A discrete density matrix theory for atoms in strong magnetic fields

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Abstract

This paper concerns the asymptotic ground state properties of heavy atoms in strong, homogeneous magnetic fields. In the limit when the nuclear charge Z tends to ∞ with the magnetic field B satisfying $B \gg Z^{4/3}$ all the electrons are confined to the lowest Landau band. We consider here an energy functional, whose variable is a sequence of one-dimensional density matrices corresponding to different angular momentum functions in the lowest Landau band. We study this functional in detail and derive various interesting properties, which are compared with the density matrix (DM) theory introduced by Lieb, Solovej and Yngvason. In contrast to the DM theory the variable perpendicular to the field is replaced by the discrete angular momentum quantum numbers. Hence we call the new functional a *discrete density matrix (DDM) functional*. We relate this DDM theory to the lowest Landau band quantum mechanics and show that it reproduces correctly the ground state energy apart from errors due to the indirect part of the Coulomb interaction energy.

1 Introduction

The ground state properties of atoms in strong magnetic fields have been the subject of intensive mathematical studies during the last decade. This paper is based on the comprehensive work of Lieb, Solovej and Yngvason [LSY94a, LSY94b], which we refer to for an extensive list of references concerning the history of this subject.

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The starting point of our investigation is the Pauli Hamiltonian for an atom with N electrons and nuclear charge Z in a homogeneous magnetic field $\mathbf{B} = (0,0,B)$ with vector potential $\mathbf{A}(\mathbf{x}) = \frac{1}{2}\mathbf{B}\times\mathbf{x}$,

$$H = \sum_{1\le j\le N}\left\{\left[\boldsymbol{\sigma}_j\cdot(-i\nabla_j + \mathbf{A}(\mathbf{x}_j))\right]^2 - \frac{Z}{|\mathbf{x}_j|}\right\} + \sum_{1\le i<j\le N}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}, \tag{1.1}$$

which acts on the Hilbert space $\bigwedge_{1\le j\le N}\mathcal{L}^2(\mathbb{R}^3;\mathbb{C}^2)$ of antisymmetric spinor-valued wave functions. Here $\boldsymbol{\sigma}$ denotes the usual Pauli spin matrices.

The units are chosen such that $\hbar = 2m_e = e = 1$, so the unit of energy is four times the Rydberg energy. The magnetic field B is measured in units $B_0 = \frac{m_e^2e^3c}{\hbar^3} = 2.35\cdot 10^9$ Gauß, the field strength for which the cyclotron radius $\ell_B = (\hbar c/(eB))^{1/2}$ equals the Bohr radius $a_0 = \hbar^2/(m_e e^2)$.

The ground state energy is defined as

$$E^{\mathrm{Q}}(N,Z,B) = \inf\{\langle\Psi, H\Psi\rangle : \Psi\in \text{domain } H, \langle\Psi,\Psi\rangle = 1\}, \tag{1.2}$$

and if there is a ground state wave function Ψ, the corresponding ground state density ρ^{Q} is given by

$$\rho^{\mathrm{Q}}(\mathbf{x}) = \rho_\Psi(\mathbf{x}) \equiv N\sum_{s_i=\pm1/2}\int |\Psi(\mathbf{x},s_1,\ldots,\mathbf{x}_N,s_N)|^2 \mathrm{d}\mathbf{x}_2\ldots\mathrm{d}\mathbf{x}_N. \tag{1.3}$$

Recall that the spectrum of the free Pauli Hamiltonian on $\mathcal{L}^2(\mathbb{R}^3;\mathbb{C}^2)$ for one electron in the magnetic field $\mathbf{B}$,

$$H_{\mathbf{A}} = \left[\boldsymbol{\sigma}\cdot(-i\nabla + \mathbf{A}(\mathbf{x}))\right]^2, \tag{1.4}$$

is given by

$$p_z^2 + 2\nu B \qquad \nu = 0,1,2,..., \quad p_z\in\mathbb{R}. \tag{1.5}$$

The projector Π_0 onto the lowest Landau band, $\nu = 0$, is represented by the kernel

$$\Pi_0(\mathbf{x},\mathbf{x}') = \frac{B}{2\pi}\exp\left\{\frac{i}{2}(\mathbf{x}_\perp\times\mathbf{x}'_\perp)\cdot\mathbf{B} - \frac{1}{4}(\mathbf{x}_\perp-\mathbf{x}'_\perp)^2B\right\}\delta(z-z')P_\downarrow, \tag{1.6}$$

where $\mathbf{x}_\perp$ and z are the components of $\mathbf{x}$ perpendicular and parallel to the magnetic field, and $P_\downarrow$ denotes the projection onto the spin-down ($s=-1/2$) component. With the decomposition $\mathcal{L}^2(\mathbb{R}^3,\mathrm{d}\mathbf{x};\mathbb{C}^2) = \mathcal{L}^2(\mathbb{R}^2,\mathrm{d}\mathbf{x}_\perp)\otimes\mathcal{L}^2(\mathbb{R},\mathrm{d}z)\otimes\mathbb{C}^2$ it can be written as

$$\Pi_0 = \sum_{m\ge0}|\phi_m\rangle\langle\phi_m|\otimes I\otimes P_\downarrow, \tag{1.7}$$

where ϕ_m denotes the function in the lowest Landau band with angular momentum $-m\le 0$, i.e., using polar coordinates (r,φ),

$$\phi_m(\mathbf{x}_\perp) = \sqrt{\frac{B}{2\pi}}\frac{1}{\sqrt{m!}}\left(\frac{Br^2}{2}\right)^{m/2}e^{-im\varphi}e^{-Br^2/4}. \tag{1.8}$$

The projector onto the subspace of $\bigwedge_{1\le j\le N}\mathcal{L}^2(\mathbb{R}^3;\mathbb{C}^2)$ where all the electrons are in the lowest Landau band is the N-th tensorial power of Π_0 and will be denoted by Π_0^N. The ground state energy of electrons restricted to the lowest Landau band is defined as

$$E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)=\inf_{\|\Psi\|=1}\langle\Psi,\Pi_0^N H\Pi_0^N\Psi\rangle. \tag{1.9}$$

The assertion that for $B\gg Z^{4/3}$ the electrons are to the leading order confined to the lowest Landau band is confirmed by the following theorem.

1.1. THEOREM (Lowest Landau band confinement). *([LSY94a], Theorem 1.2) For any fixed $\lambda=N/Z$ there is a $\delta(x)$ with $\delta(x)\to 0$ as $x\to\infty$ such that*

$$E^{\mathrm{Q}}_{\mathrm{conf}}\ge E^{\mathrm{Q}}\ge E^{\mathrm{Q}}_{\mathrm{conf}}\left(1+\delta(B/Z^{4/3})\right). \tag{1.10}$$

We now define the functional we are considering. We are only interested in $B\gg Z^{4/3}$, so we can restrict ourselves to considering all particles in the lowest Landau band. Recalling that

$$\Pi_0 H_{\mathbf{A}}\Pi_0=\sum_{m\ge 0}|\phi_m\rangle\langle\phi_m|\otimes(-\partial_z^2)\otimes P_\downarrow, \tag{1.11}$$

it is natural to define the following *discrete density matrix functional* (DDM) as

$$\mathcal{E}^{\mathrm{DDM}}_{B,Z}[\Gamma]=\sum_{m\in\mathbb{N}_0}\left(\mathrm{Tr}[-\partial_z^2\Gamma_m]-Z\int V_m(z)\rho_m(z)\mathrm{d}z\right)+\widetilde{D}(\rho,\rho), \tag{1.12}$$

where

$$\widetilde{D}(\rho,\rho)=\frac12\sum_{m,n}\int V_{m,n}(z-z')\rho_m(z)\rho_n(z')\mathrm{d}z\mathrm{d}z', \tag{1.13}$$

and the potentials V_m and $V_{m,n}$ are given by

$$V_m(z) = \int\frac{1}{|\mathbf{x}|}|\phi_m(\mathbf{x}_\perp)|^2\mathrm{d}\mathbf{x}_\perp, \tag{1.14}$$

$$V_{m,n}(z-z') = \int\frac{|\phi_m(\mathbf{x}_\perp)|^2|\phi_n(\mathbf{x}'_\perp)|^2}{|\mathbf{x}-\mathbf{x}'|}\mathrm{d}\mathbf{x}_\perp\mathrm{d}\mathbf{x}'_\perp. \tag{1.15}$$

Here Γ is a sequence of density matrices acting on $\mathcal{L}^2(\mathbb{R},\mathrm{d}z)$,

$$\Gamma=(\Gamma_m)_{m\in\mathbb{N}_0}, \tag{1.16}$$

with corresponding densities $\rho=(\rho_m)_m$, $\rho_m(z)=\Gamma_m(z,z)$. Note that $\mathcal{E}^{\mathrm{DDM}}_{B,Z}$ depends on B via the potentials V_m and $V_{m,n}$.

This functional is defined for all Γ with the properties:

(i)

$$0 \leq \Gamma_m \leq I \qquad \text{for all } m \in \mathbb{N}_0, \tag{1.17}$$

(ii)

$$\sum_m \operatorname{Tr}[(1-\partial_z^2)\Gamma_m] < \infty. \tag{1.18}$$

The corresponding energy is given by

$$E^{\mathrm{DDM}}(N,Z,B) = \inf \left\{ \mathcal{E}^{\mathrm{DDM}}_{B,Z}[\Gamma] \,\middle|\, \sum_m \operatorname{Tr}[\Gamma_m] \leq N \right\}. \tag{1.19}$$

(We do not require that N is an integer.) As we will show, E^{DDM} correctly reproduces the confined ground state energy $E^{\mathrm{Q}}_{\mathrm{conf}}$ apart from errors due to the indirect part of the Coulomb interaction energy:

1.2. THEOREM (Relation of E^{DDM} and $E^{\mathrm{Q}}_{\mathrm{conf}}$). *For some constant c_λ depending only on $\lambda = N/Z$*

$$0 \geq E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B) - E^{\mathrm{DDM}}(N,Z,B) \geq -R_L, \tag{1.20}$$

with

$$R_L = c_\lambda \min\left\{ Z^{17/15} B^{2/5}, Z^{8/3}(1+[\ln(B/Z^3)]^2) \right\}. \tag{1.21}$$

The proof will be given in Sections 5 and 6. Note that $E^{\mathrm{Q}}_{\mathrm{conf}}$ is of order $\min\{Z^{7/3}(B/Z^{4/3})^{2/5}, Z^3(1+[\ln(B/Z^3)]^2)\}$, so R_L is really of lower order.

The functional (1.12) is in fact a *reduced Hartree-Fock* approximation (in the sense of [S91]) for the quantum mechanical many body problem, i.e. Hartree-Fock theory with the exchange term dropped. The upper bound in Theorem 1.2 holds quite generally for (reduced) Hartree-Fock approximations to many body quantum mechanics with positive two-body interactions.

Hartree and Hartree-Fock approximations to H with restriction to the lowest Landau level were probably for the first time considered in [CLR70] and [CR73]. They have been studied numerically in [NLK86, NKL87].

In this paper we present a rigorous mathematical treatment of the functional (1.12). In Section 3 we show that there exists a unique solution to the minimization problem in (1.19). The corresponding minimizer is composed of eigenfunctions of one-dimensional effective mean-field Hamiltonians depending on m. Moreover, the superharmonicity of the effective mean-field potential implies monotonicity and concavity of the eigenvalues in m, which amounts to "filling the lowest angular momentum channels". This fact is important for numerical treatments of the model, for it means that at most the N lowest angular momenta have to be considered. For B/Z^3 large enough, we will show that each angular momentum channel is occupied by at most *one* particle. In Section 4 we estimate the maximum number of electrons that can be bound to the nucleus. We use Lieb's strategy to derive an upper bound analogous to [S00].

The DDM theory can also be considered as a discrete analogue of the DM functional introduced in [LSY94a]. To express this analogy we will recall its definition and main properties in the next section.

2 Comparison with the DM functional

In [LSY94a] Lieb, Solovej and Yngvason defined a density matrix (DM) functional as

$$\mathcal{E}^{\mathrm{DM}}[\Gamma] = \int_{\mathbb{R}^2} \mathrm{Tr}_{\mathcal{L}^2(\mathbb{R})}[-\partial_z^2 \Gamma_{\mathbf{x}_\perp}]\mathrm{d}\mathbf{x}_\perp - Z\int |\mathbf{x}|^{-1}\rho_\Gamma(\mathbf{x}) + D(\rho_\Gamma, \rho_\Gamma). \tag{2.1}$$

Its variable is an operator valued function

$$\Gamma : \mathbf{x}_\perp \to \Gamma_{\mathbf{x}_\perp}, \tag{2.2}$$

where $\Gamma_{\mathbf{x}_\perp}$ is a density matrix on $\mathcal{L}^2(\mathbb{R})$, given by a kernel $\Gamma_{\mathbf{x}_\perp}(z, z')$ and satisfying

$$0 \leq \Gamma_{\mathbf{x}_\perp} \leq (B/2\pi)I \tag{2.3}$$

as an operator on $\mathcal{L}^2(\mathbb{R})$. Here we denote

$$\rho_\Gamma(\mathbf{x}) = \Gamma_{\mathbf{x}_\perp}(z, z) \quad \text{and} \quad D(f, g) = \frac{1}{2}\int \frac{f(\mathbf{x})g(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}'. \tag{2.4}$$

The energy

$$E^{\mathrm{DM}}(N, Z, B) = \inf\{\mathcal{E}^{\mathrm{DM}}[\Gamma] \,|\, \Gamma \,\text{satisfies}\,(2.3)\ \text{and}\ \int \rho_\Gamma \leq N\} \tag{2.5}$$

turns out to be asymptotically equal to the confined quantum mechanical ground state energy $E^{\mathrm{Q}}_{\mathrm{conf}}$ in the following precise sense:

2.1. THEOREM (Relation of E^{DM} and $E^{\mathrm{Q}}_{\mathrm{conf}}$). *([LSY94a], Sect. 5 and 8) For some constants c_λ and c'_λ, depending only on $\lambda = N/Z$,*

$$R_U \geq E^{\mathrm{Q}}_{\mathrm{conf}}(N, Z, B) - E^{\mathrm{DM}}(N, Z, B) \geq -R_L, \tag{2.6}$$

with R_L given in (1.21) and

$$R_U = c'_\lambda \min\{Z^{5/3}B^{1/3}, Z^{8/3}[1 + \ln(Z) + (\ln(B/Z^3))^2]^{5/6}\}. \tag{2.7}$$

The DM energy fulfills the simple scaling relation

$$E^{\mathrm{DM}}(N,Z,B) = Z^3 E^{\mathrm{DM}}(\lambda,1,\eta), \tag{2.8}$$

where we introduced the parameters $\lambda = N/Z$ and $\eta = B/Z^3$. In the limit $\eta \to \infty$, $E^{\mathrm{DM}}/(\ln\eta)^2$ converges to the so-called *hyper-strong* (HS) energy $E^{\mathrm{HS}}(\lambda)$, which is the ground state energy of the functional

$$\mathcal{E}^{\mathrm{HS}}[\rho] = \int_{\mathbb{R}} \left(\frac{\mathrm{d}}{\mathrm{d}z}\sqrt{\rho(z)}\right)^2 \mathrm{d}z - \rho(0) + \frac{1}{2}\int \rho(z)^2 \mathrm{d}z \tag{2.9}$$

under the condition $\int \rho(z)\mathrm{d}z \leq \lambda$. The corresponding minimizer can be given explicitly, namely

$$\begin{aligned} \rho^{\mathrm{HS}}(z) &= \frac{2(2-\lambda)^2}{(4\sinh[(2-\lambda)|z|/4 + c(\lambda)])^2} \qquad \text{for} \quad \lambda < 2, \\ &\qquad \tanh c(\lambda) = (2-\lambda)/2, \\ \rho^{\mathrm{HS}}(z) &= 2(2+|z|)^{-2} \qquad\qquad\qquad \text{for} \quad \lambda \geq 2. \end{aligned} \tag{2.10}$$

We now discuss the relation of $\mathcal{E}^{\mathrm{DDM}}_{B,Z}$ and $\mathcal{E}^{\mathrm{DM}}$. The functional $\mathcal{E}^{\mathrm{DDM}}_{B,Z}$ is the restriction of $\mathcal{E}^{\mathrm{DM}}$ to density matrices of the form

$$\Gamma_{\mathbf{x}_\perp}(z,z') = \sum_m |\phi_m(\mathbf{x}_\perp)|^2 \Gamma_m(z,z'). \tag{2.11}$$

Therefore it is clear that

$$E^{\mathrm{DDM}}(N,Z,B) \geq E^{\mathrm{DM}}(N,Z,B). \tag{2.12}$$

In the limit $N \to \infty$ they coincide, i.e. we will show that

$$\lim_{N\to\infty} \frac{E^{\mathrm{DDM}}(N,Z,B)}{Z^3} = E^{\mathrm{DM}}(\lambda,1,\eta) \tag{2.13}$$

for all fixed λ and η. In fact, (2.13) follows immediately from Theorem 1.2 and Theorem 2.1, but it could of course also be shown directly without referring to the relation to $E^{\mathrm{Q}}_{\mathrm{conf}}$. Note that in contrast to DM, the DDM energy depends non-trivially on all the three parameters N, Z and B, like the original QM problem.

3 Properties of $\mathcal{E}^{\mathrm{DDM}}_{B,Z}$

3.1. THEOREM (Existence of a minimizer). *For each $N > 0$, $B > 0$ and $Z > 0$ there exists a minimizer Γ^{DDM} for $\mathcal{E}^{\mathrm{DDM}}_{B,Z}$ under the condition $\sum_m \mathrm{Tr}[\Gamma_m] \leq N$.*

Proof. Let $\Gamma^{(i)}$ be a minimizing sequence for $\mathcal{E}^{\mathrm{DDM}}_{B,Z}$ under the normalization condition $\sum_m \mathrm{Tr}[\Gamma_m] \leq N$, with corresponding densities $\rho^{(i)} = (\rho^{(i)}_m)_m$. Using the one-dimensional Lieb-Thirring inequality [LT76] we have

$$\int \left|\rho^{(i)}_m\right|^3 \leq \mathrm{const.}\mathrm{Tr}[-\partial_z^2 \Gamma^{(i)}_m]. \tag{3.1}$$

Moreover (cf. [LSY94a], Eq. (4.5b)),

$$\int \left(\frac{\mathrm{d}\sqrt{\rho^{(i)}_m(z)}}{\mathrm{d}z} \right)^2 \mathrm{d}z \leq \mathrm{Tr}[-\partial_z^2 \Gamma^{(i)}_m]. \tag{3.2}$$

Since the potential energy is relatively bounded with respect to the kinetic energy (compare Thm. 2.2 in [LSY94a]), the right hand sides of (3.1) and (3.2) are uniformly bounded. Hence the sequence $\rho^{(i)}_m$ is bounded in $\mathcal{L}^3(\mathbb{R}, \mathrm{d}z) \cap \mathcal{L}^1(\mathbb{R}, \mathrm{d}z)$, and $\sqrt{\rho^{(i)}_m}$ is bounded in $\mathcal{H}^1(\mathbb{R}, \mathrm{d}z)$. By the "diagonal sequence trick", there is a subsequence, again denoted by $\rho^{(i)}$, such that $\rho^{(i)}_m$ converges to some $\rho^{(\infty)}_m$ for each m, weakly in $\mathcal{L}^3(\mathbb{R}, \mathrm{d}z) \cap \mathcal{L}^p(\mathbb{R}, \mathrm{d}z)$ for some $1 < p \leq 3$ and pointwise almost everywhere. By Fatou's lemma

$$\begin{aligned} &\liminf_{i\to\infty} \sum_{m,n} \int \mathrm{d}z\mathrm{d}z' V_{m,n}(z-z') \rho^{(i)}_m(z) \rho^{(i)}_n(z) \\ &\geq \sum_{m,n} \int \mathrm{d}z\mathrm{d}z' V_{m,n}(z-z') \rho^{(\infty)}_m(z) \rho^{(\infty)}_n(z). \end{aligned} \tag{3.3}$$

Observe now that $V_m \leq C$ for some $C > 0$ and for all m. Moreover, $V_m(z) \leq 1/|z|$, so $V_m \in \mathcal{L}^p$ for all $p > 1$. By the weak convergence we can conclude that

$$\lim_{i\to\infty} \int \mathrm{d}z V_m(z) \rho^{(i)}_m(z) = \int \mathrm{d}z V_m(z) \rho^{(\infty)}_m(z) \tag{3.4}$$

for each m. Moreover, by the dominated convergence theorem, we get

$$\lim_{i\to\infty} \sum_m \int \mathrm{d}z V_m(z) \rho^{(i)}_m(z) = \sum_m \int \mathrm{d}z V_m(z) \rho^{(\infty)}_m(z). \tag{3.5}$$

Using the "diagonal sequence trick" once more, we can use the trace class property of the $\Gamma^{(i)}_m$'s to conclude that there exists a subsequence of $\Gamma^{(i)}$ and a $\Gamma^{\mathrm{DDM}} = (\Gamma^{\mathrm{DDM}}_m)_m$ such that

$$\Gamma^{(i)}_m \rightharpoonup \Gamma^{\mathrm{DDM}}_m \tag{3.6}$$

in weak operator sense, for each m. It follows from weak convergence that $0 \leq \Gamma^{\mathrm{DDM}}_m \leq 1$. Using Fatou's lemma twice, we have

$$\sum_m \mathrm{Tr}[\Gamma^{\mathrm{DDM}}_m] \leq \liminf_{i\to\infty} \sum_m \mathrm{Tr}[\Gamma^{(i)}_m] \leq N. \tag{3.7}$$

By the same argument

$$\sum_m \mathrm{Tr}[-\partial_z^2 \Gamma_z^{\mathrm{DDM}}] \leq \liminf_{i\to\infty} \sum_m \mathrm{Tr}[-\partial_z^2 \Gamma_m^{(i)}]. \tag{3.8}$$

Let now ρ_m^{DDM} denote the density of Γ_m^{DDM}. It remains to show that $\rho_m^{(\infty)} = \rho_m^{\mathrm{DDM}}$ for each m. From weak convergence it follows that

$$(1-\partial_z^2)^{1/2}\Gamma_m^{(i)}(1-\partial_z^2)^{1/2} \rightharpoonup (1-\partial_z^2)^{1/2}\Gamma_m^{\mathrm{DDM}}(1-\partial_z^2)^{1/2} \tag{3.9}$$

weakly on the dense set $\mathcal{C}_0^\infty(\mathbb{R})$. Since the operators are bounded by $\mathrm{Tr}[(1-\partial_z^2)\Gamma_m^{(i)}] \leq C$, we see that (3.9) holds weakly in $\mathcal{L}^2(\mathbb{R}, \mathrm{d}z)$. With $\eta \in \mathcal{C}_0^\infty(\mathbb{R})$ considered as a multiplication operator, it is easy to see that $(1-\partial_z^2)^{-1/2}\eta(1-\partial_z^2)^{-1/2}$ is a compact operator (it is even Hilbert-Schmidt). Thus it can be approximated in norm by finite rank operators. Using (3.9) we can therefore conclude that

$$\lim_{i\to\infty} \mathrm{Tr}[\Gamma_m^{(i)}\eta] = \mathrm{Tr}[\Gamma_m^{\mathrm{DDM}}\eta], \tag{3.10}$$

i.e. $\rho_m^{(i)} \to \rho_m^{\mathrm{DDM}}$ in the sense of distributions. Since we already know that $\rho_m^{(i)}$ converges to $\rho_m^{(\infty)}$ pointwise almost everywhere, we conclude that $\rho_m^{(\infty)} = \rho_m^{\mathrm{DDM}}$ for each m.

We have thus shown that there exists a Γ^{DDM} with $\sum_m \mathrm{Tr}[\Gamma_m^{\mathrm{DDM}}] \leq N$ and $\mathcal{E}_{B,Z}^{\mathrm{DDM}}[\Gamma^{\mathrm{DDM}}] \leq \liminf_{i\to\infty} \mathcal{E}_{B,Z}^{\mathrm{DDM}}[\Gamma^{(i)}] = E^{\mathrm{DDM}}$. □

3.2. LEMMA (Uniqueness of the density). *The density corresponding to the minimizer is unique, i.e., if there are two minimizers $\Gamma^{(1)}$ and $\Gamma^{(2)}$, their densities $\rho_m^{(1)}$ and $\rho_m^{(2)}$ are equal, for all m.*

Proof. Observe that

$$\widetilde{D}(\rho,\rho) = D(\tilde\rho,\tilde\rho), \tag{3.11}$$

where we set $\tilde\rho(\mathbf{x}) = \sum_m |\phi_m(\mathbf{x}_\perp)|^2 \rho_m(z)$. Using the positive definiteness of the Coulomb kernel and the fact that $\tilde\rho^{(1)} = \tilde\rho^{(2)}$ implies $\rho_m^{(1)} = \rho_m^{(2)}$ for all m, we immediately get the desired result. □

Having established the uniqueness of the density, we can now define a *linearized DDM functional* by

$$\mathcal{E}_{\mathrm{lin}}^{\mathrm{DDM}}[\Gamma] = \sum_m \mathrm{Tr}[h_m^{\mathrm{DDM}}\Gamma_m], \tag{3.12}$$

with the one-particle operators

$$h_m^{\mathrm{DDM}} = -\partial_z^2 - \Phi_m^{\mathrm{DDM}}(z), \tag{3.13}$$

where the potentials are given by

$$\Phi_m^{\mathrm{DDM}}(z) = ZV_m(z) - \sum_n \int \rho_n^{\mathrm{DDM}}(z')V_{m,n}(z-z')\mathrm{d}z'. \tag{3.14}$$

3.3. LEMMA (Equivalence of linearized theory). *A minimizer $\Gamma^{\rm DDM}$ for $\mathcal{E}^{\rm DDM}_{B,Z}$ under the constraint $\sum_m \mathrm{Tr}[\Gamma_m] \le N$ is also a minimizer for the linearized functional $\mathcal{E}^{\rm DDM}_{\rm lin}$ (with the same constraint).*

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

$$\mathcal{E}^{\rm DDM}_{B,Z}[\Gamma] = \mathcal{E}^{\rm DDM}_{\rm lin}[\Gamma] + \widetilde{D}(\rho_\Gamma - \rho^{\rm DDM}, \rho_\Gamma - \rho^{\rm DDM}) - \widetilde{D}(\rho^{\rm DDM}, \rho^{\rm DDM}). \tag{3.15}$$

In particular, for all $\delta > 0$,

$$\begin{aligned}\mathcal{E}^{\rm DDM}_{B,Z}[(1-\delta)\Gamma^{\rm DDM} + \delta\Gamma] \;&=\; (1-\delta)\mathcal{E}^{\rm DDM}_{\rm lin}[\Gamma^{\rm DDM}] + \delta\mathcal{E}^{\rm DDM}_{\rm lin}[\Gamma] - \widetilde{D}(\rho^{\rm DDM}, \rho^{\rm DDM}) \\ &\quad + \delta^2 \widetilde{D}(\rho_\Gamma - \rho^{\rm DDM}, \rho_\Gamma - \rho^{\rm DDM}). \end{aligned}\tag{3.16}$$

Now if there exists a $\Gamma^{(0)}$ with $\sum_m \mathrm{Tr}[\Gamma^{(0)}_m] \le N$ and $\mathcal{E}^{\rm DDM}_{\rm lin}[\Gamma^{(0)}] < \mathcal{E}^{\rm DDM}_{\rm lin}[\Gamma^{\rm DDM}]$ we can choose δ small enough to conclude that

$$\mathcal{E}^{\rm DDM}_{B,Z}[(1-\delta)\Gamma^{\rm DDM} + \delta\Gamma^{(0)}] < \mathcal{E}^{\rm DDM}_{\rm lin}[\Gamma^{\rm DDM}] - \widetilde{D}(\rho^{\rm DDM}, \rho^{\rm DDM}) = \mathcal{E}^{\rm DDM}_{B,Z}[\Gamma^{\rm DDM}], \tag{3.17}$$

which contradicts the fact that $\Gamma^{\rm DDM}$ minimizes $\mathcal{E}^{\rm DDM}_{B,Z}$. □

We now are able to construct the minimizer of $\mathcal{E}^{\rm DDM}_{B,Z}$ by means of the eigenfunctions e^i_m of the one-dimensional operators $h^{\rm DDM}_m$. If $\mu^1_m < \mu^2_m < \dots$ denote the corresponding eigenvalues, there is a $\mu \le 0$ such that

$$\Gamma^{\rm DDM}_m = \sum_{i=1}^{I_m - 1} |e^i_m\rangle\langle e^i_m| + \lambda_m |e^{I_m}_m\rangle\langle e^{I_m}_m|, \tag{3.18}$$

where $I_m = \max\{i : \mu^i_m \le \mu\}$, and $0 \le \lambda_m \le 1$ is the filling of the last level. Since λ_m is determined by the unique density $\rho^{\rm DDM}_m$, we immediately get the following corollary:

3.4. COROLLARY (Uniqueness of $\Gamma^{\rm DDM}$). *For any $B > 0$ and $Z > 0$ the minimizer of the functional $\mathcal{E}^{\rm DDM}_{B,Z}$ under the condition $\sum_m \mathrm{Tr}[\Gamma_m] \le N$ is unique.*

Note that $\Gamma^{\rm DDM}$ really depends on the three parameters N, Z and B, but we suppress this dependence for the simplicity of the notation.

Of course, the choice of μ is not unique, but I_m is unique for every m. In the following, we will choose for μ the smallest possible, i.e.

$$\mu \equiv \max\{\mu^{I_m}_m\}. \tag{3.19}$$

The energy $E^{\rm DDM}(N, Z, B)$ is a convex, non-increasing function in N. Moreover, it has the following property.

3.5. THEOREM (Differentiability of $E^{\rm DDM}$). *For $N \notin \mathbb{N}$ the energy $E^{\rm DDM}$ is differentiable in N, and the derivative is given by $\partial E^{\rm DDM}/\partial N = \mu$ with μ given above. For $N \in \mathbb{N}$, the right and left derivatives, $\partial E^{\rm DDM}/\partial N_\pm$, are given by*

$$\frac{\partial E^{\rm DDM}}{\partial N_-} = \mu, \quad \frac{\partial E^{\rm DDM}}{\partial N_+} = \min\{\mu_m^{I_m+1}\}. \tag{3.20}$$

Proof. For fixed N, Z and B define $\mathcal{E}_{\rm lin}^{\rm DDM}$ as above. Let $E_{\rm lin}(N')$ be the infimum of $\mathcal{E}_{\rm lin}^{\rm DDM}$ under the constraint $\sum_m {\rm Tr}[\Gamma_m] \leq N'$. For $0 < N_- < N < N_+$ let $\Gamma^\pm$ be the corresponding minimizers. We have, with $0 < \delta < 1$,

$$\begin{aligned} E^{\rm DDM}(N + \delta(N_\pm - N), Z, B) &\leq \mathcal{E}_{B,Z}^{\rm DDM}[(1-\delta)\Gamma^{\rm DDM} + \delta\Gamma^\pm] \\ &= E^{\rm DDM}(N,Z,B) \\ &\quad + \delta\left(E_{\rm lin}(N_\pm) - E_{\rm lin}(N)\right) + O(\delta^2). \end{aligned} \tag{3.21}$$

Dividing by $\delta(N_\pm - N)$ and taking the limit $\delta \to 0$ followed by $N_\pm \to N$, we conclude that

$$\frac{\partial E_{\rm lin}}{\partial N_-} \leq \frac{\partial E^{\rm DDM}}{\partial N_-}, \qquad \frac{\partial E^{\rm DDM}}{\partial N_+} \leq \frac{\partial E_{\rm lin}}{\partial N_+}. \tag{3.22}$$

From (3.15) we infer that $E^{\rm DDM}(N', Z, B) \geq E_{\rm lin}(N') - \widetilde{D}(\rho^{\rm DDM}, \rho^{\rm DDM})$ for all N', with equality for $N = N'$. Therefore we get the inverse inequalities in (3.22), so equality holds. The assertions of the theorem follow from

$$E_{\rm lin}(N) = \sum_{j=1}^{[N]} \mu(j) + (N - [N])\,\mu([N]+1), \tag{3.23}$$

where $[N]$ is the largest integer $\leq N$, and $\mu(j)$ is the j'th element of the set $\{\mu_m^i\}$ in increasing order. □

Corresponding to the DDM minimizer we define the *three-dimensional DDM density* as

$$\tilde\rho^{\rm DDM}(\mathbf{x}) = \sum_{m\geq 0} |\phi_m(\mathbf{x}_\perp)|^2 \rho_m^{\rm DDM}(z). \tag{3.24}$$

3.6. THEOREM (Ordering of the μ_m^i). *Assume $h_m^{\rm DDM}$ has at least M eigenvalues. Then, for $m \geq 1$,*

$$\sum_{i=1}^M \left(m\mu_{m-1}^i + (m+1)\mu_{m+1}^i - (2m+1)\mu_m^i\right) \leq -\frac{2\pi}{B}\sum_{i=1}^M \int \tilde\rho^{\rm DDM} |\phi_m e_m^i|^2 \tag{3.25}$$

(with the understanding that μ_{m-1}^i (μ_{m+1}^i) $= 0$ if $h_{m-1}^{\rm DDM}$ ($h_{m+1}^{\rm DDM}$) has less than i eigenvalues). The analogous inequality for $m = 0$ is

$$\sum_{i=1}^M \left(\mu_1^i - \mu_0^i\right) \leq Z\sum_{m=1}^M |e_0^i(0)|^2 - \frac{2\pi}{B}\sum_{i=1}^M \int \tilde\rho^{\rm DDM}|\phi_0 e_0^i|^2. \tag{3.26}$$

Proof. With $\Delta_{(2)}$ the two-dimensional Laplacian, one easily computes that

$$(2B)^{-1}\Delta_{(2)}|\phi_m|^2 = m|\phi_{m-1}|^2 + (m+1)|\phi_{m+1}|^2 - (2m+1)|\phi_m|^2 \tag{3.27}$$

for $m \geq 1$. Multiplying (3.27) with $\Phi(\mathbf{x}) = Z/|\mathbf{x}| - \tilde{\rho}^{\mathrm{DDM}} * |\mathbf{x}|^{-1}$ and integrating over $\mathbf{x}_\perp$, we therefore get, for any density matrix γ (recall the definitions (1.14), (1.15), (3.13) and (3.14)),

$$\begin{aligned}
&\mathrm{Tr}\left[\left(mh_{m-1}^{\mathrm{DDM}} + (m+1)h_{m+1}^{\mathrm{DDM}} - (2m+1)h_m^{\mathrm{DDM}}\right)\gamma\right] \\
&= -(2B)^{-1}\int \mathrm{d}\mathbf{x}\Phi(\mathbf{x})\rho_\gamma(z)\Delta_{(2)}|\phi_m(\mathbf{x}_\perp)|^2 \\
&= -\frac{2\pi}{B}\int \mathrm{d}\mathbf{x}\tilde{\rho}^{\mathrm{DDM}}|\phi_m|^2\rho_\gamma + \frac{1}{2B}\int \mathrm{d}z\Phi_m^{\mathrm{DDM}}\frac{\partial^2}{\partial z^2}\rho_\gamma,
\end{aligned} \tag{3.28}$$

where we used partial integration for the second step, and the fact that $\phi_m(\mathbf{0}) = 0$ for $m \geq 1$. To treat the last term in (3.28), note that the function

$$w \to \sum_{i=1}^{M}\int \mathrm{d}z\Phi_m^{\mathrm{DDM}}(z)|e_m^i(z+w)|^2 \tag{3.29}$$

has its maximum at $w = 0$, because otherwise one could lower the energy by shifting the eigenvectors e_m^i. Therefore the second derivative of (3.29) at $w = 0$ is negative. Setting $\gamma = \sum_{i=1}^{M}|e_m^i\rangle\langle e_m^i|$ we see that the last term in (3.28) is negative, so we can conclude that

$$\mathrm{Tr}\left[\left(mh_{m-1}^{\mathrm{DDM}} + (m+1)h_{m+1}^{\mathrm{DDM}} - (2m+1)h_m^{\mathrm{DDM}}\right)\gamma\right] \leq -\frac{2\pi}{B}\int \tilde{\rho}^{\mathrm{DDM}}|\phi_m|^2\rho_\gamma. \tag{3.30}$$

By the variational principle (3.25) holds. The proof of (3.26) is analogous, considering also the contribution from $\phi_0(\mathbf{0})$ in (3.28). □

As a corollary, we immediately get

3.7. COROLLARY (Monotonicity of $\sum_{i=1}^{M}\mu_m^i$ in m). *$\sum_{i=1}^{M}\mu_m^i$ is increasing in m for all M, and strictly increasing as long as it is < 0. Moreover, $\Gamma_m^{\mathrm{DDM}} = 0$ for $m \geq N$.*

Proof. This follows immediately from Theorem 3.6, noting that $\lim_{m\to\infty}\mu_m^i = 0$ for all i. □

3.8. Remark (Concavity of $\sum_{i=1}^{M}\mu_m^i$). The result (3.25) (together with the monotonicity) implies concavity of μ_m^1 in m. More precisely,

$$\begin{aligned}
&\tfrac{1}{2}\mu_{m-1}^1 + \tfrac{1}{2}\mu_{m+1}^1 = \\
&\frac{m}{2m+1}\mu_{m-1}^1 + \frac{m+1}{2m+1}\mu_{m+1}^1 + \frac{1}{2(2m+1)}(\mu_{m-1}^1 - \mu_{m+1}^1) \leq \mu_m^1
\end{aligned} \tag{3.31}$$

(and the same holds for $\sum_{i=1}^{M}\mu_m^i$). This is the analogue of Prop. 2.3 in [LSY94a], which states that $-\mu_1(\mathbf{x}_\perp)$ is a increasing and concave function of $|\mathbf{x}_\perp|$ (note the different sign convention).

We now introduce the parameters $\lambda = N/Z$ and $\eta = B/Z^3$. The next theorem deals with the $\eta\to\infty$ limit of $E^{\rm DDM}$ with fixed λ. To prove it we need the following Lemma.

3.9. LEMMA (Convergence to delta function). *Let $L = L(\eta)$ be the solution of the equation*

$$\eta^{1/2} = L(\eta)\sinh(L(\eta)/2). \tag{3.32}$$

Let $\psi\in\mathcal{H}^1(\mathbb{R},\mathrm{d}z)$, with $\lambda = \int|\psi|^2$ and $T = \int|\mathrm{d}\psi/\mathrm{d}z|^2$. Then, for all $m\geq 0$, $Z>0$ and $\eta = B/Z^3$,

$$\begin{aligned}\left||\psi(0)|^2 - \frac{1}{ZL^2}\int V_m(z/LZ)|\psi(z)|^2\mathrm{d}z\right|&\\ \leq \frac{1}{L}\left(\lambda\sqrt{\frac{\pi}{2}}\frac{Z^{1/2}}{(m+1)^{1/2}} + 16\lambda^{1/4}T^{3/4}\frac{(m+1)^{1/4}}{Z^{1/4}}\right).&\end{aligned} \tag{3.33}$$

Proof. After an appropriate scaling, this is a direct consequence of [BSY00], Lemma 2.1, using the estimates

$$\int|\phi_m(\mathbf{x}_\perp)|^2|\mathbf{x}_\perp|^{-1}\mathrm{d}\mathbf{x}_\perp \leq \sqrt{\frac{\pi}{2}}\frac{B^{1/2}}{(m+1)^{1/2}} \tag{3.34}$$

and

$$\int|\phi_m(\mathbf{x}_\perp)|^2|\mathbf{x}_\perp|^{1/2}\mathrm{d}\mathbf{x}_\perp \leq 2\frac{(m+1)^{1/4}}{B^{1/4}}. \tag{3.35}$$

□

3.10. THEOREM (The limit $B\gg Z^3$). *For all $\lambda>0$*

$$\lim_{\eta\to\infty}\frac{E^{\rm DDM}(\lambda Z, Z, \eta Z^3)}{Z^3(\ln\eta)^2} = E^{\rm HS}(\lambda), \tag{3.36}$$

uniformly in Z.

Remark: The uniformity in Z will be important for the proof of Theorem 3.12. It is non-trivial in contrast to DM, where one has the scaling relation (2.8), which implies that the left hand side of (3.36) (with DDM replaced by DM) is independent of Z.

Proof. The lower bound is quite easy, using the results of [LSY94a]. As shown in Section 2, we have

$$\frac{E^{\rm DDM}(\lambda Z, Z, \eta Z^3)}{Z^3} \geq \frac{E^{\rm DM}(\lambda Z, Z, \eta Z^3)}{Z^3} = E^{\rm DM}(\lambda, 1, \eta), \tag{3.37}$$

where we have used the scaling properties of E^{DM}. It is shown in [LSY94a] that the right hand side of (3.37) divided by $(\ln\eta)^2$ converges to $E^{\mathrm{HS}}(\lambda)$.

For the upper bound we assume $N\in\mathbb{N}$ for the moment. We use as trial density matrices

$$\begin{aligned}\Gamma_m(z,z') &= \frac{Z^2}{N}L\sqrt{\rho^{\mathrm{HS}}(LZz)}\sqrt{\rho^{\mathrm{HS}}(LZz')}, \quad 0\le m\le N-1\\ \Gamma_m(z,z') &= 0, \quad m\ge N,\end{aligned} \tag{3.38}$$

where ρ^{HS} is given in (2.10) and $L=L(\eta)$ is defined in (3.32). The kinetic energy is easily computed to be

$$Z^3L^2\int|\mathrm{d}\sqrt{\rho^{\mathrm{HS}}}/\mathrm{d}z|^2. \tag{3.39}$$

For the attraction term we use Lemma 3.9 to estimate

$$\begin{aligned}\frac{1}{Z^3L^2}\sum_m Z\int V_m\rho_m &\ge \frac{1}{N}\sum_{m=0}^{N-1}\left(\rho^{\mathrm{HS}}(0)-\frac{C_\lambda}{L}\left(\frac{Z^{1/2}}{(m+1)^{1/2}}+\frac{(m+1)^{1/4}}{Z^{1/4}}\right)\right)\\ &\ge \rho^{\mathrm{HS}}(0)-\frac{C'_\lambda}{L}\end{aligned} \tag{3.40}$$

for some constant C'_λ depending on λ.

For the repulsion term we first estimate

$$\sum_{0\le m,n\le N-1}V_{m,n}(z)\le\left(\frac{B}{2\pi}\right)^2\int\frac{\Theta(\sqrt{2N/B}-|\mathbf{x}_\perp|)\Theta(\sqrt{2N/B}-|\mathbf{x}'_\perp|)}{\sqrt{|\mathbf{x}_\perp-\mathbf{x}'_\perp|^2+z^2}}\mathrm{d}\mathbf{x}_\perp\mathrm{d}\mathbf{x}'_\perp, \tag{3.41}$$

which follows from monotonicity of $1/|\mathbf{x}|$ in $|\mathbf{x}_\perp|$ and the fact that $\sum_m|\phi_m|^2\le B/2\pi$. Therefore we have

$$\begin{aligned}&\frac{1}{Z^3L^2}\sum_{0\le m,n\le N-1}\int V_{m,n}(z-z')\rho_m(z)\rho_m(z')\mathrm{d}z\mathrm{d}z'\\ &\qquad\le\frac{1}{L}\xi\int f(\xi(z-z'))\rho^{\mathrm{HS}}(z)\rho^{\mathrm{HS}}(z')\mathrm{d}z\mathrm{d}z',\end{aligned} \tag{3.42}$$

where we set $\xi=(\eta/\lambda)^{1/2}/L$, and the function f is given by

$$f(z)=(2\pi)^{-2}\int\frac{\Theta(\sqrt{2}-|\mathbf{x}_\perp|)\Theta(\sqrt{2}-|\mathbf{x}'_\perp|)}{\sqrt{|\mathbf{x}_\perp-\mathbf{x}'_\perp|^2+z^2}}\mathrm{d}\mathbf{x}_\perp\mathrm{d}\mathbf{x}'_\perp. \tag{3.43}$$

We now claim that $L^{-1}\xi f(\xi z)\to\delta(z)$ as $\eta\to\infty$. Since $f(z)\le1/|z|$ we have, for any $\chi\in\mathcal{H}^1\cap\mathcal{L}^1$,

$$\left|L^{-1}\xi\int f(\xi z)\chi(z)\mathrm{d}z-\chi(0)L^{-1}\int_{-\xi}^{\xi}f(z)\mathrm{d}z\right|$$

$$= \left| L^{-1}\xi \int_{-1}^{1} f(\xi z)(\chi(z)-\chi(0))\mathrm{d}z + L^{-1}\xi \int_{|z|\geq 1} f(\xi z)\chi(z)\mathrm{d}z \right|$$

$$\leq \text{const.} L^{-1}\xi \int_{-1}^{1} f(\xi z) z^{1/2}\mathrm{d}z + L^{-1}\int_{|z|\geq 1} |\chi(z)|\mathrm{d}z \leq \text{const.} L^{-1}. \quad (3.44)$$

Now $L^{-1}\int_{|z|\leq\xi} f \to 1$ as $\eta\to\infty$, which proves our claim. And since $L(\eta)\approx \ln\eta$ for large η, this finishes the proof of Theorem 3.10, in the case where N is an integer. The proof for $N\notin\mathbb{N}$ is analogous, using (3.38) with the density matrix corresponding to $m=[N]$ multiplied by $N-[N]$ as trial density matrices. □

3.11. COROLLARY (HS limit of the density). *For fixed $\lambda = N/Z$*

$$\lim_{\eta\to\infty} \frac{1}{Z^2\ln\eta}\sum_m \rho_m^{\mathrm{DDM}}(z/Z\ln\eta) = \rho^{\mathrm{HS}}(z) \quad (3.45)$$

in the weak $\mathcal{L}^1$ sense, uniformly in Z.

Proof. The convergence of the densities in (3.45) follows from the convergence of the energies in a standard way by considering perturbations of the external potential (cf. e.g. [LSY94a]). Moreover, since the convergence in (3.36) is uniform in Z, (3.45) holds for any function $Z=Z(\beta)$, so we can conclude that (3.45) holds uniformly in Z, too. □

Using the results above we can now prove the analogue of Theorem 4.6 in [LSY94a].

3.12. THEOREM (Γ_m^{DDM} has rank at most 1 for large η). *There exists a constant C such that $\eta\geq C$ implies that Γ_m^{DDM} has rank at most 1 for all m.*

Proof. We first treat the case $\lambda<2$. From Theorems 3.5 and 3.10 and the fact that $E^{\mathrm{DDM}}(\lambda Z, Z, \eta Z^3)$ is convex in λ, we get

$$\lim_{\eta\to\infty}\frac{\mu}{Z^2(\ln\eta)^2} = \frac{dE^{\mathrm{HS}}(\lambda)}{d\lambda} < 0. \quad (3.46)$$

Suppose that μ is not the ground state energy of some h_m^{DDM}. Then $\mu\geq -Z^2/4$, because the second lowest eigenvalue of h_m^{DDM} is equal to the ground state energy of the three-dimensional operator

$$-\Delta - \Phi_m^{\mathrm{DDM}}(|\mathbf{x}|). \quad (3.47)$$

This follows because $\Phi_m^{\mathrm{DDM}}(z)$ is reflexion symmetric, so the eigenvector corresponding to the second lowest eigenvalue, $u_m(z)$, has a node at $z=0$. Therefore $u_m(|\mathbf{x}|)/|\mathbf{x}|$ is an eigenvector of (3.47), and because it does not change sign, it must be a ground state. Since $\Phi_m^{\mathrm{DDM}}(|\mathbf{x}|)\leq Z/|\mathbf{x}|$, the ground state energy of (3.47) is greater than $-Z^2/4$. So $\mu/Z^2(\ln\eta)^2$ would go to zero as $\eta\to\infty$, in contradiction to (3.46). Therefore there exists a constant C such that $\eta > C$ implies the assertion to the theorem. This constant can be chosen independent of Z, because the limit (3.46) is uniform in Z (by the same argument as in the proof of Corollary 3.11).

Now assume that $\lambda = 1 + \bar{\delta}$ for some $\bar{\delta} > 0$. From Corollary 3.11 we infer that for large enough η there is some $c_\delta > 0$ such that

$$\sum_m \int_{|z| \le c_\delta (Z \ln \eta)^{-1}} \rho_m^{\mathrm{DDM}} \ge (1 + \tfrac{1}{2}\delta) Z, \tag{3.48}$$

where $\delta = \min\{1, \bar{\delta}\}$. We now will show that for η large enough h_m^{DDM} has at most one eigenvalue, for all $0 \le m \le N$. By the same argument as above, we need to show that the three-dimensional operator (3.47) has no eigenvalues. Using $V_m(z) \le 1/|z|$ and (cf. the next section)

$$V_{m,n}(z) \ge \frac{1}{\sqrt{2}} V_{m+n}(z/\sqrt{2}) \ge \frac{1}{\sqrt{z^2 + 2(m+n+1)B^{-1}}} \ge \frac{1}{\sqrt{z^2 + 2(2N+1)B^{-1}}} \tag{3.49}$$

we can use (3.48) to estimate

$$\Phi_m^{\mathrm{DDM}}(|\mathbf{x}|) \le \frac{Z}{|\mathbf{x}|} - \frac{Z(1 + \frac{1}{2}\delta)}{\sqrt{(|\mathbf{x}| + c_\delta (Z \ln \eta)^{-1})^2 + 2(2N+1)B^{-1}}}. \tag{3.50}$$

Therefore, for η large enough,

$$\Phi_m^{\mathrm{DDM}}(|\mathbf{x}|) \le \begin{cases} Z/|\mathbf{x}| & \text{for} \quad |\mathbf{x}| \le 3\delta^{-1} c_\delta (Z \ln \eta)^{-1} \\ 0 & \text{otherwise.} \end{cases} \tag{3.51}$$

By means of the Cwikel-Lieb-Rosenbljum bound [RS78] we can estimate the number of negative eigenvalues of (3.47) as

$$\text{const.} \int |\Phi_m^{\mathrm{DDM}}(|\mathbf{x}|)|_+^{3/2} \mathrm{d}\mathbf{x} \le c'_\delta (\ln \eta)^{-3/2}, \tag{3.52}$$

which is less than 1 for η large enough. □

3.13. Remark (Chemical potential for large B/Z^3). The theorem above, together with Corollary 3.7, shows that for B/Z^3 large enough, the chemical potential is given by the ground state energy of $h_{<N-1>}^{\mathrm{DDM}}$, i.e. $\mu = \mu_{<N-1>}^1$, where $< N >$ denotes the smallest integer $\ge N$.

4 Maximal negative ionization

The DDM energy is convex and monotonously decreasing in N. Because $\widetilde{D}(\rho, \rho)$ is strictly convex in ρ, E^{DDM} is strictly convex up to some $N = N_c(Z, B)$, and constant for $N \geq N_c$. By uniqueness of Γ^{DDM} the minimizer for $N > N_c$ is equal to the one with $N = N_c$. In particular, $\sum_m \mathrm{Tr}[\Gamma_m^{\mathrm{DDM}}] = \min\{N, N_c\}$.

The "critical" N_c measures the maximal particle number that can be bound to the nucleus. We will proceed essentially as in [S00] and use Lieb's strategy [L84] to get an upper bound on N_c. In addition, the following Lemma is needed. Throughout, we use various properties of V_m stated in [BRW99], Sect. 4., and proven in [RW00].

4.1. LEMMA (Comparison of V_m and $V_{m,n}$).

$$\left(\frac{1}{V_m(z)} + \frac{1}{V_n(z)} + \frac{1}{V_m(z')} + \frac{1}{V_n(z')}\right) V_{m,n}(z - z') \geq 1 \tag{4.1}$$

Proof. Using the definition of $V_{m,n}$ it can be shown (cf. [P82]) that

$$\sqrt{2} V_{m,n}(\sqrt{2} z) = \sum_{i=0}^{m+n} c_i V_i(z) \tag{4.2}$$

for some coefficients $c_i \geq 0$ that fulfill $\sum_i c_i = 1$. Since $V_m \geq V_{m+1}$ for all m ([BRW99], 4b) we get

$$V_{m,n}(z) \geq \frac{1}{\sqrt{2}} V_{m+n}(z/\sqrt{2}) \geq \frac{1}{2} V_{m+n}(z/2), \tag{4.3}$$

where we used the fact that $aV_m(az) \leq V_m(z)$ if $a \leq 1$ ([BRW99], 4g). Moreover, using convexity of $1/V_{m+n}$ ([BRW99], 4i), we arrive at

$$V_{m,n}(z - z') \geq \left(V_{m+n}(z)^{-1} + V_{m+n}(z')^{-1}\right)^{-1}. \tag{4.4}$$

The assertion (4.1) follows if we can show that

$$\frac{1}{V_{m+n}(z)} \leq \frac{1}{V_m(z)} + \frac{1}{V_n(z)}. \tag{4.5}$$

This is of course trivial if n or m equals zero. If $n, m \geq 1$ we use $\sqrt{z^2 + m}^{-1} \geq V_m(z) \geq \sqrt{z^2 + m + 1}^{-1}$ ([BRW99], 4a) to estimate

$$\begin{aligned} \frac{1}{V_{m+n}(z)} &\leq \sqrt{z^2 + m + n + 1} \leq 2\sqrt{z^2 + (\sqrt{m} + \sqrt{n})^2/4} \\ &\leq \sqrt{z^2 + m} + \sqrt{z^2 + n} \leq \frac{1}{V_m(z)} + \frac{1}{V_n(z)}, \end{aligned} \tag{4.6}$$

which finishes the proof. □

4.2. THEOREM (Critical particle number).

$$Z \leq N_c \leq 4Z - \frac{1}{N_c} \frac{\partial E^{\mathrm{DDM}}(N_c, Z, B)}{\partial Z} \tag{4.7}$$

Remark: The factor 4 stems from the symmetrization of (4.1) in m and n. Due to this symmetrization one could expect that Lemma 4.1 holds with 1 replaced by 2 on the right hand side. This would imply that $4Z$ could be replaced by $2Z$ in (4.7).

Proof. Let e_m^i denote the eigenvectors of h_m^{DDM}, i.e.

$$h_m^{\mathrm{DDM}} e_m^i = \mu_m^i e_m^i. \tag{4.8}$$

Multiplying (4.8) with e_m^i/V_m and integrating we get

$$Z \geq \sum_n \int \frac{1}{V_m(z)} e_m^i(z)^2 V_{m,n}(z-z')\rho_n^{\mathrm{DDM}}(z')\mathrm{d}z\mathrm{d}z' + \langle e_m^i|\frac{1}{V_m}(-\partial_z^2)|e_m^i\rangle, \tag{4.9}$$

where we used that $\mu_m^i \leq 0$. Since $1/V_m$ is convex and $|z|V_m(z) \to 1$ as $|z| \to \infty$ we have $|(1/V_m)'| \leq 1$. Using this and partial integration we can estimate the last term in (4.9) by

$$\begin{aligned} \langle e_m^i|\frac{1}{V_m}(-\partial_z^2)|e_m^i\rangle &= \langle e_m^i V_m^{-1/2}| - \partial_z^2 - \frac{1}{4}\left|\frac{V_m'}{V_m}\right|^2 |e_m^i V_m^{-1/2}\rangle \\ &\geq -\frac{1}{4}\int V_m(z) e_m^i(z)^2 \mathrm{d}z. \end{aligned} \tag{4.10}$$

Summing over all m and i (and, according to Eq. (3.18), multiplying the factor corresponding to the largest μ_m^i by λ_m), we arrive at

$$NZ \geq \sum_{m,n} \int \frac{1}{V_m(z)} \rho_m^{\mathrm{DDM}}(z) V_{m,n}(z-z')\rho_n^{\mathrm{DDM}}(z')\mathrm{d}z\mathrm{d}z' - \frac{1}{4}\sum_m \int V_m \rho_m^{\mathrm{DDM}}. \tag{4.11}$$

Note that the last term in (4.11) is equal to $\partial E^{\mathrm{DDM}}/\partial Z$. To treat the first term in (4.11) we use symmetry and Lemma 4.1 to get

$$\begin{aligned} &\sum_{m,n} \int \frac{1}{V_m(z)} \rho_m^{\mathrm{DDM}}(z) V_{m,n}(z-z')\rho_n^{\mathrm{DDM}}(z')\mathrm{d}z\mathrm{d}z' \\ &= \frac{1}{4}\sum_{m,n} \int \left(\frac{1}{V_m(z)} + \frac{1}{V_n(z)} + \frac{1}{V_m(z')} + \frac{1}{V_n(z')}\right) \\ &\qquad \times \rho_m^{\mathrm{DDM}}(z) V_{m,n}(z-z')\rho_n^{\mathrm{DDM}}(z')\mathrm{d}z\mathrm{d}z' \geq \frac{1}{4}N^2. \end{aligned} \tag{4.12}$$

Inserting this into (4.11) and dividing by $N/4$ we arrive at

$$N \leq 4Z - \frac{1}{N}\frac{\partial E^{\mathrm{DDM}}}{\partial Z}. \tag{4.13}$$

The lower bound on N_c is quite easy. We just have to show that $h^{\mathrm{DDM}}_{[N+1]}$ has a bound state if $N < Z$. Using $\psi(z) = \exp(-a|z|)$ with $a > 0$ as a trial vector we compute

$$\begin{aligned}
&\langle\psi|h^{\mathrm{DDM}}_{[N+1]}|\psi\rangle \\
&= a - Z\int V_{[N+1]}(z)e^{-2a|z|}\mathrm{d}z + \sum_n \int V_{n,[N+1]}(z-z')\rho^{\mathrm{DDM}}_n(z')e^{-2a|z|}\mathrm{d}z\mathrm{d}z' \\
&\leq a - Z\int V_{[N+1]}(z)e^{-2a|z|}\mathrm{d}z + N\max_{n\leq N}\int V_{n,[N+1]}(z)e^{-2a|z|}\mathrm{d}z. \qquad (4.14)
\end{aligned}$$

Since

$$\lim_{a\to 0}\frac{1}{\ln(1/a)}\int V_{[N+1]}e^{-2a|z|} = \lim_{a\to 0}\frac{1}{\ln(1/a)}\int V_{n,[N+1]}e^{-2a|z|} = 1, \qquad (4.15)$$

$\langle\psi|h^{\mathrm{DDM}}_{[N+1]}|\psi\rangle$ will be negative for small enough a, if $N < Z$. $\square$

4.3. Remark (Explicit bound on N_c). The concavity of E^{DDM} in Z implies that $\partial E^{\mathrm{DDM}}(N,Z,B)/\partial Z \geq E^{\mathrm{DDM}}(N,2Z,B)/Z$. Using (2.12) and the bounds on E^{DM} given in [LSY94a], Thm. 4.8, (4.7) implies the upper bound

$$N_c \leq 4Z\left(1 + C\min\left\{(B/Z^3)^{2/5}, 1 + [\ln(B/Z^3)]^2\right\}\right) \qquad (4.16)$$

for some constant C independent of Z and B.

4.4. Remark (Upper bound on N_c^{DM}). The upper bound (4.16) holds also for N_c^{DM}, the critical particle number in the DM theory. In fact, the convergence in (2.13) implies that

$$N_c^{\mathrm{DM}} \leq Z\left(\liminf_{Z\to\infty}\frac{N_c(Z,\eta Z^3)}{Z}\right) \qquad (4.17)$$

for all fixed $\eta = B/Z^3$.

5 Upper bound to the QM energy

We now show that E^{DDM} is an upper bound to the quantum mechanical ground state energy. In fact it is even an upper bound to $E^{\mathrm{Q}}_{\mathrm{conf}}$. By Lieb's variational principle [L81]

$$E^{\mathrm{Q}} \leq \mathrm{Tr}[(H_{\mathbf{A}} - Z|\mathbf{x}|^{-1})\gamma] + \frac{1}{2}\int\frac{\gamma(\mathbf{x},\mathbf{x})\gamma(\mathbf{x}',\mathbf{x}') - |\gamma(\mathbf{x},\mathbf{x}')|^2}{|\mathbf{x}-\mathbf{x}'|}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \qquad (5.1)$$

for all density matrices $0 \leq \gamma \leq 1$ with $\mathrm{Tr}[\gamma] \leq N$. We choose

$$\gamma(\mathbf{x},\mathbf{x}') = \sum_m \phi_m(\mathbf{x}_\perp)\overline{\phi_m}(\mathbf{x}'_\perp)\Gamma_m(z,z'). \qquad (5.2)$$

Since $\Pi_0\gamma\Pi_0 = \gamma$, we get an upper bound even for $E^{\mathrm{Q}}_{\mathrm{conf}}$. Omitting the negative "exchange term", we compute

$$E^{\mathrm{Q}}_{\mathrm{conf}}(N, Z, B) \leq \mathcal{E}^{\mathrm{DDM}}_{B,Z}[\Gamma], \tag{5.3}$$

where $\Gamma = (\Gamma_m)_m$. Note that $\mathrm{Tr}[\gamma] = \sum_m \mathrm{Tr}[\Gamma_m]$. Therefore we immediately conclude that

$$E^{\mathrm{Q}}_{\mathrm{conf}}(N, Z, B) \leq E^{\mathrm{DDM}}(N, Z, B). \tag{5.4}$$

6 Lower bound to the QM energy

To get a lower bound on the QM energy we need to estimate the two-body interaction potential in terms of one-body potentials. One way to do this is to use the Lieb-Oxford inequality [LO81] together with the positive definiteness of the Coulomb kernel:

$$\langle\Psi|\sum_{i<j}|\mathbf{x}_i - \mathbf{x}_j|^{-1}\Psi\rangle \geq 2D(\rho, \rho_\Psi) - D(\rho, \rho) - 1.68\int \rho_\Psi^{4/3}, \tag{6.1}$$

where we can choose $\rho = \tilde{\rho}^{\mathrm{DDM}}$. However, if Ψ is an (approximate) ground state wave function in the lowest Landau band, the error term $\int \rho_\Psi^{4/3}$ will in general be greater than the energy itself. More precisely, if γ_Ψ denotes the one-particle density matrix of Ψ, we can estimate

$$\begin{aligned}\int \rho_\Psi^{4/3} &\leq \left(\int \rho_\Psi^3\right)^{1/6}\left(\int \rho_\Psi\right)^{5/6} \\ &\leq \left(\frac{3}{\pi^2}B^2\mathrm{Tr}[-\partial_z^2\gamma_\Psi]\right)^{1/6} N^{5/6} \\ &\leq \mathrm{const.}Z^{1/5}N^{14/15}B^{2/5},\end{aligned} \tag{6.2}$$

where we used [LSY94a], Lemma 4.2, to estimate $\int \rho_\Psi^3$ and the kinetic energy. For large enough B this bound is of no use.

That is why we follow the method of [LSY94a] to get an improved bound for large B. Their result is that for wave functions Ψ that satisfy $\langle\Psi|H\Psi\rangle < 0$ the bound

$$\langle\Psi|\sum_{i<j}|\mathbf{x}_i - \mathbf{x}_j|^{-1}\Psi\rangle \geq 2D(\rho^{\mathrm{DM}}, \rho_\Psi) - D(\rho^{\mathrm{DM}}, \rho^{\mathrm{DM}}) - c_\lambda Z^{8/3}\left(1 + (\ln\eta)^2\right) \tag{6.3}$$

holds. The proof of this result uses only properties of ρ^{DM} which hold also for $\tilde{\rho}^{\mathrm{DDM}}$. Therefore (6.3) holds also with ρ^{DM} replaced by $\tilde{\rho}^{\mathrm{DDM}}$, possibly with a different constant. So we can estimate

$$\begin{aligned}E^{\mathrm{Q}}_{\mathrm{conf}}(N, Z, B) \geq\ & \inf_\Psi \langle\Psi|\sum_i \left(H^{(i)}_{\mathbf{A}} - Z/|\mathbf{x}_i| + \tilde{\rho}^{\mathrm{DDM}} * |\mathbf{x}_i|^{-1}\right)\Psi\rangle \\ & - D(\tilde{\rho}^{\mathrm{DDM}}, \tilde{\rho}^{\mathrm{DDM}}) - R_L,\end{aligned} \tag{6.4}$$

where the infimum is over all Ψ with $\Pi_0^N \Psi = \Psi$ and $\|\Psi\| = 1$, and

$$R_L = c_\lambda \min\{Z^{17/15} B^{2/5}, Z^{8/3}\left(1 + (\ln \eta)^2\right)\}. \tag{6.5}$$

Because $H_{\mathbf{A}} - Z/|\mathbf{x}| + \tilde{\rho}^{\mathrm{DDM}} * |\mathbf{x}|^{-1}$ is a one-particle operator that is invariant under rotations around the z-axis, we can restrict ourselves to considering Slater determinants of angular momentum eigenfunctions, which leads to

$$\begin{aligned} E^{\mathrm{Q}}_{\mathrm{conf}}(N, Z, B) &\geq \inf_{\Gamma} \mathcal{E}^{\mathrm{DDM}}_{\mathrm{lin}}[\Gamma] - \widetilde{D}(\rho^{\mathrm{DDM}}, \rho^{\mathrm{DDM}}) - R_L \\ &= E^{\mathrm{DDM}}(N, Z, B) - R_L. \end{aligned} \tag{6.6}$$

6.1. Remark (Magnitude of the "exchange term"). One may ask for the optimal magnitude of R_L such that a bound of the form (6.6) is valid. R_L is an upper bound on the difference between $E^{\mathrm{Q}}_{\mathrm{conf}}$ and E^{DDM}, which is given by the exchange energy

$$I_\Psi = D(\rho_\Psi, \rho_\Psi) - \langle \Psi | \sum_{i<j} |\mathbf{x}_i - \mathbf{x}_j|^{-1} \Psi \rangle, \tag{6.7}$$

where Ψ is an (approximate) ground state wave function of H. The exchange energy is roughly N times the self energy of the charge distribution of one particle. This distribution has the shape of a cylinder with diameter $R \sim B^{-1/2}$ and length $L \sim \max\{Z^{-2/5} B^{-1/5}, Z^{-1} \ln(B/Z^3)^{-1}\}$, if we assume $N \sim Z$ (see also [LSY95] for heuristic arguments). Note that $L \gg R$ is equivalent to $B \gg Z^{4/3}$. In this case, we expect an exchange energy of the order

$$\begin{aligned} Z L^{-1} \ln(L/R) &\sim Z^{7/5} B^{1/5} \ln(B/Z^{4/3}) \quad \text{for} \quad Z^{4/3} \ll B \leq Z^3 \\ Z L^{-1} \ln(L/R) &\sim Z^2 \ln(B/Z^3) \ln(B/Z^2) \quad \text{for} \quad B \gg Z^3. \end{aligned} \tag{6.8}$$

Hence the exchange energy should be of order $Z^{1/2} (E^{\mathrm{DDM}})^{1/2} \times$ some factor logarithmic in B. We conjecture that (at least for appropriate Ψ in the lowest Landau band)

$$I_\Psi \leq \text{const.} \frac{1}{B} \int \rho_\Psi^2 \times \text{ some factor logarithmic in } B, \tag{6.9}$$

which is precisely of the correct order (6.8). This is in accordance with results on the homogeneous electron gas in a magnetic field [DG71, FGPY92].

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