\rm H}] \leq \lambda$, i.e.*

$$E^{\rm MH}(\lambda,\beta) = \mathcal{E}^{\rm MH}_\beta[\Gamma^{\rm H}]. \tag{2.16}$$

Proof. We follow closely the proof of the analogous theorems 2.2 and 4.3 in [LSY94a]. Let Γ_n be a minimizing sequence for $\mathcal{E}^{\rm MH}_\beta$ with $\mathrm{Tr}[\Gamma_n] \leq \lambda$. First note that $\mathrm{Tr}[H_\beta \Gamma_n]$ is bounded above, because $\mathcal{E}^{\rm MH}_\beta[\Gamma_n]$ is bounded above, and since the other contributions to the energy are bounded relative to H_β. Now we show that the magnetic-kinetic energy is bounded below by the 3-norm of ρ: Using the diamagnetic inequality (the prerequisite for the final result in [S76])

$$\langle \psi, (H_\beta + V)\psi \rangle \geq \langle |\psi|, (H_0 + V)|\psi| \rangle, \tag{2.17}$$

and the decomposition of Γ as in (2.2) , we get

$$\mathrm{Tr}[(-i\nabla + \beta\mathbf{a}(\mathbf{x}))^2\,\Gamma] \geq \sum_n w_n \int |\nabla|\psi_n||^2 . \tag{2.18}$$

Moreover, using the Cauchy-Schwarz inequality,

$$\begin{aligned} |\nabla \rho_\Gamma|^2 &= \left| \sum_n 2 w_n |\psi_n| \nabla |\psi_n| \right|^2 \\ &\leq 4 \left(\sum_n w_n |\psi_n|^2 \right) \left(\sum_n w_n \, |\nabla|\psi_n||^2 \right). && (2.19) \end{aligned}$$

Because $\nabla\rho_\Gamma = 2\rho_\Gamma^{1/2}\nabla\rho_\Gamma^{1/2}$ this gives

$$\mathrm{Tr}[(-i\nabla+\beta\mathbf{a}(\mathbf{x}))^2\,\Gamma] \geq \int \left|\nabla\rho_\Gamma^{1/2}\right|^2 \geq 3\left(\frac{\pi}{2}\right)^{4/3}\left(\int\rho_\Gamma^3\right)^{1/3}, \tag{2.20}$$

where we have used the Sobolev inequality in the last step.

We can then conclude that the corresponding sequence $\rho_n \equiv \rho_{\Gamma_n}$ is bounded in $L^3\cap\mathcal{L}^1$ and $\rho_n^{1/2}$ is bounded in $\mathcal{H}^1$. Therefore, for each $p\in(1,3]$, there exists a subsequence, again denoted by ρ_n, that converges to some ρ_∞ weakly in $\mathcal{L}^3\cap\mathcal{L}^p$, and pointwise almost everywhere. It follows from weak convergence that $\rho_\infty\geq 0$ and $\int\rho_\infty\leq\lambda$. From Fatou's lemma we infer that

$$\liminf_{n\to\infty} D[\rho_n,\rho_n] \geq D[\rho_\infty,\rho_\infty]. \tag{2.21}$$

Moreover, since $|\mathbf{x}|^{-1}\in\mathcal{L}^{3/2}+\mathcal{L}^{3+\varepsilon}$ for every $\varepsilon>0$, and choosing p the dual of $3+\varepsilon$, we see that

$$\lim_{n\to\infty}\int\frac{1}{|\mathbf{x}|}\rho_n = \int\frac{1}{|\mathbf{x}|}\rho_\infty. \tag{2.22}$$

Since the Γ_n's are trace class operators on $\mathcal{L}^2$, we can pass to a subsequence such that for some Γ^{H}

$$\lim_{n\to\infty}\mathrm{Tr}[\Gamma_n A] = \mathrm{Tr}[\Gamma^{\mathrm{H}}A] \tag{2.23}$$

for every compact operator A. (Here we used the Banach-Alaoglu Theorem and the fact that the dual of the compact operators is the trace class operators). In particular, we have

$$\Gamma_n \rightharpoonup \Gamma^{\mathrm{H}} \tag{2.24}$$

in the weak operator sense. It is clear that $\Gamma^{\mathrm{H}}\geq 0$. Now let $\phi_j\in\mathcal{C}_0^\infty(\mathbb{R}^3)$ be an orthonormal basis for $\mathcal{L}^2$. Again by Fatou's Lemma

$$\mathrm{Tr}[\Gamma^{\mathrm{H}}] = \sum_j\langle\phi_j|\Gamma^{\mathrm{H}}|\phi_j\rangle \leq \liminf_{n\to\infty}\mathrm{Tr}[\Gamma_n]\leq\lambda. \tag{2.25}$$

In the same way one shows that

$$\begin{aligned}\mathrm{Tr}[(H_\beta-\beta)\,\Gamma^{\mathrm{H}}] &= \sum_j\langle(H_\beta-\beta)^{1/2}\,\phi_j|\Gamma^{\mathrm{H}}|\,(H_\beta-\beta)^{1/2}\,\phi_j\rangle\\ &\leq \liminf_{n\to\infty}\mathrm{Tr}[(H_\beta-\beta)\,\Gamma_n].\end{aligned} \tag{2.26}$$

It remains to show that $\rho_{\Gamma^{\mathrm{H}}}=\rho_\infty$. We already mentioned that for some constant C

$$\mathrm{Tr}[H_\beta\Gamma_n] < C \tag{2.27}$$

for all n. It follows from (2.24) that

$$(1+H_\beta)^{1/2}\Gamma_n(1+H_\beta)^{1/2} \rightharpoonup (1+H_\beta)^{1/2}\Gamma^{\mathrm{H}}(1+H_\beta)^{1/2} \tag{2.28}$$

weakly on the dense set of $\mathcal{C}_0^\infty$ functions. Since the operators are bounded by (2.27), (2.28) holds weakly in $\mathcal{L}^2$.

Now consider some $f \in \mathcal{C}_0^\infty$ acting as a multiplication operator on $\mathcal{L}^2$. It is easy to see that f is relatively compact with respect to $-\Delta$, i. e. $f(1-\Delta)^{-1}$ is compact. In fact, it is Hilbert-Schmidt, because the trace of its square is given by

$$\int f(\mathbf{x})f(\mathbf{y})Y(\mathbf{x}-\mathbf{y})^2 d^3\mathbf{x}\, d^3\mathbf{y} \tag{2.29}$$

with the Yukawa-Potential $Y(\mathbf{x}) = (4\pi|\mathbf{x}|)^{-1}\exp(-|\mathbf{x}|)$, and this is bounded by Young's inequality. From [AHS78], Thm. 2.6, we infer that

$$g = (1+H_\beta)^{-1/2} f (1+H_\beta)^{-1/2} \tag{2.30}$$

is compact (it is even Hilbert-Schmidt). Thus there exists a sequence g_i of finite-rank operators which approximates g in norm. We have

$$\begin{aligned}\left|\int(\rho_n - \rho_{\Gamma^{\mathrm{H}}})f\right| &= \left|\mathrm{Tr}[(\Gamma_n - \Gamma^{\mathrm{H}})f]\right| \\ &\le \left|\mathrm{Tr}[(1+H_\beta)^{1/2}(\Gamma_n - \Gamma^{\mathrm{H}})(1+H_\beta)^{1/2} g_i]\right| \\ &\quad + 2(C+1)\lambda\|g - g_i\|, \end{aligned}\tag{2.31}$$

where we have used (2.27). Hence $\rho_n \to \rho_{\Gamma^{\mathrm{H}}}$ in the sense of distributions. Because we already know that ρ_n converges to ρ_∞ pointwise almost everywhere, we conclude that $\rho_{\Gamma^{\mathrm{H}}} = \rho_\infty$. We have thus shown that there exists a Γ^{H} with $\mathrm{Tr}[\Gamma^{\mathrm{H}}] \le \lambda$ and $\mathcal{E}_\beta^{\mathrm{MH}}[\Gamma^{\mathrm{H}}] \le \liminf_{n\to\infty} \mathcal{E}_\beta^{\mathrm{MH}}[\Gamma_n]$, from which we conclude that $\mathcal{E}_\beta^{\mathrm{MH}}[\Gamma^{\mathrm{H}}] = E^{\mathrm{MH}}(\lambda, \beta)$. □

2.5. Remark. If Γ^{H} is unique, and given any minimizing sequence for $\mathcal{E}_\beta^{\mathrm{MH}}$, the whole sequence converges weakly to Γ^{H}.

Although we cannot make an assertion about the uniqueness of Γ^{H} yet, we can state the

2.6. PROPOSITION (Uniqueness of the density). *The density ρ^{H} corresponding to the minimizer is unique.*

Proof. This follows immediately from the strict convexity of $D[\rho, \rho]$. □

For $\lambda \le \lambda_c$, the energy E^{MH} is a strictly decreasing function of λ. So the minimizers for different $\lambda \le \lambda_c$ are different, and they have the normalization $\mathrm{Tr}[\Gamma] = \lambda$. No part of the electron cloud has to be moved to infinity. The strict convexity of $D[\rho, \rho]$ implies now, for $\lambda \le \lambda_c$, a strict convexity of E^{MH} as a function of λ.

2.3 Some physical quantities and their interrelations

Since the densities of the minimizers are unique, the contributions to the Hartree energy, $\int \rho/|\mathbf{x}|$ and $D[\rho,\rho]$, are fixed. We denote them as attraction A and repulsion R, suppressing the dependence on the parameters. As a consequence, also K, the kinetic-magnetic energy, is fixed. Inserting a minimizer into (1.9) we get

$$E = K - A + R. \tag{2.32}$$

To deduce an analogue to the Feynman-Hellman theorem, we observe the following inequality: Consider two different parameters, ζ and $\bar{\zeta}$, with corresponding minimizers Γ and $\bar{\Gamma}$, and their densities ρ and $\bar{\rho}$. All the other parameters are fixed. Insert $\bar{\Gamma}$ into the functional (2.5) with parameter ζ, to conclude

$$\begin{aligned} E^{\mathrm{MH}}_{\mathrm{ext}}(\lambda,\beta,\zeta,\alpha) &< \mathcal{E}^{\mathrm{MH}}_{\lambda,\beta,\zeta,\alpha}[\bar{\Gamma}] \\ &= \mathcal{E}^{\mathrm{MH}}_{\lambda,\beta,\bar{\zeta},\alpha}[\bar{\Gamma}] - (\zeta-\bar{\zeta})\int \frac{1}{|\mathbf{x}|}\bar{\rho}_{\Gamma^{\mathrm{H}}} \\ &= E^{\mathrm{MH}}_{\mathrm{ext}}(\lambda,\beta,\bar{\zeta},\alpha) - (\zeta-\bar{\zeta})\int \frac{1}{|\mathbf{x}|}\bar{\rho}. \end{aligned} \tag{2.33}$$

Together with the same argument, where ζ and $\bar{\zeta}$ are exchanged, we get, for $\zeta > \bar{\zeta}$,

$$-\int \frac{1}{|\mathbf{x}|}\rho < \frac{E^{\mathrm{MH}}_{\mathrm{ext}}(\lambda,\beta,\zeta,\alpha) - E^{\mathrm{MH}}_{\mathrm{ext}}(\lambda,\beta,\bar{\zeta},\alpha)}{\zeta-\bar{\zeta}} < -\int \frac{1}{|\mathbf{x}|}\bar{\rho}. \tag{2.34}$$

We conclude, using the continuity (2.22), where the ρ_n are now the unique densities of the minimizers for $\bar{\zeta}_n \to \zeta$, that the Hartree energy is differentiable in ζ, and

$$\left.\frac{\partial E^{\mathrm{MH}}_{\mathrm{ext}}}{\partial \zeta}\right|_{\zeta=1} = -A. \tag{2.35}$$

In the same way, using the inequality (2.21) instead of (2.22), we show that

$$\left.\frac{\partial E^{\mathrm{MH}}_{\mathrm{ext}}}{\partial \alpha}\right|_{\alpha=1} = R. \tag{2.36}$$

Having established the differentiability in λ, ζ and in α, the scaling relation (2.7) implies differentiability in β. So, the **magnetic moment** θ,

$$\theta = \frac{\partial E^{\mathrm{MH}}}{\partial \beta}, \tag{2.37}$$

is well defined as a function of β.

Taking the partial derivatives of (2.7) in α and ζ at $\alpha = 1$ and $\zeta = 1$ gives

$$\begin{aligned} R &= -E + \lambda\mu, & (2.38) \\ -A &= 3E - \lambda\mu - 2\beta\theta. & (2.39) \end{aligned}$$

The relation (2.38) is, because of the negativity of the chemical potential μ for $\lambda < \lambda_c$, a **virial inequality**,

$$R < |E|, \tag{2.40}$$

turning into an equality at $\lambda = \lambda_c$. Inserting (2.38) into (2.39), we get

$$\beta\theta = \frac{K - |E|}{2}. \tag{2.41}$$

The equation (2.38) and the inequality (2.40) are also valid in the Regions 1 and 3, where there is a scaling relation analogous to (2.7). But this relation is without a β, so instead of (2.41), in Regions 1 and 3 the well known **virial equality**

$$K = |E| = \frac{A - R}{2} \tag{2.42}$$

holds (see also [LSY94a, B84]). Moreover, for $\lambda = \lambda_c$ we have $|E| : K : A : R = 1 : 1 : 3 : 1$.

2.4 The linearized theory

Since the density ρ^{H} of a minimizer is unique and integrable, we can define a linearized Hartree functional by

$$\mathcal{E}^{\mathrm{MH}}_{\beta,\mathrm{lin}}[\Gamma] = \mathrm{Tr}[H^{\mathrm{H}}\Gamma], \tag{2.43}$$

with the one-particle Hartree Hamiltonian

$$H^{\mathrm{H}} \equiv H_\beta - \beta - \Phi^{\mathrm{H}}(\mathbf{x}). \tag{2.44}$$

Here the Hartree potential $\Phi^{\mathrm{H}}(\mathbf{x})$ is given by

$$\Phi^{\mathrm{H}}(\mathbf{x}) = \frac{1}{|\mathbf{x}|} - \rho^{\mathrm{H}} * \frac{1}{|\mathbf{x}|}. \tag{2.45}$$

Note that H^{H} depends on λ only via ρ^{H}.
Since Φ^{H} is in $\mathcal{L}^2 + \mathcal{L}^\infty_\varepsilon$, it is relative compact with respect to H_β [AHS78], so we know that the essential spectrum of H^{H} is $[0, \infty)$.

2.7. LEMMA (Linear Hartree functional). *Let* Γ^{H} *be a minimizer of* $\mathcal{E}^{\mathrm{MH}}_\beta$ *under the constraint* $\mathrm{Tr}[\Gamma] \le \lambda$. *Then* Γ^{H} *also minimizes* $\mathcal{E}^{\mathrm{MH}}_{\beta,\mathrm{lin}}$ *(under the same constraint).*

Proof. (We proceed essentially as in [LSY94a]). For any Γ

$$\mathcal{E}^{\mathrm{MH}}_\beta[\Gamma] = \mathcal{E}^{\mathrm{MH}}_{\beta,\mathrm{lin}}[\Gamma] + D[\rho_\Gamma - \rho^{\mathrm{H}}, \rho_\Gamma - \rho^{\mathrm{H}}] - D[\rho^{\mathrm{H}}, \rho^{\mathrm{H}}]. \tag{2.46}$$

Especially, for all $\delta > 0$,

$$\begin{aligned}\mathcal{E}_\beta^{\mathrm{MH}}[(1-\delta)\Gamma^{\mathrm{H}} + \delta\Gamma] &= (1-\delta)\mathcal{E}_{\beta,\mathrm{lin}}^{\mathrm{MH}}[\Gamma^{\mathrm{H}}] + \delta\mathcal{E}_{\beta,\mathrm{lin}}^{\mathrm{MH}}[\Gamma] - D[\rho^{\mathrm{H}}, \rho^{\mathrm{H}}] \\ &\quad + \delta^2 D[\rho_\Gamma - \rho^{\mathrm{H}}, \rho_\Gamma - \rho^{\mathrm{H}}]. \end{aligned} \tag{2.47}$$

Now if there exists a Γ_0 with $\mathrm{Tr}[\Gamma_0] \leq \lambda$ and $\mathcal{E}_{\beta,\mathrm{lin}}^{\mathrm{MH}}[\Gamma_0] < \mathcal{E}_{\beta,\mathrm{lin}}^{\mathrm{MH}}[\Gamma^{\mathrm{H}}]$ we can choose δ small enough to conclude that

$$\mathcal{E}_\beta^{\mathrm{MH}}[(1-\delta)\Gamma^{\mathrm{H}} + \delta\Gamma_0] < \mathcal{E}_{\beta,\mathrm{lin}}^{\mathrm{MH}}[\Gamma^{\mathrm{H}}] - D[\rho^{\mathrm{H}}, \rho^{\mathrm{H}}] = \mathcal{E}_\beta^{\mathrm{MH}}[\Gamma^{\mathrm{H}}], \tag{2.48}$$

which contradicts the fact that Γ^{H} minimizes $\mathcal{E}_\beta^{\mathrm{MH}}$. □

The **Hartree equation**, the Euler-Lagrange equation corresponding to the minimization of the functional $\mathcal{E}_\beta^{\mathrm{MH}}$, is

$$H^{\mathrm{H}}\Gamma = \mu\Gamma. \tag{2.49}$$

The ground state energy of H^{H} is given by the chemical potential $\mu(\lambda, \beta) = (E+R)/\lambda$. For the overcritical values of $\lambda \geq \lambda_c$ the ground state energy μ of H^{H} is 0, and there is just one density corresponding to the minimizer.

We can now ensure that $\lambda_c = \lambda_c(\beta)$ is not too small. In fact we state

2.8. LEMMA (Lower bound on the critical charge).

$$\lambda_c(\beta) > 1 \qquad \text{for all } \beta \geq 0. \tag{2.50}$$

Proof. For $\beta = 0$ this was shown in [BL83], and $\lambda_c(0)$ was computed numerically to be 1.21 in [B84].

Fix $\beta > 0$. We assume that $\lambda_\rho \equiv \int \rho^{\mathrm{H}} \leq 1$, and will show that H^{H} has an eigenvalue strictly below zero. Using $\psi(r, z) = \exp(-\beta r^2/4 - a|z|)$ with some $a > 0$ as a (not normalized) test function we compute

$$\begin{aligned}\langle\psi|H^{\mathrm{H}}\psi\rangle &= \frac{2\pi}{\beta}a - 2\pi\int \Phi^{\mathrm{H}}(r,z)e^{-\frac{1}{2}\beta r^2 - 2a|z|} r\,dr\,dz \\ &\leq \frac{2\pi}{\beta}a - \int \rho^{\mathrm{H}}(\mathbf{x})\left(\phi(\mathbf{0}) - \phi(\mathbf{x})\right) d^3\mathbf{x}, \end{aligned} \tag{2.51}$$

where $\phi(\mathbf{x})$ is the potential generated by the charge distribution $\exp(-\frac{1}{2}\beta r^2 - 2a|z|)$, i.e.

$$\phi(\mathbf{y}) = \int \frac{e^{-\frac{1}{2}\beta r^2 - 2a|z|}}{|\mathbf{x} - \mathbf{y}|} d^3\mathbf{x}. \tag{2.52}$$

Note that $\phi(\mathbf{0}) > \phi(\mathbf{y})$ for $\mathbf{y} \neq \mathbf{0}$, so we can choose a small enough to conclude that H^{H} has an eigenvalue strictly below zero and binds more charge than λ_ρ. □

Lemma 2.8 shows that in Hartree theory there are always negative ions. The following lemma gives an upper bound on the maximal negative ionization.

2.9. LEMMA (Upper bound on the critical charge). *For some constant C independent of β*

$$\lambda_c(\beta) \le 2 + \frac{1}{2}\min\left\{1+\beta, C\left(1+[\ln\beta]^2\right)\right\}. \tag{2.53}$$

Proof. This follows from Lemma 4.9 and the bound on N_c given in [S00] (see Remark 4.10 below). □

2.5 The minimizer has $L^{\|} = 0$

Let H be the operator

$$H = H_\beta - \beta - \Phi(\mathbf{x}), \tag{2.54}$$

where the potential is given by

$$\Phi(\mathbf{x}) = \frac{1}{|\mathbf{x}|} - \frac{1}{|\mathbf{x}|} * \rho. \tag{2.55}$$

The function ρ is assumed to be *axially symmetric*, non-negative, and $\rho \in \mathcal{L}^1 \cap \mathcal{L}^q$, where $q > 3/2$. This implies that $|\mathbf{x}|^{-1} * \rho$ is a bounded, continuous function going to zero at infinity. The operator H is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^3)$. Since $\Phi \in \mathcal{L}^2 + \mathcal{L}^\infty_\varepsilon$, it is a relatively compact perturbation of H_β [AHS78], so we know that the essential spectrum of H is given by $[0, \infty)$. The symmetry of ρ implies that H is axially symmetric, i.e. it commutes with the rotations generated by the parallel component of the angular momentum,

$$L^{\|} = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right). \tag{2.56}$$

For $m \ge 0$ let now Ψ_m be a ground state of H, if there is one, with angular momentum $L^{\|}\Psi_m = -m\Psi_m$. Note that we can restrict ourselves to considering non-negative m's, since $(H \restriction L^{\|} = -m)$ is antiunitarily equivalent to $(H + 2\beta m \restriction L^{\|} = m)$ by complex conjugation, so in the ground state m is certainly non-negative. Writing

$$\Psi_m(\mathbf{x}) = e^{-im\varphi} r^m f(r, z), \tag{2.57}$$

where (r, φ) denote polar coordinates for (x, y), we see that f is a ground state for

$$\widetilde{H}_m = -\frac{\partial^2}{\partial r^2} - \frac{2m+1}{r}\frac{\partial}{\partial r} - \frac{\partial^2}{\partial z^2} + \frac{\beta^2}{4}r^2 - (m+1)\beta - \Phi(r, z) \tag{2.58}$$

on $\mathcal{L}^2(\mathbb{R}^3, r^{2m}d\mathbf{x})$. If $\widetilde{H}_m$ has a ground state, it is unique and strictly positive ([RS78]; to apply the theorems therein note that the first three terms in $\widetilde{H}_m$ are just the radial part of the Laplacian in $2m+3$ dimensions). So Ψ_m is the only ground state of H with $L^{\|} = -m$. Moreover, f is a bounded, continuous function [LL97], and hence

$$|\Psi_m(r, \phi, z)| \leq \text{const.} r^m, \tag{2.59}$$

for small r and some constant independent of z. In particular, $\Psi_m(\mathbf{0}) = 0$ if $m > 0$.

We now are able to prove the main result of this subsection:

2.10. THEOREM ($m = 0$ in the ground state of H). *Let H be a Hamiltonian as in (2.54), with ρ axially symmetric and non-negative. If* $\inf \operatorname{spec} H$ *is an eigenvalue, the corresponding eigenvector is unique and has zero angular momentum, for all values of $\beta \geq 0$.*

Proof. For $\rho = 0$, i.e. the hydrogen atom, this was shown in [AHS81] (and also in [GS95]). So we can restrict ourselves to considering the case $\int \rho > 0$.

Let Ψ_m be a normalized ground state for H, with angular momentum $-m$. Define

$$f(\mathbf{b}) = -\int |\Psi_m(\mathbf{x})|^2 \Phi(\mathbf{x} - \mathbf{b}) d^3\mathbf{x}. \tag{2.60}$$

The function f is continuous and bounded. It achieves its minimal value at $\mathbf{b} = \mathbf{0}$, because otherwise one could lower the energy by translating $|\Psi_m|^2$. Strictly speaking,

$$f(\mathbf{b}) - f(\mathbf{0}) = \langle \widetilde{\Psi}_m | H | \widetilde{\Psi}_m \rangle - \langle \Psi_m | H | \Psi_m \rangle \geq 0, \tag{2.61}$$

with $\mathbf{b} = (b_1, b_2, b_3)$ and

$$\widetilde{\Psi}_m(\mathbf{x}) = e^{-\frac{i}{2}\beta(b_2 x - b_1 y)} \Psi_m(\mathbf{x} + \mathbf{b}). \tag{2.62}$$

The phase in (2.62) is chosen such that the kinetic energy remains invariant. (Note that translating H_β is equivalent to changing the gauge of the magnetic potential.)

In the sense of distributions,

$$\Delta f(\mathbf{b}) = 4\pi \left(|\Psi_m(\mathbf{b})|^2 - |\Psi_m|^2 * \rho_-(\mathbf{b}) \right), \tag{2.63}$$

with $\rho_-(\mathbf{x}) \equiv \rho(-\mathbf{x})$. The function $|\Psi_m|^2 * \rho_-$ is pointwise strictly positive and continuous. Assume now that $m > 0$. Since, by (2.59), $|\Psi_m(\mathbf{x})| \leq C|\mathbf{x}|^m$ for some $C > 0$, there is an $R > 0$ such that

$$\Delta f(\mathbf{b}) < 0 \quad \text{for} \quad |\mathbf{b}| < R, \tag{2.64}$$

i.e. f is superharmonic in some open region containing $\mathbf{0}$. This contradicts the fact that f achieves its minimum at $\mathbf{b} = \mathbf{0}$. As a consequence, a ground state of H must have angular momentum $m = 0$. □

An analogous result holds also for the restriction of H to the lowest Landau band. This fact will be used in the proof of Theorem 3.6.

2.11. COROLLARY ($m = 0$ in the ground state of $\Pi_0 H \Pi_0$). *Let Π_0 be the projector onto the lowest Landau band. If $\Pi_0 H \Pi_0$ has a ground state, the ground state wave function Ψ_0 is given by*

$$\Psi_0(\mathbf{x}) = \sqrt{\frac{\beta}{2\pi}} \exp\left(-\frac{\beta}{4} r^2\right) \psi(z) \tag{2.65}$$

for some $\psi(z)$ with $\int |\psi(z)|^2 dz = \|\Psi_0\|_2^2$.

Proof. Mimicking the proof of the last theorem, we see that if $\Pi_0 H \Pi_0$ has a ground state, the corresponding wave function $\Psi_0 = \Pi_0 \Psi_0$ has $L^{\|} = 0$. Hence it is given by (2.65). □

Let now ρ be the Hartree density ρ^{H}, the unique density of the minimizer of $\mathcal{E}_\beta^{\mathrm{MH}}$ (depending on λ and β). Applying Lemma (2.7) and the theorem above, we immediately get

2.12. COROLLARY (Uniqueness of Γ^{H}). *The functional $\mathcal{E}_\beta^{\mathrm{MH}}$ has a unique minimizer Γ^{H} under the condition $\mathrm{Tr}[\Gamma] \leq \lambda$, which is proportional to the projection onto the positive function $\sqrt{\rho^{\mathrm{H}}}$. In particular, Γ^{H} has rank 1. Moreover, ρ^{H} minimizes the is density functional (1.11) under the condition $\int \rho \leq \lambda$. It is $\mathcal{C}^\infty$ away from the origin, continuous at $\mathbf{x} = \mathbf{0}$, and strictly positive.*

The properties of ρ^{H} stated above follow from the fact that ρ^{H} minimizes $\hat{\mathcal{E}}_\beta^{\mathrm{MH}}$, and therefore satisfies the variational equation

$$-\Delta\sqrt{\rho^{\mathrm{H}}} + \left(\frac{\beta^2}{4} r^2 - \beta - \Phi^{\mathrm{H}}\right) \sqrt{\rho^{\mathrm{H}}} = \mu \sqrt{\rho^{\mathrm{H}}}, \tag{2.66}$$

where μ is the chemical potential of the MH theory. Note that Corollary 2.12 proves the assertion made in the Introduction that both $\mathcal{E}^{\mathrm{MH}}$ and $\hat{\mathcal{E}}^{\mathrm{MH}}$ have the same ground state energy and density.

3 The limits of Region 2

3.1 The limit of very weak magnetic fields

The limit $\beta \to 0$ is rather easy to handle:

3.1. THEOREM (Hartree energy for small β). *In the limit $\beta \to 0$,*

$$E^{\mathrm{MH}}(\lambda, \beta) = E^{\mathrm{H}}(\lambda) - \beta\lambda + O(\beta^2). \tag{3.1}$$

Proof. Fix $\lambda > 0$, and let ρ_β be the minimizer of the density functional $\hat{\mathcal{E}}_\beta^{\mathrm{MH}}$ under the constraint $\int \rho \leq \lambda$. Using ρ_0 as a trial function we get

$$E^{\mathrm{MH}}(\lambda, \beta) \leq \hat{\mathcal{E}}_\beta^{\mathrm{MH}}[\rho_0] = E^{\mathrm{MH}}(\lambda, 0) - \beta\lambda + \frac{\beta^2}{4} \int r^2 \rho_0. \tag{3.2}$$

It is well known that ρ_0 falls off more quickly that the inverse of any polynomial, so $\int r^2\rho_0$ is finite [BBL81].

For the converse, we estimate

$$E^{\mathrm{MH}}(\lambda, \beta) = \hat{\mathcal{E}}_\beta^{\mathrm{MH}}[\rho_\beta] \geq \hat{\mathcal{E}}_0^{\mathrm{MH}}[\rho_\beta] - \beta\lambda \geq E^{\mathrm{MH}}(\lambda, 0) - \beta\lambda. \tag{3.3}$$

The observation $E^{\mathrm{MH}}(\lambda, 0) = E^{\mathrm{H}}(\lambda)$ then leads to (3.1). □

3.2 Lowest Landau band confinement in Hartree theory

We now show that for large β most of the charge is confined to the lowest Landau band. To do this, we write the Hartree functional as

$$\mathcal{E}_\beta^{\mathrm{MH}}[\Gamma] = \mathrm{Tr}\left[\left(H_\beta - \beta - \frac{1}{|\mathbf{x}|}\right)\Gamma\right] + \tfrac{1}{2}\mathrm{Tr}_2\left[\Gamma \otimes \Gamma \frac{1}{|\mathbf{x}-\mathbf{y}|}\right], \tag{3.4}$$

where Tr_2 means the trace over the doubled space $\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{x}) \otimes \mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{y})$. Let Π_0 be the projector onto the lowest Landau band, and let $\Pi_> = 1 - \Pi_0$. We will use the decomposition

$$H_\beta - \beta = \Pi_0(H_\beta - \beta)\Pi_0 + \Pi_>(H_\beta - \beta)\Pi_> \tag{3.5}$$

and

$$\frac{1}{|\mathbf{x}|} = \Pi_0 \frac{1}{|\mathbf{x}|}\Pi_0 + \Pi_> \frac{1}{|\mathbf{x}|}\Pi_> + \Pi_0 \frac{1}{|\mathbf{x}|}\Pi_> + \Pi_> \frac{1}{|\mathbf{x}|}\Pi_0. \tag{3.6}$$

The off-diagonal terms can be bound using

$$\left(\sqrt{\varepsilon}\Pi_0 - \frac{1}{\sqrt{\varepsilon}}\Pi_>\right)\frac{1}{|\mathbf{x}|}\left(\sqrt{\varepsilon}\Pi_0 - \frac{1}{\sqrt{\varepsilon}}\Pi_>\right) \geq 0 \tag{3.7}$$

for some $0 < \varepsilon < 1$, with the result that

$$\frac{1}{|\mathbf{x}|} \leq (1+\varepsilon)\Pi_0 \frac{1}{|\mathbf{x}|}\Pi_0 + \left(1 + \frac{1}{\varepsilon}\right)\Pi_> \frac{1}{|\mathbf{x}|}\Pi_>. \tag{3.8}$$

In the same way one shows that, see [LSY94a],

$$\begin{aligned} \frac{1}{|\mathbf{x}-\mathbf{y}|} &\geq (1-3\varepsilon)\Pi_0 \otimes \Pi_0 \frac{1}{|\mathbf{x}-\mathbf{y}|}\Pi_0 \otimes \Pi_0 \\ &+ \left(1 - \frac{3}{\varepsilon}\right)\Pi_> \otimes \Pi_> \frac{1}{|\mathbf{x}-\mathbf{y}|}\Pi_> \otimes \Pi_> \\ &+ \left(1 - 2\varepsilon - \frac{1}{\varepsilon}\right)\Pi_0 \otimes \Pi_> \frac{1}{|\mathbf{x}-\mathbf{y}|}\Pi_0 \otimes \Pi_> \\ &+ \left(1 - \varepsilon - \frac{2}{\varepsilon}\right)\Pi_> \otimes \Pi_0 \frac{1}{|\mathbf{x}-\mathbf{y}|}\Pi_> \otimes \Pi_0. \end{aligned} \tag{3.9}$$

Moreover, we will use

$$\mathrm{Tr}_2\left[\Pi_\# \otimes \Pi_> \frac{1}{|\mathbf{x}-\mathbf{y}|}\Pi_\# \otimes \Pi_> \Gamma \otimes \Gamma\right] \le \mathrm{Tr}[\Pi_\# \Gamma] \sup_{\mathbf{a}} \mathrm{Tr}\left[\Pi_> \Gamma \Pi_> \frac{1}{|\mathbf{x}-\mathbf{a}|}\right], \tag{3.10}$$

where # stands for either 0 or >. If we restrict ourselves to considering Γ's with $\mathrm{Tr}[\Gamma] \le \lambda$ we therefore have

$$\begin{aligned}\mathcal{E}_\beta^{\mathrm{MH}}[\Gamma] &\ge (1-3\varepsilon)\mathcal{E}_\beta^{\mathrm{MH}}[\Pi_0\Gamma\Pi_0] + 3\varepsilon\lambda\left(\frac{8}{3}\right)^2 \inf\mathrm{spec}\ \left(H_\beta - \beta - \frac{1}{2|\mathbf{x}|}\right) \\ &+ \mathrm{Tr}[\Pi_>\Gamma]\left(\frac{\beta}{2} + \inf_{\mathbf{a}}\inf\mathrm{spec}\ \left(\tfrac{1}{2}H_\beta - \frac{2}{\varepsilon}\frac{1}{|\mathbf{x}|} - \frac{2\lambda}{\varepsilon}\frac{1}{|\mathbf{x}-\mathbf{a}|}\right)\right), \end{aligned} \tag{3.11}$$

where we have used that

$$\Pi_>(H_\beta - \beta)\Pi_> \ge \tfrac{1}{2}\Pi_>(H_\beta + \beta)\Pi_> \tag{3.12}$$

and that

$$\Pi_0\left(H_\beta - \beta - \frac{\delta}{2|\mathbf{x}|}\right)\Pi_0 \ge \delta^2\Pi_0\left(H_\beta - \beta - \frac{1}{2|\mathbf{x}|}\right)\Pi_0 \tag{3.13}$$

for $\delta \ge 1$, which can easily be seen by scaling $z \to \delta^{-1}z$.

Now we use the comparison with the hydrogen atom, Proposition (2.1):

$$\inf\mathrm{spec}\ \left(H_\beta - \beta - \frac{1}{2|\mathbf{x}|}\right) \ge \max\{1,\lambda^{-1}\}E^{\mathrm{MH}}(\lambda,\beta). \tag{3.14}$$

By the same argument as in the proof of this inequality, we can set $\mathbf{a} = \mathbf{0}$ in (3.11). Using the diamagnetic inequality we see that $\frac{1}{2}H_\beta - c|\mathbf{x}|^{-1} \ge -\frac{1}{2}c^2$, so finally

$$\begin{aligned}\mathcal{E}_\beta^{\mathrm{MH}}[\Gamma] &\ge (1-3\varepsilon)\mathcal{E}_\beta^{\mathrm{MH}}[\Pi_0\Gamma\Pi_0] + 3\varepsilon\left(\frac{8}{3}\right)^2 \max\{1,\lambda\}E^{\mathrm{MH}}(\lambda,\beta) \\ &+ \frac{1}{2}\left(\beta - \frac{4(1+\lambda)^2}{\varepsilon^2}\right)\mathrm{Tr}[\Pi_>\Gamma]. \end{aligned} \tag{3.15}$$

Now if β is large enough, we can set $\varepsilon^2 = 4(1+\lambda)^2/\beta$ to conclude

3.2. LEMMA (Comparison with the confined Hartree theory).

$$E_{\mathrm{conf}}^{\mathrm{MH}}(\lambda,\beta) \le E^{\mathrm{MH}}(\lambda,\beta)(1 - \mathrm{const.}(1+\lambda)^2\beta^{-1/2}), \tag{3.16}$$

where

$$E_{\mathrm{conf}}^{\mathrm{MH}}(\lambda,\beta) = \inf_{\mathrm{Tr}[\Pi_0\Gamma]\le\lambda} \mathcal{E}_\beta^{\mathrm{MH}}[\Pi_0\Gamma\Pi_0]. \tag{3.17}$$

Note that the constant in (3.16) can be chosen such that (3.16) is valid for all values of $\beta > 0$ and $\lambda > 0$.

3.3. Remark. Equation (3.15) can be used to estimate the part of the Hartree state $\Gamma^{\rm H}$ not confined to the lowest Landau band. In fact, if $\varepsilon^2 > 4(1+\lambda)^2/\beta$ in (3.15), and with $\Gamma = \Gamma^{\rm H}$, we get

$$\mathrm{Tr}[\Pi_> \Gamma^{\rm H}] \leq -\mathrm{const.}(1+\lambda)\frac{\varepsilon E^{\rm MH}(\lambda,\beta)}{\beta - 4(1+\lambda)^2\varepsilon^{-2}}. \tag{3.18}$$

Using the simple lower bound on $E^{\rm MH}$, given in Lemma 2.3, and optimizing over ε gives

$$\mathrm{Tr}[\Pi_> \Gamma^{\rm H}] \leq \mathrm{const.}(1+\lambda)^3\beta^{-1/2}. \tag{3.19}$$

3.3 Confinement for the mean field Hamiltonian

An analogous result as in the previous subsection holds also for the linearized theory. The following estimate will be used in Subsection 4.4:

3.4. LEMMA (Confinement for the mean field Hamiltonian). *Let H be given as in (2.54), with $\rho \geq 0$ and $\int \rho \leq \lambda$. Then for all $\beta > 0$*

$$\inf \mathrm{spec}\ H \geq \inf \mathrm{spec}\ \Pi_0 H \Pi_0 + (2+\lambda)\beta^{-1/2}E^{\rm hyd}(\beta,2). \tag{3.20}$$

Proof. For $0 < \varepsilon < 1$ we use again (3.5) and (3.8), and the analogous inequality in the other direction for $|\mathbf{x}|^{-1} * \rho$, to conclude that

$$\begin{aligned} H &\geq \Pi_0 \left(H_\beta - \beta - (1+\varepsilon)\frac{1}{|\mathbf{x}|} + (1-\varepsilon)\frac{1}{|\mathbf{x}|} * \rho \right) \Pi_0 \\ &\quad + \Pi_> \left(H_\beta - \beta - (1+\varepsilon^{-1})\frac{1}{|\mathbf{x}|} + (1-\varepsilon^{-1})\frac{1}{|\mathbf{x}|} * \rho \right) \Pi_> \\ &\geq (1-\varepsilon)\Pi_0 H \Pi_0 + \varepsilon \Pi_0 \left(H_\beta - \beta - \frac{2}{|\mathbf{x}|} \right) \Pi_0 \\ &\quad + \tfrac{1}{2}\Pi_> \left(H_\beta + \beta - \frac{4\varepsilon^{-1}}{|\mathbf{x}|} - \frac{2\varepsilon^{-1}}{|\mathbf{x}|} * \rho \right) \Pi_>, \end{aligned} \tag{3.21}$$

where we have also used (3.12). With the aid of the inequality (2.3) one easily sees that

$$\inf \mathrm{spec}\ \left(H_\beta - \frac{4\varepsilon^{-1}}{|\mathbf{x}|} - \frac{2\varepsilon^{-1}}{|\mathbf{x}|} * \rho \right) \geq \inf \mathrm{spec}\ \left(H_\beta - \frac{(4+2\lambda)\varepsilon^{-1}}{|\mathbf{x}|} \right). \tag{3.22}$$

Using again $\frac{1}{2}H_\beta - c|\mathbf{x}|^{-1} \geq -\frac{1}{2}c^2$ we finally get

$$H \geq (1-\varepsilon)\Pi_0 H \Pi_0 + \varepsilon E^{\rm hyd}(\beta,2) + \tfrac{1}{2}\Pi_> \left(\beta - (2+\lambda)^2\varepsilon^{-2} \right). \tag{3.23}$$

In particular, if we choose $\varepsilon = (2+\lambda)\beta^{-1/2}$, we arrive at the desired result, as long as β is large enough to ensure $\varepsilon < 1$. But if $\beta \leq (2+\lambda)^2$, (3.20) holds trivially because of the positivity of ρ. $\square$

3.4 The limit of very strong magnetic fields

In the investigation of the limit $\beta \to \infty$ some special concepts from earlier studies are involved: The right scaling, the restriction to the lowest Landau band, the effects of the superharmonicity on the distribution of the density in the perpendicular directions, and the high field limit of the Coulomb interaction.

We consider pure states $\Lambda = |\chi\rangle\langle\chi|$ defined by the wave functions with $L^{\|} = 0$ in the lowest Landau band,

$$\chi(\mathbf{x}) = \sqrt{\frac{\beta}{2\pi}} e^{-\beta(\mathbf{x}^{\perp})^2/4} \sqrt{L}\psi(Lx^{\|}). \tag{3.24}$$

We denote here the perpendicular and parallel components of the coordinates as $\mathbf{x} = (\mathbf{x}^{\perp}, x^{\|})$. The scaling factor $L = L(\beta)$ has been defined in [BSY00] as the solution of the equation

$$\beta^{1/2} = L(\beta) \sinh[L(\beta)/2]. \tag{3.25}$$

Note that

$$L(\beta) = \ln \beta + O(\ln \ln \beta) \tag{3.26}$$

as $\beta \to \infty$. In the following we use the scaled coordinates

$$z = L(\beta)x^{\|}, \qquad \mathbf{r} = \sqrt{\beta}\mathbf{x}^{\perp}, \qquad r = |\mathbf{r}|. \tag{3.27}$$

With the density matrix $\Lambda = |\chi\rangle\langle\chi|$, we calculate the contributions to $\mathcal{E}_{\beta}^{\mathrm{MH}}[\Lambda]$. The normalization of Λ, we denote it as λ_ψ, is equal to $\|\psi\|_2^2$. We restrict the set of ψ to real valued wave functions, since they minimize the kinetic energy, if the density $|\psi|^2$ is kept fixed.

3.5. LEMMA (The strong field limits). *Given the state Λ defined by real valued $\psi \in \mathcal{H}^1(\mathbb{R})$ as in (3.24), the contributions to the energy in the magnetic Hartree theory, magnetic-kinetic energy $K_{\beta,\psi}$, attraction $A_{\beta,\psi}$, and repulsion $R_{\beta,\psi}$, are in the following way related to the kinetic energy, $K_\psi = \int (d\psi/dz)^2 dz$, attraction-energy $A_\psi = \psi(0)^2$, and repulsion-energy $R_\psi = \frac{1}{2}\int \psi(z)^4 dz$ of the density $\psi(z)^2$ in the HS-theory:*

$$K_{\beta,\psi} = L^2 K_\psi, \tag{3.28}$$

$$\left|\frac{1}{L^2}A_{\beta,\psi} - A_\psi\right| \leq \frac{C}{L}\left(\lambda_\psi + \lambda_\psi^{1/4} K_\psi^{3/4}\right), \tag{3.29}$$

$$\left|\frac{1}{L^2}R_{\beta,\psi} - R_\psi\right| \leq \frac{C\lambda_\psi}{L}\left(\lambda_\psi + \lambda_\psi^{1/4} K_\psi^{3/4}\right). \tag{3.30}$$

Proof. The equation for the kinetic energy is obvious by definition of Λ. We calculate the energy of attraction as

$$A_{\beta,\psi} = L^2 \int_0^\infty e^{-r^2/2} \left[\int_{-\infty}^\infty V_{\beta,r}(z)\psi^2(z)dz\right] rdr, \tag{3.31}$$

where

$$V_{\beta,r}(z) = \frac{1}{L\sqrt{L^2r^2/\beta + z^2}}. \tag{3.32}$$

For the term in square brackets we use Lemma 2.1 of [BSY00],

$$\left|[...] - \psi(0)^2\right| \le \lambda_\psi/r + 8\lambda_\psi^{1/4}K_\psi^{3/4}r^{1/2}, \tag{3.33}$$

to estimate the difference to the expected limit in the HS-theory:

$$\left|\frac{1}{L^2}A_{\beta,\psi} - A_\psi\right| \le \frac{1}{L}\left(\lambda_\psi\sqrt{\pi/2} + 8\cdot 2^{1/4}\Gamma(5/4)\lambda_\psi^{1/4}K_\psi^{3/4}\right). \tag{3.34}$$

For the repulsion $R_{\beta,\psi}$ we calculate

$$\left|\frac{1}{L^2}R_{\beta,\psi} - R_\psi\right| \le \frac{1}{2}\int_{\mathbb{R}^4} d^2\mathbf{r}d^2\mathbf{r}'(\frac{1}{2\pi})^2 e^{-(\mathbf{r}^2+\mathbf{r}'^2)/2}[...], \tag{3.35}$$

where

$$[...] = \left|\int_{\mathbb{R}^2} dzdz'\left(V_{\beta,|\mathbf{r}-\mathbf{r}'|}(z-z') - \delta(z-z')\right)\psi^2(z)\psi^2(z')\right| \tag{3.36}$$

$$\le \frac{1}{L}\left(\frac{\lambda_\psi^2}{|\mathbf{r}-\mathbf{r}'|} + 8\lambda_\psi^{5/4}K_\psi^{3/4}|\mathbf{r}-\mathbf{r}'|^{1/2}\right). \tag{3.37}$$

The inequality is supplied by Lemma 2.2 of [BSY00], with an adaptation due to the different notation concerning the normalization. After inserting (3.37) in (3.35), the integrals can be evaluated as

$$\left|\frac{1}{L^2}R_{\beta,\psi} - R_\psi\right| \le \frac{1}{L}\left((\sqrt{\pi}/4)\lambda_\psi^2 + 4\sqrt{2}\Gamma(5/4)\cdot\lambda_\psi^{5/4}K_\psi^{3/4}\right). \tag{3.38}$$

$\square$

3.6. THEOREM (Magnetic Hartree energy for large β). *In the limit $\beta\to\infty$ with λ fixed,*

$$\lim_{\beta\to\infty}\frac{E^{\rm MH}(\lambda,\beta)}{(\ln\beta)^2} = E^{\rm HS}(\lambda). \tag{3.39}$$

Proof. Combining all the bounds of the Lemma, and using $\lambda_\psi^{1/4}K_\psi^{3/4} \le \frac{1}{4}\lambda_\psi + \frac{3}{4}K_\psi$ to simplify, gives

$$\left|\frac{1}{L^2}\mathcal{E}_\beta^{\rm MH}[\Lambda] - \mathcal{E}^{\rm HS}[|\psi|^2]\right| \le \frac{C}{L(\beta)}(1+\lambda_\psi)(\lambda_\psi + K_\psi). \tag{3.40}$$

For the **upper bound** on $E^{\rm MH}(\lambda,\beta)$ we specify ψ as $\psi_\lambda^{\rm HS}$, the minimizing wave function for the HS-theory. See equation (3.6) in [LSY94a] or the following

(4.30). It remains ψ_2^{HS}, for all $\lambda > 2$, so these wave functions are normalized to $\|\psi\|_2^2 = \lambda_\psi = \min\{\lambda, 2\}$. Since the variational principle with fixed norm can be replaced by a variational principle with bounded norm, as we have remarked in the Subsection 2.1, the wave function ψ_2^{HS} is good for the upper bounds for all $\lambda \geq 2$. K_ψ is the kinetic energy in the hyperstrong theory. Using the virial equation (2.42), we may replace K_ψ on the right side of (3.40) by $|E^{\mathrm{HS}}(\lambda)|$. With this choice of ψ the equation (3.40) gives the upper bound

$$\frac{1}{L^2} E^{\mathrm{MH}}(\lambda, \beta) \leq E^{\mathrm{HS}}(\lambda) + \frac{C}{L(\beta)} \left(\lambda + \left|E^{\mathrm{HS}}(\lambda)\right|\right). \tag{3.41}$$

To derive a **lower bound**, we use the error bound, when confining the theory to the lowest Landau band, which we have estimated in the Subsection 3.2. By Lemma 3.2 we have, for β large enough,

$$E^{\mathrm{MH}}(\lambda, \beta) \geq (1 - \mathrm{const.}(1+\lambda)^2 \beta^{-1/2})^{-1} E^{\mathrm{MH}}_{\mathrm{conf}}(\lambda, \beta). \tag{3.42}$$

Also this confined Hartree theory has rotation invariant minimizers, since the lowest Landau band is mapped onto itself by rotations around the z-axis. Moreover, since the potential is superharmonic, also the minimizer of this confined theory has $L^{\|} = 0$. See Corollary 2.11 of Subsection 2.5. The variational principle can therefore be restricted to states $\Lambda = |\chi\rangle\langle\chi|$, where the wave functions χ are specified as in equation (3.24), with general $\psi \in \mathcal{H}^1(\mathbb{R})$, normalized to $\|\psi\|_2^2 = \lambda$:

$$E^{\mathrm{MH}}_{\mathrm{conf}}(\lambda, \beta) = \inf_{\Lambda,\ \mathrm{Tr}[\Lambda]=\lambda,\ \Lambda=|\chi\rangle\langle\chi|} \mathcal{E}^{\mathrm{MH}}_\beta[\Lambda]. \tag{3.43}$$

The comparison with HS-theory in (3.40) is now used as a lower bound

$$\frac{1}{L(\beta)^2} \mathcal{E}^{\mathrm{MH}}_\beta[\Lambda] \geq \mathcal{E}^{\mathrm{HS}}[|\psi|^2] - \frac{C}{L(\beta)}(1+\lambda)(\lambda + K_\psi). \tag{3.44}$$

The right side of this inequality can be considered as a functional similar to the HS-functional, but with the constant $1 - C(1+\lambda)/L(\beta)$ in front of the kinetic energy. With an appropriate scale transformation, this is equivalent to a HS-functional multiplied with $(1-(1+\lambda)C/L(\beta))^{-1}$, as long as this parameter is positive. Taking the infima of both sides, we conclude that

$$\frac{1}{L(\beta)^2} E^{\mathrm{MH}}_{\mathrm{conf}}(\lambda, \beta) \geq \left(1 - C\frac{(1+\lambda)}{L(\beta)}\right)^{-1} E^{\mathrm{HS}}(\lambda) - C\frac{(1+\lambda)\lambda}{L(\beta)} \tag{3.45}$$

for β large enough. Considering the limit $\beta \to \infty$ at constant λ we infer

$$\liminf_{\beta\to\infty} \frac{1}{L(\beta)^2} E^{\mathrm{MH}}_{\mathrm{conf}}(\lambda, \beta) \geq E^{\mathrm{HS}}(\lambda). \tag{3.46}$$

Combining this with (3.42) proves, in union with (3.41), the theorem. $\square$

3.7. Remark. To be precise, we specify the asymptotics:

$$\frac{E^{\mathrm{MH}}(\lambda,\beta)}{L(\beta)^2} \leq \left(1 - C\frac{\lambda}{L(\beta)}\right) E^{\mathrm{HS}}(\lambda) + C\frac{\lambda}{L(\beta)}, \tag{3.47}$$

$$\frac{E^{\mathrm{MH}}(\lambda,\beta)}{L(\beta)^2} \geq \left(1 - C\frac{(1+\lambda)^2}{\beta^{1/2}}\right)^{-1} \left(1 - C\frac{1+\lambda}{L(\beta)}\right)^{-1} E^{\mathrm{HS}}(\lambda) - C\frac{\lambda+\lambda^2}{L(\beta)}, \tag{3.48}$$

as long as the terms in braces are positive.

3.8. Remark. The convergence both of the energy of the atom, and of the energy per unit charge, when divided by $(\ln\beta)^2$, is uniform in λ on bounded sets of λ.

Analyzing the limit $N \to \infty$ of many particle quantum mechanics, we will be led to the linearized mean field theory, where we need the

3.9. LEMMA (Generalized strong field limits). *Given two states which are defined by real valued $\psi \in \mathcal{H}^1(\mathbb{R})$ and real valued $\varphi \in \mathcal{H}^1(\mathbb{R})$ as in (3.24), with densities $\rho_{\beta,\psi} = \beta/2\pi e^{-\beta(\mathbf{x}^\perp)^2/2} L\psi(Lx^\parallel)^2$, the following estimate for the Coulomb repulsion holds:*

$$\left|\frac{1}{L^2} D[\rho_{\beta,\varphi}, \rho_{\beta,\psi}] - \frac{1}{2}\int_{-\infty}^{+\infty} \varphi(z)^2 \psi(z)^2 dz\right| \leq \frac{C\lambda_\varphi}{L}\left(\lambda_\psi + \lambda_\psi^{1/4} K_\psi^{3/4}\right). \tag{3.49}$$

Proof. As for $R_{\beta,\psi}$ in the proof of Lemma 3.5, with $\psi(z)^2$ in (3.36) changed to $\varphi(z)^2$. □

4 The mean field limit

We now prove the theorems that we have stated in the introduction. We will derive appropriate upper and lower bounds to the quantum mechanical energy of symmetric states obeying Bose statistics.

The atom with many interacting particles will be compared to models with independent particles in an effective field. In this comparison the upper bound is rather easy: One uses symmetric wave functions of product form as trial wave functions. Then one adds the "self energies" of the one-particle densities.

The production of lower bounds is not so easy. For the Regions 1 and 2 we will use the Lieb-Oxford bound, [LO81], and then we will borrow a part of the kinetic energy to estimate the correction in comparison to the mean field model. But this method breaks down in the presence of magnetic fields, when they are too strong. In Region 3 its use is restricted to the subregion $\beta \lesssim N^{4/3}$. This situation is similar to the case of fermionic electrons, discussed in Sect. 7 of [LSY94a].

For $\beta \gtrsim N^{4/3}$ we have to borrow some kinetic energy at the level of quantum mechanics for N particles. Here we develop a new way of producing bounds, extending the method of [BSY00].

4.1 Upper bounds

4.1. LEMMA (Upper bounds for Regions 1 **and** 2**).** *The Hartree energies provide upper bounds to the quantum mechanical energies for each N, λ and β:*

$$\frac{E(N,\lambda,\beta)}{N} \le \frac{E^{\mathrm{MH}}(\lambda,\beta)}{\lambda}. \tag{4.1}$$

Proof. We apply the variational principle, using N-fold products of 1-particle states Γ as N-particle states

$$E(N,\lambda,\beta) \le N\mathrm{Tr}[(H_\beta - \beta)\Gamma] - N\int \frac{1}{|\mathbf{x}|}\rho_\Gamma + \lambda \frac{N(N-1)}{N^2} D[\rho_\Gamma, \rho_\Gamma] \tag{4.2}$$

for all Γ with $\mathrm{Tr}[\Gamma] \le 1$. Setting $\Gamma = \Gamma^{\mathrm{H}}/\lambda$ we see that the inequality holds, for each β and λ. □

4.2. LEMMA (Upper bound for Region 3**).** *In the limit $\beta \to \infty$, the energies of the hyperstrong theory are asymptotic upper bounds to the quantum mechanical energies for each N:*

$$\limsup_{\beta\to\infty} \frac{E(N,\lambda,\beta)}{N(\ln\beta)^2} \le \frac{E^{\mathrm{HS}}(\lambda)}{\lambda}. \tag{4.3}$$

To be precise:

$$\frac{E(N,\lambda,\beta)}{N\,L(\beta)^2} \le \left(1 - C\frac{\lambda}{L(\beta)}\right)\frac{E^{\mathrm{HS}}(\lambda)}{\lambda} + \frac{C}{L(\beta)}. \tag{4.4}$$

Proof. This results from combining Lemma 4.1 with Theorem 3.6. □

4.2 Lower bounds for Regions 1 and 2

4.3. LEMMA (Lower bounds for Regions 1 **and** 2**).** *In the limit $N \to \infty$, the Hartree energies are asymptotic lower bounds to the quantum mechanical energies,*

$$\liminf_{N\to\infty} \frac{E(N,\lambda,\beta)}{N} \ge \frac{E^{\mathrm{MH}}(\lambda,\beta)}{\lambda}, \tag{4.5}$$

uniformly in β for bounded β.

Proof. We use the Lieb-Oxford inequality [LO81]

$$\langle\Psi|\sum_{i<j} |\mathbf{x}_i - \mathbf{x}_j|^{-1}|\Psi\rangle \ge D[\rho_\Psi, \rho_\Psi] - C\int \rho_\Psi^{4/3} \tag{4.6}$$

(Ψ is normalized as $\|\Psi\|_2 = 1$, the constant can be chosen to be $C = 1.68$), which, together with Hölder's inequality $\int \rho^{4/3} \leq (\int \rho^3)^{1/6} (\int \rho)^{5/6}$, implies that

$$\langle \Psi | H_{N,\lambda,\beta} \Psi \rangle \geq \frac{N}{\lambda} \mathcal{E}^{\mathrm{MH}}_\beta [\Gamma_\Psi \lambda / N] - C \lambda N^{-1/6} \left(\int \rho_\Psi^3 \right)^{1/6}, \tag{4.7}$$

where Γ_Ψ is the one-particle reduced density matrix of Ψ, and ρ_Ψ is its density. Now if $\langle \Psi | H_{N,\lambda,\beta} \Psi \rangle \leq 0$, which we can of course assume, then

$$\langle \Psi | \sum_i (H_{\beta,i} - \beta) \Psi \rangle \leq -\langle \Psi | \sum_i (H_{\beta,i} - \beta - 2|\mathbf{x}_i|^{-1}) \Psi \rangle \leq -N E^{\mathrm{hyd}}(\beta, 2), \tag{4.8}$$

with E^{hyd} defined in (2.9). Together with (2.20) this implies that

$$\left(\int \rho_\Psi^3 \right)^{1/3} \leq \frac{1}{3} \left(\frac{2}{\pi} \right)^{4/3} N \left(\beta - E^{\mathrm{hyd}}(\beta, 2) \right), \tag{4.9}$$

so finally

$$\frac{1}{N} E(N, \lambda, \beta) \geq \frac{1}{\lambda} E^{\mathrm{MH}}(\lambda, \beta) - C \lambda N^{-2/3} \left(\beta - E^{\mathrm{hyd}}(\beta, 2) \right)^{1/2}. \tag{4.10}$$

□

4.4. Remark. Note that the convergence of the energies in Region 2, including Region 1, is uniform in β for bounded β. So if $\beta \to 0$ as $N \to \infty$ we get the usual Hartree energy without magnetic field. It is even possible to let $\beta \to \infty$ with N as long as $\beta \leq \mathrm{const.} N^{4/3}$. In fact, in (4.10) we have an error term of order $N^{-2/3} \beta^{1/2}$ (note that $E^{\mathrm{hyd}} \sim (\ln \beta)^2$ for large β), and this is of lower order than E^{MH} as long as $\beta \leq \mathrm{const.} N^{4/3}$.

4.3 Restriction to independent particles

An essential ingredient is the positive definiteness of the repulsive pair interaction. The method exploiting positive definiteness of a function W uses the inequality

$$\begin{aligned} \sum_{i<j} W(\mathbf{x}_i - \mathbf{x}_j) \ \geq \ & \sum_{i=1}^N \int_{-\infty}^{+\infty} W(\mathbf{x}_i - \mathbf{y}) \sigma(\mathbf{y}) d^3\mathbf{y} \\ & - \frac{1}{2} \iint \sigma(\mathbf{x}) W(\mathbf{x} - \mathbf{y}) \sigma(\mathbf{y}) d^3\mathbf{x}\, d^3\mathbf{y} - N \frac{W(\mathbf{0})}{2}. \end{aligned} \tag{4.11}$$

Actually we need a function W which is positive definite, finite at the origin, and a lower bound to the Coulombic repulsive potential. Also the cutoff near the origin should vanish in the limits $N \to \infty$, $\beta \to \infty$, but still with $W(\mathbf{0})/N(\ln \beta)^2$ going to 0. If we choose for W the spherical symmetric cutoff potential

$$V_{\mathrm{cutoff}}(\mathbf{x}) = \frac{1 - e^{-\mu |\mathbf{x}|}}{|\mathbf{x}|}, \tag{4.12}$$

it turns out that this does not suffice for our purposes. The cutoff length μ^{-1} should be of the order of the typical lengths of the atom, and this would require a coupling of the limits $N \to \infty$ and $\beta \to \infty$, or more precisely, β is not allowed to increase arbitrarily fast with N.

To get a useful lower bound for the entire Region 3, we have to push down $W(\mathbf{0})$ even further, without changing the effective interaction to much. To achieve this, we split V_{cutoff} (we restrict the parameter to $\mu > 1$) into its effective part V_μ and the long range tail V_{long},

$$V_\mu(\mathbf{x}) = \frac{e^{-|\mathbf{x}|} - e^{-\mu|\mathbf{x}|}}{|\mathbf{x}|}, \qquad \mu > 1, \tag{4.13}$$

$$V_{\text{long}}(\mathbf{x}) = \frac{1 - e^{-|\mathbf{x}|}}{|\mathbf{x}|}, \tag{4.14}$$

and borrow some kinetic energy.

The **construction of W** proceeds in several steps. We begin with the observation that V_μ is integrable in $x^\|$ for any $\mathbf{x}^\perp$. It has moreover the property of being decreasing in $|\mathbf{x}|$. So the integrals along lines with fixed $\mathbf{x}^\perp$ can be bounded by the integral along the line, where $\mathbf{x}^\perp = 0$:

$$\int_{-\infty}^{\infty} V_\mu(\mathbf{x}) dx^\| \le 2 \ln \mu. \tag{4.15}$$

We now use Lemma 6.3 of [BSY00], the **operator inequality**, which holds for $\alpha > 0$, $F > 0$, and for each $b > 0$, b independent of α and F,

$$\alpha p_x^2 + F\delta(x) \ge F \cdot w_{F/\alpha,b}(x), \tag{4.16}$$

where

$$w_{D,b}(x) = D \frac{b^2}{2b+1} e^{-bD|x|} \tag{4.17}$$

and $p_x^2 = -(\partial/\partial x)^2$. These functions have the properties of being positive definite and producing delta-function sequences in the limit $bD \to \infty$ coupled with $b \to \infty$. (The variable x will in the application be replaced by $x^\|$.) We extend this lemma to the

4.5. PROPOSITION (Operator inequalities). *Let $V(x)$ define a positive Borel measure $V(x)dx$, with $\int_{-\infty}^{+\infty} V(x)dx \le F$, $F > 0$, $\alpha > 0$. For each $b > 0$ the operator inequality*

$$\alpha p_x^2 + V(x) \ge (V * w_{F/\alpha,b})(x) \tag{4.18}$$

holds, in the sense of an inequality for quadratic forms, with the Sobolev space $\mathcal{H}^1(\mathbb{R})$ as the form domain.

Proof. For $\psi \in \mathcal{H}^1(\mathbb{R})$ consider the wave functions $\psi_y(x) = \psi(x+y)$. By (4.16) there holds for each y the inequality

$$\langle \psi_y | (\alpha p^2 + F\delta) | \psi_y \rangle \geq F \langle \psi_y | w_{F/\alpha,b} | \psi_y \rangle. \tag{4.19}$$

Both sides of this inequality are Borel measurable functions of y. Observe $\langle \psi_y | p^2 | \psi_y \rangle = \langle \psi | p^2 | \psi \rangle$, $\langle \psi_y | w(x) | \psi_y \rangle = \langle \psi | w(x-y) | \psi \rangle$, and integrate both sides of (4.19) with $V(y)dy$. Divide by F, and use $\int_{-\infty}^{+\infty} V(x)dx/F \leq 1$ in front of the kinetic energy term. □

We may consider $\alpha(p_i^{||})^2 + V_\mu(\mathbf{x}_i - \mathbf{x}_j)$ as a 1-particle Hamiltonian acting in $\mathcal{L}^2(\mathbb{R}, dx_i^{||})$, which is parametrized by the perpendicular coordinates and by $\mathbf{x}_j$. However, the operator inequality (4.18) is also valid if the operators act in the extended space $\mathcal{L}^2(\mathbb{R}^{3N}, d^3\mathbf{x}_1 ... d^3\mathbf{x}_N)$, so we can apply this proposition, with $F = 2 \ln \mu$, to

$$\alpha(p_i^{||})^2 + V_\mu(\mathbf{x}_i - \mathbf{x}_j). \tag{4.20}$$

We add the missing long range tail and define

$$W(\mathbf{x}) = \int V_\mu(\mathbf{x}-\mathbf{y}) \delta^2(\mathbf{y}^\perp) w_{2\ln\mu/\alpha,b}(y^{||}) d^3\mathbf{y} + \frac{1 - e^{-|\mathbf{x}|}}{|\mathbf{x}|}, \tag{4.21}$$

where $w_{...}(x^{||})$ is defined in (4.17). The essential effect of the convolution of V_μ with the distribution

$$\underline{w}(\mathbf{x}) = \delta(\mathbf{x}^\perp) w(x^{||}) \tag{4.22}$$

is the lowering of the value of the interactions at the points of coincidences of particles,

$$W(\mathbf{0}) \leq \left(\int V_\mu dx^{||} \right) w_{2\ln\mu/\alpha,b}(0) + 1 < \frac{2b}{\alpha} (\ln \mu)^2 + 1. \tag{4.23}$$

Thus we have shown, that $W(\mathbf{x})$ is a lower bound to the Coulomb potential, when some borrowed part of the kinetic energy is added,

$$W = V_\mu * \underline{w} + V_{\text{long}} \leq \alpha(p^{||})^2 + V_\mu + V_{\text{long}} \leq \alpha(p^{||})^2 + 1/|\mathbf{x}|. \tag{4.24}$$

Now the function $W = V_\mu * \underline{w} + V_{\text{long}}$ is also positive definite, since the distribution $\underline{w}$ and all the involved functions are positive definite. So we can refer to the technique (4.11) of reduction to one-particle models.

4.6. PROPOSITION (Bounds by independent particles). *Considered as quadratic forms, the N-particle Hamiltonians $H_{N,\lambda,\beta}$ are bounded from below by sums of one-particle Hamiltonians and constants:*

$$H_{N,\lambda,\beta} \geq \sum_{i=1}^{N} h_i - \frac{1}{2} \frac{\lambda}{N} \iint \sigma(\mathbf{x}) W(\mathbf{x}-\mathbf{y}) \sigma(\mathbf{y}) d^3\mathbf{x}\, d^3\mathbf{y} - \lambda \frac{b}{\alpha} (\ln \mu)^2 - \frac{\lambda}{2}, \tag{4.25}$$

where

$$h_i = H_{\beta,i} - \beta - \frac{\alpha\lambda}{2}(p_i^{\|})^2 - \frac{1}{|\mathbf{x}_i|} + \frac{\lambda}{N}\int W(\mathbf{x}_i - \mathbf{y})\sigma(\mathbf{y})d^3\mathbf{y}, \tag{4.26}$$

and where $W(\mathbf{x})$ *is defined in (4.21). The parameters* α, b *have to be positive,* $\mu > 1$, $\sigma(\mathbf{x})$ *should be an element of* $\mathcal{L}^1(\mathbb{R}^3)$*.*

Proof. From $H_{\beta,i}$ we borrow a part of $(p_i^{\|})^2 = -(\partial/\partial x_i^{\|})^2$ to use (4.24),

$$\alpha(p_i^{\|})^2 + \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \geq W(\mathbf{x}_i - \mathbf{x}_j), \tag{4.27}$$

sum over all pairs $i \neq j$, and multiply with $\lambda/2N$. This gives

$$\alpha\lambda\frac{N-1}{2N}\sum_{i=1}^{N}(p_i^{\|})^2 + \frac{\lambda}{N}\sum_{i<j}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \geq \frac{\lambda}{N}\sum_{i<j}W(\mathbf{x}_i - \mathbf{x}_j). \tag{4.28}$$

Inserting (4.28) and (4.11) into (1.3) completes the proof. □

To ascertain any use to the inequality, $\alpha\lambda < 2$ is requested. In the next subsection, the density σ will be chosen to be an approximately minimizing Hartree density, and the parameters will be adapted to the limit $N, \beta \to \infty$.

4.4 The lower bound for Region 3

We choose $\sigma = N\rho$, with

$$\rho(\mathbf{x}) = \frac{\beta}{2\pi}\exp\left(-\frac{\beta(\mathbf{x}^{\perp})^2}{2}\right)\frac{1}{\lambda}L\rho_\lambda^{\mathrm{HS}}(Lx^{\|}). \tag{4.29}$$

The minimizing density $\rho_\lambda^{\mathrm{HS}}$ for the hyperstrong theory is, see [LSY94a],

$$\begin{aligned} \rho_\lambda^{\mathrm{HS}}(z) &= \frac{2(2-\lambda)^2}{(4\sinh[(2-\lambda)|z|/4 + c(\lambda)])^2} \qquad \text{for} \quad \lambda < 2, && (4.30)\\ &\qquad \tanh c(\lambda) = (2-\lambda)/2, \\ \rho_\lambda^{\mathrm{HS}}(z) &= 2(2+|z|)^{-2} \qquad\qquad\qquad\qquad \text{for} \quad \lambda \geq 2. && (4.31) \end{aligned}$$

Note that $\|\rho\|_1 = \min\{1, 2/\lambda\}$, $\quad \|\rho\|_\infty = (\beta/2\pi)L(\beta)\rho_\lambda^{\mathrm{HS}}(0)/\lambda \leq C\beta L(\beta)$.

We want to study the lower bound to $N^{-1}E(N,\lambda,\beta)$, due to Proposition 4.6,

$$\inf\text{ spec }\{h\} - \frac{\lambda}{2}\iint\rho(\mathbf{x})W(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d^3\mathbf{x}\,d^3\mathbf{y} - \frac{\lambda}{N}\left(\frac{b}{\alpha}(\ln\mu)^2 + \frac{1}{2}\right), \tag{4.32}$$

which we expect to be asymptotically proportional to $(\ln \beta)^2$. For simplicity, we will restrict our considerations to $\beta > C_\beta$ for some $C_\beta > 1$ in the following. We choose the parameters as

$$\mu = \beta^{1/2+\delta}, \alpha = N^{-\varepsilon}, b = N^{\eta}, \tag{4.33}$$

with $\delta, \varepsilon, \eta$ all greater than zero, $\varepsilon + \eta < 1$. This guarantees first of all the relative vanishing of the constant which stems from $W(\mathbf{0})$:

$$\frac{\lambda}{N}\left(\frac{b}{\alpha}(\ln \mu)^2 + \frac{1}{2}\right)/(\ln \beta)^2 \to 0, \tag{4.34}$$

as $\beta, N \to \infty$. It remains to study the Hamiltonian h and the self energy of ρ due to the interaction $W = V_\mu * \underline{w} + V_{\text{long}}$.

The inequality

$$\iint \rho(\mathbf{x})(V_\mu * \underline{w})(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d^3\mathbf{x}\,d^3\mathbf{y} \le \iint \rho(\mathbf{x})V_\mu(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})d^3\mathbf{x}\,d^3\mathbf{y} \tag{4.35}$$

can be observed in Fourier space, where $\widetilde{V}_\mu$ and $\widetilde{\underline{w}}$ are positive, and $\widetilde{\underline{w}} \le 1$. We add V_{long}, and use the pointwise inequality in $\mathbf{x}$-space $(V_\mu + V_{\text{long}})(\mathbf{x}) \le V^C(\mathbf{x}) \equiv 1/|\mathbf{x}|$. So the self-energy of ρ due to W is smaller than the self-energy $D[\rho,\rho]$ due to the interaction by the Coulomb potential V^C.

The potential $(V_\mu * \underline{w} + V_{\text{long}}) * \rho$ in the Hamiltonian h is now changed to $V^C * \rho$. First we give a bound to the difference of $V_\mu * \underline{w} * \rho$ to $V_\mu * \rho$ in the form of an operator inequality, which follows from

$$\begin{aligned} |\langle\psi|V_\mu * (\underline{w} * \rho - \rho)|\psi\rangle| &\le \|(|\psi|^2 * V_\mu)\cdot(\underline{w} * \rho - \rho)\|_1 \\ &\le \|\underline{w} * \rho - \rho\|_1 \, \| |\psi|^2 * V_\mu\|_\infty \\ &= \|\underline{w} * \rho - \rho\|_1 \sup_{\mathbf{y}} \langle\psi|V_{\mu,\mathbf{y}}|\psi\rangle, \end{aligned} \tag{4.36}$$

where $V_{\mu,\mathbf{y}} = V_\mu(\mathbf{x}-\mathbf{y})$. Since $V_\mu \le V^C$, and, with $E^{\text{hyd}}(\beta) \equiv E^{\text{hyd}}(\beta, \zeta = 1)$,

$$H_\beta - \beta - V^C_{\mathbf{y}} \ge E^{\text{hyd}}(\beta), \tag{4.37}$$

the last term in (4.36) is bounded by

$$\langle\psi|V^C_{\mathbf{y}}|\psi\rangle \le \langle\psi|H_\beta - \beta - E^{\text{hyd}}(\beta)|\psi\rangle, \tag{4.38}$$

multiplied with $\|\underline{w} * \rho - \rho\|_1$.

We observe, see Remark 2.2,

$$E^{\text{hyd}}(\beta) = \lim_{\lambda\to 0}\frac{E^{\text{MH}}(\lambda,\beta)}{\lambda}, \qquad \lim_{\lambda\to 0}\frac{E^{\text{HS}}(\lambda)}{\lambda} = -\frac{1}{4}. \tag{4.39}$$

The precise bound in the Remark 3.7 gives thus (see also [AHS81])

$$E^{\mathrm{hyd}}(\beta) \geq \left(-\frac{1}{4} - C\frac{1}{L(\beta)}\right) L^2(\beta) \geq -C(\ln\beta)^2 \tag{4.40}$$

for $\beta > C_\beta$. An analogous bound holds also for $E^{\mathrm{hyd}}(\beta, 2)$. Note that $L(\beta)$ can be replaced by $(\ln\beta)$ (and vice versa), since for $\beta > C_\beta > 1$ there are positive constants C_1 and C_2 such that $C_1 \leq \ln(\beta)/L(\beta) \leq C_2$.

To complete the estimate (4.36), we need a bound to $\|\underline{w} * \rho - \rho\|_1$. There, the integrals in perpendicular coordinates can be done explicitly. Note that for all λ we have $|d\rho_\lambda^{\mathrm{HS}}/dz| \leq \rho_\lambda^{\mathrm{HS}}$. Using this and the monotonicity of $\rho_\lambda^{\mathrm{HS}}$ in $|z|$ we can estimate

$$\begin{aligned} \left|\rho_\lambda^{\mathrm{HS}}(z-y) - \rho_\lambda^{\mathrm{HS}}(z)\right| &\leq |y| \sup_{x\in[z-y,z]} \left|\frac{d\rho_\lambda^{\mathrm{HS}}}{dz}(x)\right| \\ &\leq |y| \left(\rho_\lambda^{\mathrm{HS}}(z-y) + \rho_\lambda^{\mathrm{HS}}(z) + \Theta(|y|-|z|)\rho_\lambda^{\mathrm{HS}}(0)\right). \end{aligned} \tag{4.41}$$

Since for $|y| \geq 1$ (4.41) is obviously true even without the last term, we see that (4.41) holds with $\Theta(|y|-|z|)$ replaced by $\Theta(1-|z|)$. This implies

$$\begin{aligned} \|\rho * \underline{w} - \rho\|_1 &\leq \frac{1}{\lambda}\int dx^{\|} d\eta L w(\eta) \\ &\quad \times \left(\left|\rho_\lambda^{\mathrm{HS}}(Lx^{\|} - L\eta) - \rho_\lambda^{\mathrm{HS}}(Lx^{\|})\right| + \left(\left(\textstyle\int w\right)^{-1} - 1\right)\rho_\lambda^{\mathrm{HS}}(Lx^{\|})\right) \\ &\leq \lambda^{-1}\textstyle\int \rho_\lambda^{\mathrm{HS}}(1 - \int w) + 2\lambda^{-1}\left(\int \rho_\lambda^{\mathrm{HS}} + \rho_\lambda^{\mathrm{HS}}(0)\right) L \displaystyle\int |\eta| w(\eta) d\eta. \end{aligned} \tag{4.42}$$

Now $\int \rho_\lambda^{\mathrm{HS}} \leq \lambda$, $\rho_\lambda^{\mathrm{HS}}(0) \leq \frac{1}{2}\lambda$, $(1-\int w) \leq (2b)^{-1}$ and $\int |\eta| w \leq \alpha/(2b\ln\mu)$, so we get

$$\|\rho * \underline{w} - \rho\|_1 \leq \frac{1}{2b} + \frac{3}{2}\frac{\alpha L(\beta)}{b\ln\mu} \leq C(N^{-\eta} + N^{-\eta-\varepsilon}L(\beta)/\ln\beta) \leq C' N^{-\eta}. \tag{4.43}$$

Finally, we add to V_μ the short-range term

$$V_{\mathrm{short}}(\mathbf{x}) = \frac{e^{-\mu|\mathbf{x}|}}{|\mathbf{x}|}, \tag{4.44}$$

and we find the pointwise bound to $(V^C - V_\mu) * \rho$ as

$$\|V_{\mathrm{short}}\|_1 \|\rho\|_\infty \leq C\mu^{-2}\beta L(\beta) = C\beta^{-2\delta}L(\beta). \tag{4.45}$$

We collect the bounds we have obtained so far:

$$\frac{E(N,\lambda,\beta)}{N} \geq \inf\ \mathrm{spec}\ \{h_b\} - \lambda D[\rho,\rho] - C\lambda(\ln\beta)^2\left(N^{\varepsilon+\eta-1} + N^{-\eta} + \beta^{-2\delta}L(\beta)^{-1}\right), \tag{4.46}$$

with the one-particle Hamiltonian

$$h_b = (H_\beta - \beta)\left(1 - C\lambda N^{-\eta} - 2\lambda N^{-\varepsilon}\right) - V^C + \lambda V^C * \rho, \tag{4.47}$$

where we have used $(p^{\|})^2 \leq H_\beta - \beta$. We now use (4.8) to estimate the error terms in the kinetic energy. Then we apply the statements of the subsection on the confinement in the mean field theory, Lemma 3.4, to estimate

$$\begin{aligned} \frac{E(N,\lambda,\beta)}{N} \geq\ & \inf\ \mathrm{spec}\ \left\{\Pi_0\left(H_\beta - \beta - V^C + \lambda V^C * \rho\right)\Pi_0\right\} - \lambda D[\rho,\rho] \\ & -C\lambda(\ln\beta)^2\left(N^{-\eta} + N^{-\varepsilon} + N^{\varepsilon+\eta-1} + \frac{\beta^{-2\delta}}{L(\beta)} + \frac{2+\lambda}{\lambda}\beta^{-1/2}\right). \end{aligned} \tag{4.48}$$

Corollary 2.11 states that the minimizer of the operator in question has $L^{\|} = 0$. The search for the infimum of the spectrum can therefore be restricted to the use of the same type of wave-functions as in the investigations on the limit of very strong magnetic fields in Subsection 3.4, Lemma 3.5 and 3.9, and these investigations can be applied, too. We choose $\varepsilon = \eta = 1/3$ and get the lower bound

$$\begin{aligned} & \frac{E(N,\lambda,\beta)}{N\,L^2(\beta)} \\ & \geq \left(\inf\ \mathrm{spec}\ \left\{p_z^2 - \delta(z) + \rho_\lambda^{\mathrm{HS}}(z)\right\} - \frac{1}{2\lambda}\int(\rho_\lambda^{\mathrm{HS}}(z))^2 dz\right)\left(1 - C\frac{1+\lambda}{L(\beta)}\right)^{-1} \\ & \quad - C\left(\lambda N^{-1/3} + L(\beta)^{-1}\left(\lambda\beta^{-2\delta} + 1 + \lambda\right) + (2+\lambda)\beta^{-1/2}\right). \end{aligned} \tag{4.49}$$

The operator in curly brackets is the Hamiltonian for the linearized HS theory, with ground state energy $(E^{\mathrm{HS}} + \frac{1}{2}\int(\rho_\lambda^{\mathrm{HS}})^2)/\lambda$ (cf. eq. (2.38)). So our final result can be stated as

4.7. LEMMA (Lower bound for Region 3). *If $L(\beta) > C(1+\lambda)$, then*

$$\frac{E(N,\lambda,\beta)}{N\,L^2(\beta)} \geq \frac{E^{\mathrm{HS}}(\lambda)}{\lambda}\left(1 - C\frac{1+\lambda}{L(\beta)}\right)^{-1} - C\left(\lambda N^{-1/3} + \frac{1+\lambda}{L(\beta)}\right). \tag{4.50}$$

Hence the convergence of the lower bound, in the limit $N \to \infty$, $\beta \to \infty$, is proven.

4.8. Remark. The limits $N \to \infty$ and $\beta \to \infty$ can be considered independently of each other, in any succession or combination.

4.5 Critical particle number

Recall that $\underline{E}(N, Z, B)$ denotes the ground state energy of the unscaled Hamiltonian (1.1).

4.9. LEMMA (Limit of the critical charge). *Define*

$$N_c(Z, B) = \max\{N|\underline{E}(N, Z, B) < \underline{E}(N-1, Z, B)\}. \tag{4.51}$$

We have

$$\liminf_{Z\to\infty} \frac{N_c(Z, \beta Z^2)}{Z} \geq \lambda_c(\beta). \tag{4.52}$$

Proof. This follows from the convergence of the energies, by analogous arguments as in [BL83] or [LSY94a]. □

4.10. Remark. In [S00], Theorem 3, the following upper bound on N_c is proven:

$$N_c < 2Z + 1 + \frac{Z}{2} \min\left\{\left(1 + \frac{B}{Z^2}\right), C\left(1 + \left[\ln\left(\frac{B}{Z^2}\right)\right]^2\right)\right\} \tag{4.53}$$

for some constant C independent of B and Z. Inserting (4.53) into (4.52) this proves Lemma 2.9.

4.6 Convergence of the density matrices

4.11. LEMMA (Ground states are Hartree minimizers). *For fixed λ and β, let Ψ_N be an ε-approximate ground state of $H_{N,\lambda,\beta}$ defined in (1.3), i.e.*

$$\langle \Psi_N, H_{N,\lambda,\beta}\Psi_N\rangle \leq E(N, \lambda, \beta) + \varepsilon(N) \tag{4.54}$$

for all N, with $0 < \varepsilon = o(N)$. Let Γ_N be the corresponding one-particle reduced density matrix. Then $\lambda\Gamma_N/N$ is a minimizing sequence for $\mathcal{E}_\beta^{\mathrm{MH}}$, i.e.

$$\lim_{N\to\infty} \mathcal{E}_\beta^{\mathrm{MH}}[\lambda\Gamma_N/N] = E^{\mathrm{MH}}(\lambda, \beta). \tag{4.55}$$

Proof. Let ρ_N be the density of Γ_N. We have

$$\begin{aligned}
E^{\mathrm{MH}} &\leq \mathcal{E}_\beta^{\mathrm{MH}}[\lambda\Gamma_N/N] = \frac{\lambda}{N}\mathrm{Tr}[(H_\beta - \beta - |\mathbf{x}|^{-1})\Gamma_N] + \frac{\lambda^2}{N^2}D[\rho_N, \rho_N] \\
&= \frac{\lambda}{N}\langle\Psi_N|H_{N,\lambda,\beta}\Psi_N\rangle - \frac{\lambda^2}{N^2}\langle\Psi_N|\sum_{i<j}|\mathbf{x}_i - \mathbf{x}_j|^{-1}\Psi_N\rangle + \frac{\lambda^2}{N^2}D[\rho_N, \rho_N] \\
&\leq \frac{\lambda}{N}(E(N, \lambda, \beta) + \varepsilon) + \frac{\lambda^2}{N^2}C\int \rho_N^{4/3}, \qquad (4.56)
\end{aligned}$$

where we used again the Lieb-Oxford inequality for the last step. By an analogous argument as in Lemma 4.3 we see that the right side of (4.56) converges to E^{MH} as $N \to \infty$. □

Since $\lambda\Gamma_N/N$ is a minimizing sequence for $\mathcal{E}_\beta^{\mathrm{MH}}$, and Γ^{H} is unique, we know that $\lambda\Gamma_N/N \rightharpoonup \Gamma^{\mathrm{H}}$ in weak operator sense. If $\lambda \leq \lambda_c$, there is even norm convergence. To show this we need the following general lemma:

4.12. LEMMA (Weak convergence implies norm convergence). *Let a_N be a sequence of positive trace class operators on a Hilbert space. Suppose that $a_N \rightharpoonup a$ in weak operator sense, for some positive trace class operator a. If $\lim_{N\to\infty} \mathrm{Tr}[a_N] = \mathrm{Tr}[a]$, then $a_N \to a$ in trace norm, i.e.*

$$\|a_N - a\|_1 \equiv \mathrm{Tr}[|a_N - a|] \to 0 \quad \text{as} \quad N \to \infty. \tag{4.57}$$

Proof. See [S79], Thm. 2.20. □

4.13. THEOREM (Convergence of the density matrices). *Let Γ_N be as in Lemma 4.11, and let $\lambda \leq \lambda_c$. Then for each fixed β*

$$\lim_{N\to\infty} \|\lambda\Gamma_N/N - \Gamma^{\mathrm{H}}\|_1 = 0. \tag{4.58}$$

Proof. Since Γ^{H} is unique, $\lambda\Gamma_N/N$ converges weakly to Γ^{H} by Lemma 4.11 and the proof of Theorem 2.4. Apply Lemma 4.12 to $a_N = \lambda\Gamma_N/N$ and $a = \Gamma^{\mathrm{H}}$, and note that $\mathrm{Tr}[\lambda\Gamma_N/N] = \lambda$ and $\mathrm{Tr}[\Gamma^{\mathrm{H}}] = \min\{\lambda, \lambda_c\}$. □

4.7 Bose condensation

Bose condensation, as defined in [PO56], means that the largest eigenvalue of the one-particle reduced density matrix of the ground state for the N-particle Hamiltonian is of order N as $N \to \infty$, or equivalently, if $\liminf_{N\to\infty} \|\Gamma_N\|/\mathrm{Tr}[\Gamma_N] > 0$. This is shown to be the case for our model.

4.14. THEOREM (Bose condensation in the mean field limit). *Let Γ_N be as in Lemma 4.11. Then for each fixed β and λ*

$$\lim_{N\to\infty} \frac{\|\Gamma_N\|}{\mathrm{Tr}[\Gamma_N]} = \frac{\min\{\lambda, \lambda_c\}}{\lambda}. \tag{4.59}$$

In particular, if $\lambda \leq \lambda_c$, and if φ_N denotes the normalized eigenvector corresponding to the largest eigenvalue of Γ_N with appropriate phase-factor, we have

$$\lim_{N\to\infty} \frac{\|\Gamma_N\|}{\mathrm{Tr}[\Gamma_N]} = 1, \quad \lim_{N\to\infty} \|\varphi_N - \varphi_{\mathrm{H}}\|_2 = 0, \tag{4.60}$$

where $\varphi_{\mathrm{H}} = \lambda^{-1/2}\sqrt{\rho^{\mathrm{H}}}$ is the normalized ground state of H^{H}.

Proof. We use the notations of the proof of Theorem 4.13. The first assertion is easily proved, using that

$$|\|a_N\| - \|a\|| \leq \|a_N - a\| \leq \|a_N - a\|_1 \tag{4.61}$$

and $\|a\| = \min\{\lambda, \lambda_c\}$. To prove the second we denote $P = |\varphi_{\mathrm{H}}\rangle\langle\varphi_{\mathrm{H}}|$ and $P_N = |\varphi_N\rangle\langle\varphi_N|$, and compute

$$\begin{aligned} \mathrm{Tr}[a_N P] &= \|a_N\|\langle\varphi_N|P\varphi_N\rangle + \mathrm{Tr}[a_N^{1/2} P a_N^{1/2}(1-P_N)] \\ &\leq \|a_N\|\langle\varphi_N|P\varphi_N\rangle + \mathrm{Tr}[a_N] - \|a_N\|, \end{aligned} \tag{4.62}$$

where we have used $P \leq 1$ in the last step. Therefore $\langle\varphi_N|P\varphi_N\rangle \to 1$ as $N \to \infty$, which gives immediately the desired result. □

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