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ASYMPTOTICS OF HEAVY ATOMS IN HIGH MAGNETIC FIELDS: I. LOWEST LANDAU BAND REGIONS

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Abstract: The ground state energy of an atom of nuclear charge Ze in a magnetic field B is evaluated exactly to leading order as $Z \to \infty$. In this and a companion work [28] we show that there are 5 regions as $Z \to \infty$: $B \ll Z^{4/3}$, $B \sim Z^{4/3}$, $Z^{4/3} \ll B \ll Z^3$, $B \sim Z^3$, $B \gg Z^3$. Regions 1,2,3,4 (and conceivably 5) are relevant for neutron stars. Different regions have different physics and different asymptotic theories. Regions 1,2,3 are described by a simple density functional theory of the semiclassical Thomas-Fermi form. Here we concentrate mainly on regions 4,5 which cannot be so described, although 3,4,5 have the common feature (as shown here) that essentially all electrons are in the lowest Landau band. Region 5 does have, however, a simple non-classical density functional theory (which can be solved exactly). Region 4 does not, but, surprisingly it can be described by a novel density *matrix* functional theory!

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I. INTRODUCTION

The observed characteristics of pulsars agree well with the theory that they are in fact rapidly rotating neutron stars endowed with a surface magnetic field of the order $10^{12} - 10^{13}$ G or even stronger [1]. This field results, presumably, from the trapping of magnetic field lines during the gravitational collapse from which the neutron star emerged, and it is huge by earthly standards. The strongest stationary fields yet produced in the laboratory are of the order 10^6 G, whereas fields as large as 10^7 G can, so far, only be sustained for a few milliseconds [2,3]. More importantly, the magnetic field of a neutron star is large compared with the natural atomic unit $B^* = m_e^2 e^3 c/\hbar^3 = 2.35 \times 10^9$ G, which is the field for which the lowest cyclotron (or Landau) energy of an electron, $\frac{1}{2}\hbar Be/m_e c$, is equal to the Rydberg energy, $\frac{1}{2}m_e e^4/\hbar^2$, of a hydrogen atom. In fields of such strength the magnetic forces are at least as important as the Coulomb forces and have a decisive effect on the structure of matter. Since B is 10^3–10^4 times as large as the natural unit B^*, an asymptotic analysis in B is certainly called for.

The interior of a neutron star is presumably composed of highly dense nuclear matter with an exotic mixture of elementary particles at the core. On the other hand the outermost surface layer, through which all information about the interior has to pass, is believed to consist mainly of iron atoms. Iron has a nuclear charge number Z and an electron number N equal to 26 — which is large enough to justify an asymptotic treatment. The properties of heavy atoms in high magnetic fields are thus of considerable interest in astrophysics and have been studied by a number of authors using a variety of approximation methods [4-26] since the discovery of pulsars in the late sixties. Among the pioneering papers on this subject those of Kadomtsev [4], Ruderman [6] and Mueller, Rau and Spruch [7] should particularly be mentioned. The review article of Ruderman [12] summarizes the heuristic picture that emerged from these early investigations.

Although the above mentioned works provide valuable insights, there remained considerable uncertainty about the status of the approximations used, and it seemed desirable to supplement them with precise statements about the qualitatively different regimes of parameters and the exact leading approximation in each regime. In [27] we announced the results of such an analysis of the ground state properties of the atomic Hamiltonian with a homogeneous magnetic field of strength B in the asymptotic limit when Z, N, and B tend to infinity. The present paper contains the details of this work for the case that the field B is strong enough to confine the electrons to the lowest Landau band in leading order. The remaining cases, with partial overlap with the one treated here, are the subject of a separate publication [28].

From the mathematical point of view the present paper is the more interesting part of our work. It contains a novel construct — the single-particle density matrix theory of Sect. IV — that is half way between the full quantum theory and its semiclassical approximation. It reduces the problem to the computation of a fixed, finite number of functions instead of (as in Hartree-Fock theory) a number that tends to infinity as the size of the atom tends to infinity. It resolves a problem that at first seemed to us to be beyond the reach of exact asymptotic analysis.

The $Z \to \infty$ limit of the ground state of ordinary matter without a magnetic field was studied rigorously in [29-31] and shown to be described exactly by Thomas-Fermi (TF) theory. Since TF theory is already fairly accurate for iron with $Z = 26$, the leading contribution for $Z \to \infty$ to the energy in a magnetic field can be expected to be relevant also for the surface properties of a neutron star. Before we turn to a discussion of this asymptotic, heavy atom, regime we should mention that there also exists considerable physics literature on hydrogen and other light atoms in high magnetic fields, cf., e.g., [32-37]. The mathematically rigorous paper [38] also deals mainly with hydrogen but contains several interesting theorems for atoms of arbitrary size.

For the convenience of the reader we now give a brief summary of our main results including the cases treated in [28]. For a more detailed survey we refer to [27] and [39].

Our starting point is the Pauli Hamiltonian for an N-electron atom with nuclear charge Ze in a magnetic field with vector potential $\mathbf{A}$ such that curl $\mathbf{A} = \mathbf{B}$:

$$H_N = \sum_{i=1}^{N} \left\{ (\mathbf{p}^i + \mathbf{A}(x^i))^2 + \boldsymbol{\sigma}^i \cdot \mathbf{B} - Z|x^i|^{-1} \right\} + \sum_{1 \le i < j \le N} |x^i - x^j|^{-1}. \tag{1.1}$$

As usual, we assume the nucleus to be fixed in space (i.e., at the origin), which amounts to saying that the nuclear mass is infinitely larger than m_e. For hydrogen the ratio is 1836, and otherwise it is roughly proportional to Z. H_N operates on the Hilbert space $\mathcal{H}_N = \bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$ of antisymmetric (fermionic) spinor valued functions. Here $\boldsymbol{\sigma}$ stands for the Pauli spin matrices, and $\mathbf{p} = -i\nabla$. The superscript index i denotes the particle label (i.e., the factor in the wedge product on which the operators act), and $x^i \in \mathbf{R}^3$. Our units are such that $\hbar = c = 2m_e = e = 1$. The electron charge is $-e$, hence the $+\mathbf{A}(x)$ appearing in (1.1). We consider only the case of a constant magnetic field $\mathbf{B} = (0, 0, B)$, $B \ge 0$, and choose the symmetric gauge with $\mathbf{A}(x) = \frac{1}{2}\mathbf{B} \times x$. Note that B now denotes the value of the field in units of $4B^*$.

We are interested in the ground state energy

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

and the quantum ground-state electron density ρ^{Q}

$$\rho^{\mathrm{Q}}(x) := \rho_\Psi(x) := N \sum_{s^i = \pm 1/2} \int \left| \Psi(x, x^2, \ldots, x^N; s^1, \ldots, s^N) \right|^2 dx^2 \cdots dx^N \tag{1.3}$$

where Ψ is a quantum ground state wave function †, $s^i = \pm 1/2$ are spin variables, and we have suppressed the dependence on N, Z and B. Note: *unless stated otherwise, all integrals are over* $\mathbf{R}^3$. It turns out that the asymptotic limits of these quantities as $Z \to \infty$, with B depending on Z, and N/Z fixed, *can be described exactly* in terms of fairly simple functionals of the density alone, or, in some cases, of density *matrices* of a particular kind. More precisely, the energy $E^{\rm Q}$ and the density $\rho^{\rm Q}$ converge, after a suitable scaling, respectively to the infimum and to the unique minimizing density of the appropriate functional as $Z \to \infty$.

There are *five* types of such functionals corresponding to five asymptotic regimes of the parameters. In describing them it is convenient to use the notation $B \ll Z^n$ to indicate that $B/Z^n \to 0$ as $Z \to \infty$, and write $B \sim Z^n$ if $B/Z^n \to$ const. $\neq 0$ in this limit. The five parameter regions are the following:

Region 1: $B \ll Z^{4/3}$: The effect of the magnetic field is negligible. Standard TF theory with $B = 0$ can be applied.

Region 2: $B \sim Z^{4/3}$: A modified B-dependent TF theory is asymptotically exact. The atomic radius behaves as $Z^{-1/3}$ as in standard TF theory.

Region 3: $Z^{4/3} \ll B \ll Z^3$: The magnetic field is so strong that it confines the electrons to the lowest Landau band. Semiclassical analysis is still possible, leading to a simplified version of the B-dependent TF functional of region 2. The atom shrinks with increasing B; the radius is proportional to $Z^{1/5}B^{-2/5} = Z^{-1/3}(B/Z^{4/3})^{-2/5}$.

In all three regions 1, 2 and 3 the electronic density of an atom is *spherical* to leading order, and stable atoms are approximately neutral. *Although B affects the energy and density to leading order, it does not spoil the sphericity!!* The analysis in these regions is semiclassical with $(B/Z^3)^{1/5}$ playing the role of an effective Planck's constant.

Region 4: $B \sim Z^3$: The atom is no longer spherical, but has the form of a long cylinder with a radius smaller than $(2N/B)^{1/2}$. The length scale along the field is Z^{-1}. Semiclassical analysis breaks down, and the asymptotic theory is given by a new type of functional of one-particle density matrices. For sufficiently large values of B/Z^3 it reduces to a functional of the density alone.

Region 5: $B \gg Z^3$: The atom is essentially a one-dimensional "needle". The length scale is $Z^{-1}[\ln(B/Z^3)]^{-1}$, whereas the effective range of the Coulomb forces (i.e., the distance over which the Coulomb forces contribute to the total energy in leading order) is smaller by a factor

† To simplify the discussion we assume that a unique ground state exists. It is in fact not necessary to know this, however, for our limit theorems apply also to "approximate ground states" in the sense of [30], Sect. III.

$[\ln(B/Z^3)]^{-1}$. Consequently, in the limit $B/Z^3 \to \infty$ *the Coulomb potential reduces to a delta function* and the density and the ground state energy can be given in *closed form.* The maximum number of electrons that the nucleus can bind is now $N = 2Z$, in sharp contrast to the cases 1–3 where only Z electrons can be bound to leading order. This is closely related to enhanced binding — as discussed in Sect. IX.

Regions 4 and 5 will mainly concern us in the present paper. We note that $B/B^* \approx 10^4 \approx (26)^3 = Z^3$, so regions 3 and 4 are of direct physical interest. Eventually, region 5 might prove to be physically important. One might question the physical importance of relativistic effects, which are neglected here. It it is believed [6] that they do not play an important role, at least until $B/B^* = \alpha^{-2} = (137)^2 \approx (26)^3$, which is the value of B for which $m_e c^2 = \hbar\times$(cyclotron frequency)$= \hbar Be/m_e c$. It can be argued, however, that relativistic effects are not crucial even for very much larger values of B because the interesting electronic motion is in the direction parallel to the field; the energy of this motion depends on B only in the combination $\ln(B/Z^3)$ for large B. The perpendicular motion is frozen into the lowest Landau level (which anyway is largely insensitive to relativistic corrections).

For later reference, we include a few more details about the semiclassical regions 1–3 considered in [28]. In a TF type theory [31] one considers a functional $\mathcal{E}[\rho]$ of a one-particle density $\rho(x)$ given by

$$\mathcal{E}[\rho] = \int \tau(\rho(x))dx - Z\int |x|^{-1}\rho(x)dx + D(\rho,\rho), \tag{1.4}$$

with the notation

$$D(f,g) = \tfrac{1}{2}\int\int f(x)g(y)|x-y|^{-1}dxdy. \tag{1.5}$$

Here τ is some positive convex function that satisfies $\tau(0) = \tau'(0) = 0$ and grows at least as fast as $\rho^{\frac{3}{2}+\varepsilon}$ at ∞ to ensure that $\mathcal{E}$ is bounded below. The energy corresponding to such a functional and a given electron number N is the infimum of $\mathcal{E}[\rho]$ over all positive ρ with $\int \rho(x)dx \le N$.

The original idea behind TF theory is that for large atoms the electrons should behave locally as a free Fermi gas. Hence, if τ is chosen to be the kinetic energy of this gas as a function of the density the TF energy should give a good approximation to the true ground state energy. In the case of conventional TF theory with $B = 0$ one has $\tau(\rho) = \tau_0(\rho) = \frac{3}{5}(3\pi^2)^{2/3}\rho^{5/3}$. For free electrons in a magnetic field the kinetic energy is more complicated. It is coveniently described in terms of its Legendre transform (pressure); one has $\tau(\rho) = \tau_B(\rho) = \sup_v[\rho v - P_B(\rho)]$ with

$$P_B(v) = 2^{-1/2}(3\pi^2)^{-1}B[v^{3/2} + 2\sum_{\nu\ge1}[v - 2B\nu]_+^{3/2}], \tag{1.6}$$

where $[t]_+ = t$ if $t \geq 0$ and 0 if $t < 0$. The function τ_B converges to the simpler function τ_0 if $B \to 0$. For large B (or small ρ) it simplifies also and becomes equal to $\tau_\infty(\rho) = \frac{4}{3}\pi^4\rho^3/B^2$.

We shall refer to the TF functional with the kinetic energy τ_B as the **magnetic Thomas-Fermi** (MTF) functional and denote it by $\mathcal{E}^{\rm MTF}$. The TF functional with τ_∞ is called the **strong Thomas-Fermi** (STF) functional, denoted $\mathcal{E}^{\rm STF}$, whereas the usual functional with τ_0 is denoted $\mathcal{E}^{\rm TF}$. For the corresponding TF energies we write $E^{\rm MTF}(N,Z,B)$, $E^{\rm STF}(N,Z,B)$ and $E^{\rm TF}(N,Z)$, respectively. These energies have simple scaling properties:

Reg. 1 $$E^{\rm TF}(N,Z) = Z^{7/3}E^{\rm TF}(N/Z,1), \tag{1.7}$$

Reg. 2 $$E^{\rm MTF}(N,Z,B) = Z^{7/3}E^{\rm MTF}(N/Z,1,B/Z^{4/3}), \tag{1.8}$$

Reg. 3 $$E^{\rm STF}(N,Z,B) = Z^{7/3}(B/Z^{4/3})^{2/5}E^{\rm STF}(N/Z,1,1), \tag{1.9}$$

and corresponding relations hold also for the densities. Hence $\mathcal{E}^{\rm TF}$ has only one nontrivial parameter, $\lambda := N/Z$, $\mathcal{E}^{\rm MTF}$ has two, namely λ and $\beta := B/Z^{4/3}$, whereas $\mathcal{E}^{\rm STF}$ has again only one, namely λ. Moreover,

$$\lim_{\beta\to 0} E^{\rm MTF}(\lambda,1,\beta) = E^{TF}(\lambda,1) \tag{1.10}$$

and

$$\lim_{\beta\to\infty} E^{\rm MTF}(\lambda,1,\beta)/\beta^{2/5} = E^{\rm STF}(\lambda,1,1). \tag{1.11}$$

The basic result of [28] on the parameter regions 1, 2, 3 is the following[†]:

1.1. THEOREM (Energy asymptotics for regions 1,2,3). *Let N/Z be fixed and suppose $B/Z^3 \to 0$ as $Z \to \infty$. Then*

$$E^{\rm Q}(N,Z,B)/E^{\rm MTF}(N,Z,B) \to 1 \qquad \textit{as} \quad Z\to\infty.$$

Note that although this is a statement about $E^{\rm MTF}$, it describes the relation of $E^{\rm TF}$ and $E^{\rm STF}$ to $E^{\rm Q}$ as well because of (1.10) and (1.11), and thus covers all three regions 1–3. For the corresponding limit theorem for the densities we refer to [27] and [39].

Theorem 1.1 above generalizes Theorem 1 of [23], which is the analogous statement for $B/Z^{4/3}$ fixed. The generalization requires an extension of the Lieb-Thirring inequality [40] for the sum of the negative eigenvalues of a one-particle Hamiltonian with a magnetic field.

We conclude this summary of the results of [28] with a few historical remarks. TF theory with a magnetic field was apparently first written down in [4]. In the present terminology this was

[†] In this and the following theorems $N/Z := \lambda$ is fixed for convenience, but it is a trivial matter to relax this condition to $N/Z \to \lambda$ as $Z \to \infty$

the STF theory, where only the lowest Landau band for the electrons is considered. It was further studied by physicists in several publications, e.g., [7, 11, 13, 15, 19, 21, 24]. The earliest references to a TF theory taking all Landau levels into account, i.e., the MTF theory, are probably [17] and [18]. This theory is also discussed in [22, 25] together with its extension to a Thomas-Fermi-Dirac theory. The first rigorous results on its relation to quantum mechanics were obtained in [23].

We now turn to the discussion of regions 4 and 5, which are not covered by TF type theories. A basic fact, which simplifies the analysis in these regions (and also in region 3) is that for $B \gg Z^{4/3}$ the electrons are confined to the lowest Landau band in leading order. To state this result more precisely we recall first that the spectrum of the Pauli Hamiltonian on $L^2(\mathbf{R}^3;\mathbf{C}^2)$ for one electron in the magnetic field $\mathbf{B}$,

$$H_{\mathbf{A}} := (\mathbf{p}+\mathbf{A}(x))^2 + \mathbf{B}\cdot\boldsymbol{\sigma} = ((\mathbf{p}+\mathbf{A}(x))\cdot\boldsymbol{\sigma})^2, \tag{1.12}$$

with $\mathbf{A} = \mathbf{B}\times x/2$ as before, is given by

$$\epsilon_{p\alpha s} = 2\left(\alpha + \frac{1}{2} + s\right)B + p^2, \tag{1.13}$$

where α is a non-negative integer, $s = \pm 1/2$ is the spin component and p the momentum component along the magnetic field [41]. The eigenspace corresponding to (1.13) for fixed $\nu = \alpha + \frac{1}{2} + s$ is called the ν^{th} Landau band. In the lowest Landau band the density of states per unit area perpendicular to the field is $B/(2\pi)$, while for higher bands it is twice as large due to spin degeneracy.

The projector Π_0 on the lowest Landau band with $\nu = 0$ is given by the kernel (see e.g. [25], Appendix)

$$\Pi_0(x,x') = \frac{B}{2\pi}\exp\left\{\frac{i}{2}(x_\perp \times x'_\perp)\cdot\mathbf{B} - \tfrac{1}{4}(x_\perp - x'_\perp)^2 B\right\}\delta(x_3 - x'_3)P^{\downarrow}, \tag{1.14}$$

where $x_\perp = (x_1, x_2)$ is the component of $x \in \mathbf{R}^3$ perpendicular to the field and $P^{\downarrow}$ is the projector in the vectors in $\mathbf{C}^2$ with spin component $s = -\frac{1}{2}$.

The projector in the physical Hilbert space $\bigwedge^N L^2(\mathbf{R}^3;\mathbf{C}^2)$ onto the subspace where all electrons are in the lowest Landau band is the N'th tensorial power of Π_0 and will be denoted Π_0^N.

An important step in the proof of the limit theorems discussed further below is the following key result on the asymptotic confinement of the electrons to the lowest Landau band. It is proved in Sect. VI.

1.2. THEOREM (Confinement to lowest Landau band). *Define the ground state energy for electrons restricted to the lowest Landau band to be*

$$E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B) = \inf\{(\Psi, H_N\Psi) : \quad \Pi_0^N\Psi = \Psi \quad \textit{and} \quad (\Psi,\Psi) = 1\} \tag{1.15}$$

and let $E^{\mathrm{Q}}(N,Z,B)$ denote the usual unrestricted ground state energy for H_N. We make the additional assumption that

$$\lambda = N/Z \leq \Lambda$$

for some arbitrary, but henceforth fixed number $\Lambda > 0$. As before $\beta = B/Z^{4/3}$.

Our conclusion is that there is some constant $\delta = \delta(\lambda^{2/3}\beta, \Lambda)$ such that $\delta(\lambda^{2/3}\beta, \Lambda) \to 0$ as $\lambda^{2/3}\beta \to \infty$ and

$$(1-\delta)E^{\mathrm{Q}}(N,Z,B) \geq E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B). \tag{1.16}$$

Since $E^{\mathrm{Q}}_{\mathrm{conf}} \geq E^{\mathrm{Q}}$ (by definition), we have in particular that $E^{\mathrm{Q}}/E^{Q}_{\mathrm{conf}} \to 1$ as $\lambda^{2/3}\beta \to \infty$.

Theorem 1.2 amounts to the assertion that the ground state energy can be calculated (to leading order in β^{-1}) by confining all the electrons to the lowest Landau band. It is not asserted that $\Pi_0^N\Psi = \Psi$ for the true ground state of H_N. One immediate consequence should be noted right away: In the lowest Landau band the spin points in a fixed direction and hence *we can forget about the spin* when discussing regions 3, 4 and 5. Henceforth, the arena of the game will therefore simply be $\bigwedge^N L^2(\mathbf{R}^3)$ rather than $\bigwedge^N L^2(\mathbf{R}^3;\mathbf{C}^2)$.

Let us now consider the ground state wave function Ψ of an atom with large N and Z in a field such that $B/Z^{4/3}$ is also large but B/Z^3 not necessarily small. According to Theorem 1.2 we may, to leading order, assume that all electrons are in the lowest Landau band. In this band the kinetic energy associated with the motion along the field (including the spin contribution) is zero, which means that

$$\Pi_0 H_{\mathbf{A}} \Pi_0 = -\frac{\partial^2}{\partial x_3^2}\Pi_0 \tag{1.17}$$

Anticipating the fact that all exchange and correlation terms can be neglected for Z large enough (which, however, is by no means easy to prove when $B \gg Z^5$), we can thus reasonably expect that $E^{\mathrm{Q}} = (\Psi, H_N\Psi)$ is correctly given to leading order by the expression

$$\int -\frac{\partial^2}{\partial x_3^2} K_\Psi(x_\perp, x_3; x_\perp, x_3')|_{x_3'=x_3}\,dx - Z\int \rho_\Psi(x)|x|^{-1}dx + D(\rho_\Psi,\rho_\Psi), \tag{1.18}$$

where

$$K_\Psi(x;x') = N\int \Psi(x,x^2,\ldots,x^N)\overline{\Psi(x',x^2,\ldots,x^N)}dx^2\ldots dx^N, \tag{1.19}$$

$$\rho_\Psi(x) = K_\Psi(x;x). \tag{1.20}$$

The important point to note is that since only differentiation along the x_3 direction enters in the kinetic energy (1.17), it is *not* the full one-body density matrix $K_\Psi(x;x')$ that is relevant but only its "semi-diagonal" part

$$\Gamma^\Psi_{x_\perp}(x_3,x_3') = K_\Psi(x_\perp,x_3;x_\perp,x_3')$$

with respect to the variables perpendicular to the field. Furthermore, the kernel $\Pi_0(x,x')$ has the property that $\Pi_0(x_\perp,x_3;x_\perp,x_3') = (B/2\pi)\delta(x_3-x_3')$ from which it follows easily that for Ψ in the lowest Landau band and each value of $x_\perp$ one has (see Lemma 4.1) $0 \le \Gamma^\Psi_{x_\perp}(x_3,x_3') \le (B/2\pi)I$ as operators on $L^2(\mathbf{R})$. The physics behind this inequality is the Pauli principle and the fact that the density of states per unit area perpendicular to the field is $B/(2\pi)$ in the lowest Landau band.

The above considerations suggest a functional that does not depend on the density alone, but rather on functions $\Gamma : x_\perp \mapsto \Gamma_{x_\perp}(x_3,y_3)$ from $\mathbf{R}^2$ to density *matrices* on $L^2(\mathbf{R})$, satisfying the condition

$$0 \le \Gamma_{x_\perp} \le (B/2\pi)I \quad \text{as an operator on } L^2(\mathbf{R}). \tag{1.21}$$

The functional is defined in analogy with (1.18) as

$$\mathcal{E}^{\rm DM}[\Gamma] := \int_{\mathbf{R}^2} {\rm Tr}_{L^2(\mathbf{R})}[-\partial_3^2\Gamma_{x_\perp}]dx_\perp - Z\int |x|^{-1}\rho_\Gamma(x)dx + D(\rho_\Gamma,\rho_\Gamma), \tag{1.22}$$

where $\rho_\Gamma(x) = \Gamma_{x_\perp}(x_3,x_3)$ and $\partial_3 = \partial/\partial x_3$. Since the functional only contains derivatives with resect to the x_3 direction it might appear to be unbounded below; it turns out, however, that the "hard core" condition (1.21) prevents collapse. We define

$$E^{\rm DM}(N,Z,B) := \inf\{\mathcal{E}^{\rm DM}[\Gamma] : \int \rho_\Gamma \le N,\ \Gamma \text{ satisfies (1.21)}\}. \tag{1.23}$$

The DM theory has two nontrivial parameters, $\lambda = N/Z$ and $\eta := B/(2\pi Z^3)$; the energy obeys the **scaling relation**

Reg. 4
$$E^{\rm DM}(N,Z,B) = Z^3E^{\rm DM}(N/Z,1,B/Z^3). \tag{1.24}$$

The main limit theorem for strong fields, to be proved in Sect. VIII, can now be stated as follows

1.3. THEOREM (Energy asymptotics for regions 3,4,5). *Let N/Z be fixed and suppose $B/Z^{4/3} \to \infty$ as $Z \to \infty$. Then*

$$E^{\rm Q}(N,Z,B)/E^{\rm DM}(N,Z,B) \to 1 \qquad \textit{as} \;\; Z \to \infty.$$

Notice that there is an overlap in the parameter regions covered by Theorems 1.1 and 1.3. In fact, both theorems apply to region 3 described above.

The functional $\mathcal{E}^{\rm DM}$ has a unique minimizer for a given N, and the associated variational problem amounts to finding, for each value of $x_\perp$, the eigenfunctions of a *one-dimensional* Schrödinger operator with a potential that has to be determined in a self consistent way from the charge density

ρ_Γ. The important point is that the number of eigenfunctions that have to be considered at each point $x_\perp$ is *finite* and depends only on the parameters λ and η, but is *independent of* N. This makes the problem vastly more simple than the corresponding minimization problem for the full one-body density matrix, which is totally unmanageable as $N \to \infty$. In fact, for large values of B/Z^3 the minimization problem for $\mathcal{E}^{\rm DM}$ can easily be attacked on the computer since only the first few eigenfunctions have to be taken into account. Conversely, if $B/Z^3 \to 0$, the number of eigenfunctions tends to infinity and we recover the semiclassical theory described by $\mathcal{E}^{\rm STF}$.

In Theorem 4.6 we show that there is a critical value for B/Z^3, above which at most *one* eigenfunction enters for each fixed $x_\perp$. In this case $\mathcal{E}^{\rm DM}$ collapses to a density functional, since the kinetic term $\int {\rm Tr}_{L^2(\mathbf{R})}(-\partial_3^2\Gamma_{x_\perp})dx_\perp$ can be replaced by $\int(-\partial_3\sqrt{\rho_\Gamma(x)})^2dx$. We shall refer to this special form of the density matrix functional as the **super-strong functional** and denote it by $\mathcal{E}^{\rm SS}$. More precisely, this is the functional of the density ρ given by

$$\mathcal{E}^{\rm SS}[\rho] := \int\left(\frac{\partial}{\partial x_3}\sqrt{\rho(x)}\right)^2 dx - Z\int |x|^{-1}\rho(x)dx + D(\rho,\rho). \tag{1.25}$$

As a historical remark we note that essentially the same density functional was written down in 1971 by Kadomtsev and Kudryavtsev [8] who estimated its ground state energy by a simple variational ansatz. In Sect. III we show that as $B/Z^3 \to \infty$ the energy $\mathcal{E}^{\rm SS}$ converges, after an appropriate rescaling, to the energy of a functional of a *one-dimensional* density, called the **hyper-strong functional**. It is defined as

$$\mathcal{E}^{\rm HS}[\rho] := \int_{\mathbf{R}}\left(\frac{d}{dx}\sqrt{\rho(x)}\right)^2 dx - \rho(0) + \tfrac{1}{2}\int_{\mathbf{R}}\rho(x)^2dx, \tag{1.26}$$

where ρ is now a density depending on the one-dimensional variable $x \in \mathbf{R}$. In Theorem 3.1 we show that the minimizer of $\mathcal{E}^{\rm HS}$ can be evaluated *exactly*. Combining the solution with Theorem 1.3 we thus obtain the following result for the quantum mechanical ground state energy in region 5. (See (3.7) and (8.10).)

1.4. THEOREM (Energy asymptotics for region 5). *If $Z \to \infty$ and $B/Z^3 \to \infty$ with $N/Z = \lambda$ fixed, then*

$$E^{\rm Q}(N,Z,B)/(Z^3[\ln(B/Z^3)]^2) \to \begin{cases} -\frac14\lambda + \frac18\lambda^2 - \frac1{48}\lambda^3, & \text{for } \lambda \le 2 \\ -\frac16, & \text{for } \lambda \ge 2 \end{cases}.$$

This is one of the few cases in atomic physics where the quantum mechanical ground state can be evaluated in closed form.

One of the remarkable corollaries of Theorem 1.4, which will be proved in Sect. IX, is the following — which we call a theorem because of its physical importance. In a normal $B = 0$

atom [42-44], the maximum number of electrons, $N_c^{\rm Q}$, that can be bound to a nucleus, satisfies $N_c^{\rm Q}/Z \to 1$ as $Z \to \infty$. The situation is the same in regions 1, 2, 3 where a TF type theory continues to be valid and atoms are spherical; *cf.* Theorems 3.18 and 3.23 in [31]. The asymptotic neutrality result in [42] can be extended to regions 1, 2, 3 by using the methods in [44]. The situation in regions 4 and 5 is very different (although we must admit we prove this assertion only for region 5): *the ionization can be proportional to Z itself.* In these two regions the atom also happens to be non- spherical. Of course this ionization result applies only to a single atom and cannot be expected to hold for bulk matter because the Coulomb repulsion of very many ionized atoms would eventually be overwhelming.

1.5. THEOREM (Ionization of atoms). *The maximal number, $N_c^{\rm Q}$, of electrons that can be bound to an atom of nuclear charge Z, defined by*

$$N_c^{\rm Q} = \max\{N : E^{\rm Q}(N,Z,B) < E^{\rm Q}(N-1,Z,B)\}, \tag{1.27}$$

satisfies

$$\liminf N_c^{\rm Q}/Z \geq 2 \quad \textit{as} \quad Z \to \infty \quad \textit{and} \quad B/Z^3 \to \infty. \tag{1.28}$$

We *conjecture* that the $Z \to \infty$ limiting value of $N_c^{\rm Q}/Z$ (and $N_c^{\rm DM}/Z$ in the density matrix theory) is an increasing function of B/Z^3. In any event, $N_c^{\rm Q}/Z = 2$ for $B \gg Z^3$ and this is probably the largest value of that ratio. Theorem 1.5 should not be confused with a theorem of Lieb [45] that $N_c^{\rm Q} < 2Z+1$, which is not relevant here because that theorem does not include the $\boldsymbol{\sigma}\cdot\mathbf{B}$ term of the Pauli Hamiltonian. This point, which we confess confused us for some time, is discussed in Sect. IX.

Another property that holds for regions 4 and 5, but not 1, 2, 3, is that *atomic binding energies are on the scale of the atomic energy itself.* In a TF type theory atoms do not bind together [29-31] but in region 5 they do bind, and presumably also in the DM theory in region 4. This translates into the following (also proved in Sect. IX).

1.6. THEOREM (Strong atomic binding). *Let $E_{\rm b}^{\rm Q}(Z_1,Z_2,B)$ denote the binding energy (defined in Sect. IX) of a neutral molecule consisting of two nuclei of charges Z_1 and Z_2. It is always true that* $\lim E_{\rm b}^{\rm Q}(Z_1,Z_2,B)/[E^{\rm Q}(Z_1,Z_1,B)+E^{\rm Q}(Z_2,Z_2,B)] > 0$ *as $Z_{1,2} \to \infty$ and $B/Z_{1,2}^3 \to \infty$, provided Z_1/Z_2 is bounded away from 0 and ∞. In particular, if $Z_1 = Z_2 = Z$ then*

$$E_{\rm b}^{\rm Q}(Z,Z,B)/2|E^{\rm Q}(Z,Z,B)| \to 3, \quad \textit{as } Z \to \infty.$$

In view of the somewhat conflicting statements in the literature about atomic binding in a strong magnetic field (see e.g. [6, 9, 10, 12, 16, 20, 26]), we emphasize that this is a *theorem* about quantum mechanics in the limit considered. It does not necessarily contradict the Hartree-Fock calculations of [16] and [20] that seem to indicate that iron is weakly bound in fields of the order $10^{12} - 10^{13}$ G.

In this overview we have concentrated on the properties of the energy for brevity. In all cases, however, corresponding results for the electron density can also be proved. The precise statements can be found in Theorems 8.1 and 8.2 in Sect. VIII.

We conclude the introduction with a few remarks about the organization of the paper. It was found convenient to discuss first the properties of all the asymptotic functionals and then the quantum mechanical limit theorems. For the former we start with the functional $\mathcal{E}^{\rm SS}$, although it is in reality a special case of $\mathcal{E}^{\rm DM}$. The main reason is that we think it is easier to assimilate the latter after some acquaintance with the former. Also, it turns out that certain results about $\mathcal{E}^{\rm SS}$ are needed in our discussion of the density matrix functional. We proceed by considering the hyper-strong functional $\mathcal{E}^{\rm HS}$, and finally the density matrix functional $\mathcal{E}^{\rm DM}$. We turn to the quantum mechanical limit theorems in Sect. V by deriving a variational upper bound for the quantum mechanical energy. In the next section we prove the result on confinement in the lowest Landau band (Theorem 1.2). The most difficult problem, treated in Sect. VII, is to estimate the negative exchange energy from below, because the Lieb-Oxford inequality [46], although universally valid, is not strong enough if B is of order higher than Z^5. Our exchange bound is given in Theorem 7.1. After the problem has been reduced in this way to the study of a one-body Hamiltonian the completion of the proof of Theorem 1.3 turns out to be fairly simple.

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II. THE SUPER-STRONG MAGNETIC FIELD DENSITY FUNCTIONAL

In this section we introduce a density functional $\mathcal{E}^{\rm SS}[\rho]$ that is very different from the Thomas-Fermi functional discussed in [28] and in the Introduction. It involves derivatives of the density $\rho(x)$, and in some respects resembles a density functional appropriate for bosons rather than fermions. Nevertheless, as we shall show in Sect. VIII, this functional correctly gives the limiting energy for an atom in a magnetic field $B \gg Z^3$.

Our functional $\mathcal{E}^{\rm SS}$ involves a parameter $\eta = B/(2\pi Z^3)$. The functional makes sense for all $\eta > 0$, and we shall first undertake the usual task of proving existence and uniqueness of a minimizing density ρ. However, as the motivation for $\mathcal{E}^{\rm SS}$ comes from quantum mechanics with η large, the $\mathcal{E}^{\rm SS}$ theory is physically significant mainly in that case, where the theory is asymptotically exact if $Z \to \infty$ as well. In Sect. III, we show how to extract the $\eta \to \infty$ limit of the super-strong theory. Oddly enough, this limiting theory (which we call the **hyper-strong theory**) can be solved *exactly.* One point worth noting is that the errors, in this hyper-strong theory, turn out to be *non*-negligible in the sense that they are typically approximately of the order $1/|\ln \eta|$. Thus, while the hyper-strong limit is the correct mathematical limit for $B/Z^3 \to \infty$, it is worthwhile studying the somewhat more complicated functional $\mathcal{E}^{\rm SS}$ without taking the limit $\eta \to \infty$. This claim is supported by the fact, which we show in Sects. IV and VIII, that the super-strong theory is also correct (as $Z \to \infty$) for large but finite values of the parameter η, without taking the limit $\eta \to \infty$. Another reason for studying the super-strong theory, even in the limit as $\eta \to \infty$, is that it contains more information than the hyper-strong theory; in particular it tells us about the cross-sectional density in the atom, whereas the hyper-strong theory deals only with the cross-sectional integral of the density.

The super-strong energy functional is defined by (1.25). Note that the first term (the kinetic energy) involves only the derivative in the x_3 direction. The last two terms are familiar. The first term is the kinetic energy in the x_3 direction — the kinetic energy in the $x_\perp = (x_1, x_2)$ direction being absent on account of the assertion in Theorem 1.2 that all the electrons can be assumed to be in the lowest Landau band, and hence have zero kinetic energy in the $x_\perp$ direction.

As usual, we have the condition on the particle number

$$\int \rho = N, \tag{2.1}$$

but now (1.25) has to be supplemented by another, strange looking condition:

$$\int_{\mathbf{R}} \rho(x_\perp, x_3) dx_3 \le \frac{B}{2\pi} \text{ for each } x_\perp = (x_1, x_2). \tag{2.2}$$

This condition comes from the fact, to be explicated in Theorem 4.6, that for large B/Z^3 at most one eigenstate (the ground state, of course) in the x_3 direction is occupied by an electron. That fact, together with (1.21), leads to (2.2).

The domain of definition of $\mathcal{E}^{\rm SS}$ is the set $\mathcal{C}^{\rm SS}$ of nonnegative measurable functions ρ satisfying the conditions

(a) $\int \rho(x)dx < \infty$

(b) $\int_{\mathbf{R}} \rho(x_\perp, x_3) dx_3 \le C$ for some $C < \infty$ independent of $x_\perp$ (2.3)

(c) The distributional derivative $\partial\sqrt{\rho}/\partial x_3$ is a function in $L^2(\mathbf{R}^3)$.

The functional $\mathcal{E}^{\rm SS}$ is easily shown to be strictly convex on $\mathcal{C}^{\rm SS}$. Note, however, that $\mathcal{E}^{\rm SS}$ is *not* convex as a functional of $\psi = \sqrt{\rho}$. The proof of the convexity is the same as in [31], Theorem 7.1.

As a preliminary to our theorems here, we note some properties of functions in $\mathcal{C}^{\rm SS}$.

(i) For almost every $x_\perp$ the function $\psi := \sqrt{\rho}$ is a Hölder continuous function of x_3 with exponent 1/2. This is so because $\psi(x_\perp, \cdot)$ is in $H^1(\mathbf{R})$ for almost every $x_\perp \in \mathbf{R}^2$. To be precise

$$\begin{aligned}|\psi(x_\perp, a) - \psi(x_\perp, b)| &= \left|\int_a^b (\partial\psi/\partial x_3) dx_3\right| \le \left|\int_a^b dx_3\right|^{1/2} \left|\int_a^b (\partial\psi/\partial x_3)^2 dx_3\right|^{1/2} \\ &\le |a-b|^{1/2} \left|\int (\partial\psi/\partial x_3)^2 dx_3\right|^{1/2}. \end{aligned} \tag{2.4}$$

(ii) $\rho \in L^3(\mathbf{R}^3)$ and, for some universal constant K,

$$\int\limits_{\mathbf{R}^3} \rho^3 \le KC^2 \int\limits_{\mathbf{R}^3} (\partial\psi/\partial x_3)^2, \tag{2.5}$$

where C is the constant in (2.3). Inequality (2.5) follows easily from the Sobolev inequality in $\mathbf{R}$, $K\int(\partial f/\partial x)^2 \ge \left(\int f^6\right)\left(\int f^2\right)^{-2}$. After scaling, we see from (2.2) that the C of interest in our problem can be taken to be unity.

The following lemma is useful for proving the existence of minimizers for $\mathcal{E}^{\rm SS}$.

2.1. LEMMA (Energy of one-dimensional Coulomb problem). *For $Z > 0$ and $a > 0$, let $\widehat{h}_{Z,a}$ be the operator on $L^2(\mathbf{R})$ given by*

$$\widehat{h}_{Z,a} = -\frac{d^2}{dx^2} - \frac{Z}{\sqrt{x^2+a^2}}.$$

Then the eigenvalues, $-\widehat{\mu}_n$, satisfy

$$\begin{gathered}\widehat{\mu}_1 \le Z^2\{1 + [\sinh^{-1}(1/Za)]^2\} \\ \widehat{\mu}_{2n} \text{ and } \widehat{\mu}_{2n+1} \le Z^2/4n^2, \quad n = 1, \ldots.\end{gathered}$$

Proof: By scaling, we see that $\widehat{h}_{Z,a} = Z^2$ times an operator that depends only on Za. Therefore we can assume $Z = 1$. With $T := \int_{\mathbf{R}} (d\psi/dx)^2$ and $\psi \in H^1(\mathbf{R})$, (which we can assume to be real),

$$\begin{aligned}(\psi, \widehat{h}_{1,a}\psi) &= T - \int_{\mathbf{R}} \psi(x)^2 (x^2+a^2)^{-1/2} dx \\ &= T - \int\limits_{|x|\le 1} \frac{d}{dx}\left[\int_0^x (y^2+a^2)^{1/2} dy\right] \psi^2(x) dx - \int\limits_{|x|\ge 1} \psi(x)^2 (x^2+a^2)^{-1/2} dx\end{aligned}$$

$$
\begin{aligned}
&\geq T + 2 \int_{|x|\leq 1} \left[\int_0^x (y^2+a^2)^{-1/2}dy\right]\psi(x)\frac{d\psi(x)}{dx}dx \\
&\quad - \int_0^1 (y^2+a^2)^{-1/2}dy[\psi(1)^2+\psi(-1)^2] - \int_{\mathbf{R}} \psi^2 \\
&\geq T - 2\sinh^{-1}(a^{-1}) \int_{\mathbf{R}} \left|\psi(x)\frac{d\psi(x)}{dx}\right| dx - \int_{\mathbf{R}} \psi^2 \\
&\geq T - 2\sinh^{-1}(a^{-1}) I^{1/2}T^{1/2} - I
\end{aligned}
$$

with $I = \int \psi^2$. The fourth line was obtained from the third by noting that $\psi(1)^2 \leq 2\int_1^\infty \psi(x)[d\psi(x)/dx]dx$. The bound on $\widehat{\mu}_1$ is obtained by minimizing the last expression with respect to T.

To estimate $\widehat{\mu}_{2n}$ we first replace $-Z(|x|^2+a^2)^{-1/2}$ with the lower bound $-Z|x|^{-1}$. Thus, if ψ_{2n} denotes the $2n$-th normalized eigenfunction,

$$-\mu_{2n} \geq (\psi_{2n},\ (p^2 - Z|x|^{-1})\psi_{2n}).$$

Since the potential $x \mapsto Z(|x|^2+a^2)^{-1/2}$ is symmetric about $x=0$, the eigenfunction ψ_{2n} must have a node at $x=0$. The eigenvalues of the operator on the right side of this inequality, when restricted to functions with a node at the origin, are precisely the same as the eigenvalues of the hydrogen atom restricted to radial functions. Thus we obtain $\widehat{\mu}_{2n} \leq Z^2/4n^2$. Since $\widehat{\mu}_{2n+1} \leq \widehat{\mu}_{2n}$, the lemma follows. ■

2.2. THEOREM (Unique minimizer for $\mathcal{E}^{\mathrm{SS}}$). *For each N, Z and $B>0$ there is a unique (and hence axially symmetric) $\rho^{\mathrm{SS}} \in \mathcal{C}^{\mathrm{SS}}$ satisfying the conditions (2.2) and*

$$\int \rho^{\mathrm{SS}} \leq N, \tag{2.6}$$

and such that

$$\mathcal{E}^{\mathrm{SS}}[\rho^{\mathrm{SS}}] = E^{\mathrm{SS}}(N,Z,B) := \inf\left\{\mathcal{E}^{\mathrm{SS}}[\rho]\ :\ \rho\in\mathcal{C}^{\mathrm{SS}}, \int\rho\leq N, \quad \rho \text{ satisfies } (2.2)\right\}. \tag{2.7}$$

The energy $E^{\mathrm{SS}}(N,Z,B)$ is a monotonically nonincreasing, convex function of N, and in fact

$$E^{\mathrm{SS}}(N,Z,B) = \inf\{\mathcal{E}^{\mathrm{SS}}[\rho]\ :\ \rho\in\mathcal{C}^{\mathrm{SS}}, \int\rho = N,\ \rho \text{ satisfies } (2.2)\}.$$

Moreover, if $\rho^{(n)}$ is any minimizing sequence for (2.7) (i.e. $\mathcal{E}^{\mathrm{SS}}[\rho^{(n)}] \to E^{\mathrm{SS}}(N,Z,B)$ and $\int\rho^{(n)}(x)dx \leq N, \int\rho^{(n)}(x)dx_3 \leq B/2\pi$), then each of the three terms in the energy (1.25) converges to the corresponding term for ρ^{SS}.

Remark: ρ^{SS} depends on N, Z and B, but our notation suppresses this for simplicity.

Proof: We begin by finding a lower bound for $\mathcal{E}^{\rm SS}[\rho]$ that behaves like $NZ^2\left[\ln(B/Z^2N)\right]^2$ for $B/(Z^2N)$ large. To do so we ignore the third (repulsion) term in (1.25). For each $\rho \in \mathcal{C}^{\rm SS}$ satisfying (2.1) and (2.2) we define

$$\lambda(\rho;x_\perp) = \int_{\mathbf{R}} \rho(x_\perp,x_3)dx_3 \le B/2\pi.$$

By Lemma 2.1 we have that

$$\mathcal{E}^{\rm SS}[\rho] \ge -\int_{\mathbf{R}^2} \lambda(\rho;x_\perp)Z^2\{1+[\sinh^{-1}(1/(Z|x_\perp|)]^2\}dx_\perp.$$

We know that $\int_{\mathbf{R}^2}\lambda(\rho;x_\perp)dx_\perp = N$. Since the factor in braces $\{\ \}$ is a decreasing function of $|x_\perp|$, a lower bound for $\mathcal{E}^{\rm SS}[\rho]$ is obtained as follows: We have

$$\mathcal{E}^{\rm SS}[\rho] \ge -\frac{Z^2B}{2\pi}\int\limits_{|x_\perp|<\sqrt{2N/B}} \left\{1+\left[\sinh^{-1}(1/Z|x_\perp|)\right]^2\right\}dx_\perp. \tag{2.8}$$

The function $\sinh^{-1}(t)$ behaves like t for small t and like $\ln t$ for large t. From this we conclude that the expression (2.8) is bounded below† by $-(\text{const.})NZ^2[1+[\ln(B/Z^2N)]^2]$.

Now fix N and B and let $\rho^{(1)},\rho^{(2)},\ldots$ be a minimizing sequence in $\mathcal{C}^{\rm SS}$, i.e. $\mathcal{E}^{\rm SS}[\rho^{(n)}] \to E^{\rm SS}(N,Z,B)$ as $n\to\infty$ and $\int\rho^{(n)} \le N$ for each n. The kinetic energy $T[\rho^{(n)}] := \int(\partial\sqrt{\rho^{(n)}}/\partial x_3)^2$ is bounded. The reason is that we can write $\mathcal{E}^{\rm SS}[\rho] := \frac{1}{2}T[\rho] + \widetilde{\mathcal{E}}^{\rm SS}[\rho]$. By the same argument as above, $\widetilde{\mathcal{E}}^{\rm SS}[\rho]$ is bounded below, and hence $\frac{1}{2}T[\rho^{(n)}]$ must be bounded above. By inequality (2.5) the $L^3(\mathbf{R}^3)$ norm of $\rho^{(n)}$ is uniformly bounded in n.

By the Banach-Alaoglu Theorem there is a subsequence (which we continue to denote by $\rho^{(n)}$) that converges weakly in $L^3(\mathbf{R}^3)$ to some function $\rho^\infty \in L^3(\mathbf{R}^3)$. (Of course $\rho^\infty \ge 0$ since weak limits of nonnegative functions are nonnegative; and $\int\rho^\infty \le N$ since otherwise, for some ball K we would have $N < \int_K\rho^\infty = \lim_{n\to\infty}\int_K\rho^{(n)} \le N$.) By Mazur's theorem we can take convex combinations of the $\rho^{(n)}$'s so that the new sequence (which we denote again by $\rho^{(n)}$) converges *strongly* to ρ^∞ in $L^3(\mathbf{R}^3)$. Moreover, we can require that the new $\rho^{(n)}$ be a convex combination only of the old subsequence starting with n, i.e., the subsequence $\rho^{(n)},\rho^{(n+1)},\rho^{(n+2)},\ldots$. Since $\rho^{(n)}$ is a bounded sequence in $L^1(\mathbf{R}^3)$, we can also demand that $\rho^{(n)}$ converges strongly to ρ^∞ in $L^p(\mathbf{R}^3)$ for some fixed $3 \ge p > 1$. We choose $p = 6/5$. Since $\rho \mapsto \mathcal{E}^{\rm SS}[\rho]$ is convex, this new, strongly convergent sequence is also minimizing. By the standard proof of the Riesz-Fischer theorem that L^p is complete we can pass to a further subsequence and demand that the following holds:

(i) $\lim\limits_{n\to\infty}\rho^{(n)}(x) = \rho^\infty(x)$ for almost every x.

† Throughout we shall use (const.) to denote any positive universal constant.

(ii) There is a function $G \in L^3(\mathbf{R}^3) \cap L^{6/5}(\mathbf{R}^3)$ such that $\rho^{(n)}(x) \le G(x)$ for all x and n.

By (i) and Fatou's Lemma, ρ^∞ satisfies condition (2.2). Let us investigate the convergence properties of the three terms $T[\rho] - A[\rho] + R[\rho]$ that define $\mathcal{E}^{\rm SS}[\rho]$ according to (1.25). Clearly,

$$\lim_{n\to\infty} A[\rho^{(n)}] = A[\rho^\infty]$$

thanks to the strong convergence of $\rho^{(n)}$ to ρ^∞ in $L^3(\mathbf{R}^3)$. (Actually, weak convergence would suffice here.) Next

$$\lim_{n\to\infty} R[\rho^{(n)}] = R[\rho^\infty]$$

by dominated convergence (since $\rho^{(n)} \le G$ and $G \in L^{6/5}(\mathbf{R}^3)$; but $(x, y) \mapsto$
$G(x)G(y)V|x-y|^{-1}$ is in $L^1(\mathbf{R}^3 \times \mathbf{R}^3)$ by Young's inequality).

The difficult term is $T[\rho^{(n)}]$. We claim that $\rho^\infty \in \mathcal{C}^{\rm SS}$ and that

$$\liminf_{n\to\infty} T[\rho^{(n)}] \ge T[\rho^\infty]. \tag{2.9}$$

To prove (2.9) we use the fact that

$$\left\{\int_{\mathbf{R}^3} |\partial\phi/\partial x_3|^2\right\}^{1/2} = \sup\left\{\int_{\mathbf{R}^3} \phi(\partial f/\partial x_3) \ :\ f \in C_0^\infty(\mathbf{R}^3) \text{ and } \int_{\mathbf{R}^3} f^2 = 1\right\}$$

for all functions $\phi \in L^2(\mathbf{R}^3)$. Implicit in this equation is the assertion that the finiteness of the right side implies that the distributional derivative of ϕ is an $L^2(\mathbf{R}^3)$ function. Now, for each fixed $f \in C_0^\infty(\mathbf{R}^3)$ with $\int f^2 = 1$ we have

$$\liminf_{n\to\infty}\left\{\int (\partial\sqrt{\rho^{(n)}}/\partial x_3)^2\right\}^{1/2} \ge \liminf_{n\to\infty}\left|\int \sqrt{\rho^{(n)}}\partial f/\partial x_3\right| = \left|\int \sqrt{\rho^\infty}\partial f/\partial x_3\right|,$$

where the last equality is a consequence of dominated convergence. This implies (2.9).

We have shown that $E^{\rm SS}(N, Z, B) = \lim_{n\to\infty}\mathcal{E}^{\rm SS}[\rho^{(n)}] \ge \mathcal{E}^{\rm SS}[\rho^\infty]$, from which it is evident that ρ^∞ is a minimizer. The uniqueness property follows trivially from the strict convexity of $\rho \mapsto \mathcal{E}^{\rm SS}[\rho]$. In fact this convexity also implies the convexity of $E^{\rm SS}(N, Z, B)$ in N. The monotonicity of E is a trivial consequence of its definition (2.7). The fact that $E^{\rm SS}$ agrees with the energy defined using the strong condition $\int \rho = N$ follows easily from the fact that extra charge can always be "added at infinity" as in ref. [30].

It remains to prove that when $\rho^{(n)}$ is any minimizing sequence then the three terms in (1.25) converge to those for $\rho^{\rm SS}$. First, by the Banach-Alaoglu theorem, $\rho^{(n)} \rightharpoonup \widehat{\rho}$ weakly in $L^3(\mathbf{R}^3)$ for some subsequence and some $\widehat{\rho}$. By the proof we just gave, $\widehat{\rho}$ is minimizing. But the minimizer is unique and hence $\widehat{\rho} = \rho^{\mathrm{SS}}$. We also remark that the uniqueness implies that $\rho^{(n)} \rightharpoonup \rho^{\mathrm{SS}}$ without the necessity of passing to a subsequence.

By the weak convergence of $\rho^{(n)}$ to ρ^{SS}, $\int Z|x|^{-1}\rho^{(n)}(x)dx$ converges to $\int Z|x|^{-1}\rho^{\mathrm{SS}}(x)dx$ and hence the middle term in (1.25) behaves properly. We conclude that

$$\lim_{n\to\infty} T[\rho^{(n)}] + R[\rho^{(n)}] = T[\rho^{\mathrm{SS}}] + R[\rho^{\mathrm{SS}}]$$

and therefore it suffices to prove that $\liminf_{n\to\infty} T[\rho^{(n)}] \geq T[\rho^{\mathrm{SS}}]$ and $\liminf_{n\to\infty} R[\rho^{(n)}] \geq R[\rho^{\mathrm{SS}}]$.

By Mazur's theorem there are convex combinations (call them $\widetilde{\rho}^{(n)}$) of the $\rho^{(n)}$'s so that $\widetilde{\rho}^{(n)}$'s converge strongly in $L^3(\mathbf{R}^3)$ to ρ^{SS} and satisfy (i) and (ii) above. As we saw, this implies that $\liminf_{n\to\infty} T[\widetilde{\rho}^{(n)}] \geq T[\rho^{\mathrm{SS}}]$. However, $\rho \mapsto T[\rho]$ is convex and this convexity implies that $\liminf_{n\to\infty} T[\rho^{(n)}] \geq \liminf_{n\to\infty} T[\widetilde{\rho}^{(n)}]$, which is the desired conclusion. The same strategy proves that $\liminf_{n\to\infty} R[\rho^{(n)}] \geq R[\rho^{\mathrm{SS}}]$. ∎

The $\mathcal{E}^{\mathrm{SS}}$ functional has a natural scaling which is given by defining a scaled density by $\widetilde{\rho}(x) = Z^{-4}\rho(Z^{-1}x)$. Then $\mathcal{E}^{\mathrm{SS}}[\rho] = Z^3\mathcal{E}^{\mathrm{SS}}[\widetilde{\rho}]$. Moreover, if ρ satisfies (2.1) and (2.2) then $\widetilde{\rho}$ satisfies $\int_{\mathbf{R}} \widetilde{\rho}dx_3 \leq B/(2\pi Z^3)$ and $\int \widetilde{\rho} \leq N/Z$. We can then conclude that the energy E^{SS} satisfies the **scaling relation** $E^{\mathrm{SS}}(N, Z, B) = Z^3 E^{\mathrm{SS}}(N/Z, 1, B/Z^3)$ (compare (1.24)). There are thus two non-trivial parameters in the theory $\lambda = N/Z$ and $\eta = B/(2\pi Z^3)$.

Having proved the existence of a unique minimizer, we wish next to establish some of its properties. To begin with we can note, that there is a number N_c^{SS} (which *a-priori* might be $+\infty$) such that the energy E^{SS} is a strictly decreasing function of N for $N < N_c^{\mathrm{SS}}$ and is constant for $N \geq N_c^{\mathrm{SS}}$. Whenever $N \leq N_c^{\mathrm{SS}}$ the minimizer satisfies $\int \rho^{\mathrm{SS}} = N$ and not $\int \rho^{\mathrm{SS}} < N$. When $N > N_c^{\mathrm{SS}}$ the minimizer satisfies $\int \rho^{\mathrm{SS}} = N_c^{\mathrm{SS}}$.

Given ρ^{SS} (for $N \leq N_c^{\mathrm{SS}}$) we can form the function

$$\begin{aligned} \phi_{x_\perp}^{\mathrm{SS}}(x_3) &= Z|x|^{-1} - |x|^{-1} * \rho^{\mathrm{SS}} \\ &= Z(|x_\perp|^2 + x_3^2)^{-1/2} - \int \rho^{\mathrm{SS}}(y)(|x_\perp - y_\perp|^2 + |x_3 - y_3|^2)^{-1/2} dy. \end{aligned} \tag{2.10}$$

As long as $x \neq 0$, $\phi_{x_\perp}^{\mathrm{SS}}$ is a continuous function of $x = (x_\perp, x_3)$. This follows easily from the facts that $\rho \in L^3(\mathbf{R}^3)$ and $|x|^{-1} \in L^{3/2}_{\mathrm{loc}}(\mathbf{R}^3)$.

For each $x_\perp \neq 0$ there is a well defined Schrödinger equation associated with the energy functional

$$\mathcal{W}_{x_\perp}(\psi) := \int_{\mathbf{R}} (\partial\psi/\partial x_3)^2 - \int_{\mathbf{R}} \phi_{x_\perp}^{\mathrm{SS}}(x_3)\psi(x_3)^2 dx_3. \tag{2.11}$$

The ground state energy is

$$-\mu_1^{\mathrm{SS}}(x_\perp) := \inf\{\mathcal{W}_{x_\perp}(\psi) \, : \int |\psi|^2 = 1\} \tag{2.12}$$

and we note that $\mu_1^{\rm SS}(x_\perp) \geq 0$ (since $\phi_{x_\perp}^{\rm SS}(x_3) \to 0$ as $x = (x_\perp, x_3) \to \infty$). We also note that whenever $\mu_1^{\rm SS}(x_\perp) > 0$ there is a unique, nonnegative minimizing ψ (denoted by $\psi_{x_\perp}$) for (2.12). It satisfies the Schrödinger equation

$$-\psi'' - \phi_{x_\perp}^{\rm SS}\psi = -\mu_1^{\rm SS}(x_\perp)\psi. \tag{2.13}$$

Since $\phi_{x_\perp}^{\rm SS}(x_3)$ is axially symmetric, ie., depends only on $|x_\perp|$ it is evident that $\mu_1^{\rm SS}(x_\perp)$ and $\psi_{x_\perp}(x)$ are axially symmetric in $x_\perp$.

The following property of $\mu_1^{\rm SS}(x_\perp)$ will play an important role in our discussion of $\rho^{\rm SS}$.

2.3. PROPOSITION (Subharmonicity of $\mu_1^{\rm SS}(x_\perp)$). *For each $N \geq 0$ the function $x_\perp \mapsto \mu_1^{\rm SS}(x_\perp)$ is a subharmonic function on $\mathbf{R}^2 \setminus \{0\}$ and is a decreasing convex function of $|x_\perp|$. It is strictly decreasing on the set $\{x_\perp, : \mu^{\rm SS}(x_\perp) > 0\}$. This allows us to define*

$$r^{\rm SS} = \sup\{r \ : \ \mu_1^{\rm SS}(x_\perp) > 0 \text{ for } |x_\perp| < r\}. \tag{2.14}$$

When $|x_\perp| > r^{\rm SS}$ there are no $L^2(\mathbf{R})$ solutions to (2.13).

Proof: Subharmonicity is a property that only has to be checked locally. If $\mu^{\rm SS}(x_\perp^0) = 0$ then $\mu_1^{\rm SS}$ obviously satisfies the mean value inequality at $x_\perp^0$. Thus, we can henceforth assume $\mu_1^{\rm SS}(x_\perp^0) > 0$, in which case there is surely a minimizing ψ for the $x_\perp^0$ problem (2.13). We denote it here simply by ψ^0.

Consider the following function, for $x = (x_\perp, x_3) \in \mathbf{R}^3$. It is the energy of a one-dimensional wire, with one-dimensional charge density $\psi^0(x)^2$, as a function of its position in the field $\phi^{\rm SS}$. Namely,

$$F(x) = \int_{\mathbf{R}} \phi_{x_\perp}^{\rm SS}(x_3 + y)\psi^0(y)^2 dy. \tag{2.15}$$

We observe that F is subharmonic on $\mathbf{R}^3 \setminus L$, where $L = \{(x_\perp, x), : x_\perp = 0\}$ is the vertical line through the origin. This follows straightforwardly from (2.10).

For $x_\perp$ close to our base point $x_\perp^0$, we shall use the function $\psi^0(\cdot + x_3)$, with x_3 arbitrary, as a variational function in (2.11) for the energy $-\mu_1^{\rm SS}(x_\perp)$. Thus

$$G(x_\perp) := \mu_1^{\rm SS}(x_\perp^0) - \mu_1^{\rm SS}(x_\perp) \leq \mathcal{W}_{x_\perp}(\psi^0(\cdot + x_3)) - \mathcal{W}_{x_\perp^0}(\psi^0) = F(x_\perp^0, 0) - F(x_\perp, x_3). \tag{2.16}$$

This inequality holds for every $x_3 \in \mathbf{R}$. The right side of (2.16) is a superharmonic function of $x = (x_\perp, x_3)$ on $\mathbf{R}^3 \setminus L$ and we set

$$H(x_\perp) := \inf_{x_3}[F(x_\perp^0, 0) - F(x_\perp, x_3)].$$

It is not hard to prove by verifying the mean value inequality, that the infimum over x_3 of a continuous superharmonic function on $\mathbf{R}^3$ is superharmonic on $\mathbf{R}^2$.

We conclude that G in (2.16) is bounded above by the superharmonic function H and that $G(x_\perp^0) = H(x_\perp^0) = 0$. Hence G satisfies the mean-value inequality around $x_\perp^0$ appropriate for a superharmonic function (since H does).

It is immediate that $\mu_1^{\rm SS}(x_\perp)$ is a strictly monotone decreasing function of $|x_\perp|$ on the set where $\mu_1^{\rm SS}(x_\perp) > 0$. This follows from the fact that $\mu_1^{\rm SS}$ is axially symmetric, $\mu_1^{\rm SS} \geq 0$ and $\mu_1^{\rm SS}$ vanishes at infinity. On any open set of the form $\Omega_a := \{x_\perp \ : |x_\perp| > a\}$, $\mu_1^{\rm SS}$ cannot attain its supremum (by the strong maximum principle) unless $\mu_1^{\rm SS}$ is a constant function.

Since $\Delta\mu_1^{\rm SS} \geq 0$ we have (with $r = |x_\perp|$)

$$\frac{d^2}{dr^2}\mu_1^{\rm SS}(r) + \frac{1}{r}\frac{d}{dr}\mu_1^{\rm SS}(r) \geq 0$$

and hence $\mu_1^{\rm SS}$ is a convex function of $|x_\perp|$.

It remains to show that there is no $L^2(\mathbf{R})$ solution to (2.13) with $\mu_1^{\rm SS}(x_\perp) = 0$ and with $|x_\perp| > r^{\rm SS}$. If there is a solution to (2.13) for some point $x_\perp^0$ satisfying these conditions we can form $F(x)$ as in (2.15). This F is subharmonic and $F(x_\perp, x_3) - F(x_\perp^0, 0)$ achieves its maximum (namely zero) at an interior point $(x_\perp^0, 0)$ of the open set $A = \{(x_\perp, x_3), : |x_\perp| > r^{\rm SS}\}$. Then F is constant in A. But that means $F(x_\perp^0, y) = F(x_\perp^0, 0)$ for all y, i.e. we can take ψ^0, translate it vertically by y, and still have a ground state solution to (2.13). This would violate uniqueness of the ground state – among other things. ■

Let us now consider (for fixed B and N) the following **linearized problem** defined by the functional

$$\mathcal{E}_{\rm lin}^{\rm SS}[\rho] := T[\rho] - \int \rho(x)\phi_{x_\perp}^{\rm SS}(x_3)dx \tag{2.17}$$

with

$$T[\rho] = \int (\partial\sqrt{\rho}/\partial x_3)^2. \tag{2.18}$$

We seek the energy and a minimizer for

$$e(N) := \inf\{\mathcal{E}_{\rm lin}^{\rm SS}[\rho] \ : \ \rho \in \mathcal{C}^{\rm SS}, \ \rho \text{ satisfies (2.2) and } \int \rho \leq N\}. \tag{2.19}$$

Note that the same N appears twice; once in (2.17) and once in $\int \rho \leq N$. Problem (2.19) has a simple solution. Define a radius $R^{\rm SS}$ using (2.14), by

$$R^{\rm SS} = \min(\sqrt{2N/B}, \ r^{\rm SS}). \tag{2.20}$$

The required solution is

$$\widehat{\rho}(x_\perp, x_3) = \frac{B}{2\pi}\begin{cases}\psi_{x_\perp}(x_3)^2, & \text{for } |x_\perp| \le R^{\rm SS} \\ 0, & \text{otherwise}\end{cases} \quad ,$$

where $\psi_{x_\perp}$ is the normalized solution to (2.13). We then have

$$e(N) = -\int\limits_{|x_\perp|\le R^{\rm SS}} \mu_1^{\rm SS}(x_\perp)dx_\perp. \tag{2.21}$$

If $R^{\rm SS} = \sqrt{2N/B} \le r^{\rm SS}$ our solution is clearly unique and has $\int\widehat{\rho} = N$. We note here that the positive level sets of $\mu_1^{\rm SS}$ all have zero measure since $\mu_1^{\rm SS}$ is strictly decreasing. When $R^{\rm SS} = r^{\rm SS} < \sqrt{2N/B}$ our minimizer has $\int\widehat{\rho} < N$. It is also unique since there are no $L^2(\mathbf{R})$ solutions to (2.13) with $|x_\perp| > r^{\rm SS}$. The next theorem implies that the case $r^{\rm SS} < \sqrt{2N/B}$ does not occur when $N \le N_c^{\rm SS}$.

2.4. THEOREM (Equivalence of the linear and nonlinear problems). *Let $\rho^{\rm SS}$ be the unique minimizer for the nonlinear problem as in Theorem 2.2. Then $\rho^{\rm SS}$ is the unique minimizer $\widehat{\rho}$ for the linear problem defined by (2.19).*

Remarks: (1). The theorem tells us that for $N \le N_c^{\rm SS}$, the minimizer $\rho^{\rm SS}$ satisfies the Euler-Lagrange equation

$$-\frac{\partial^2}{\partial x_3^2}\sqrt{\rho^{\rm SS}} - \phi_{x_\perp}^{\rm SS}\sqrt{\rho^{\rm SS}} = -\mu_1^{\rm SS}(x_\perp)\sqrt{\rho^{\rm SS}}. \tag{2.22}$$

Here $-\mu_1^{\rm SS}(x_\perp)$ is the ground state energy of the Schrödinger operator with potential $\phi_{x_\perp}^{\rm SS}$.

(2). For $N \le N_c^{\rm SS}$ we have $\int\rho^{\rm SS} = N$ and thus the alternative $R^{\rm SS} < \sqrt{2N/B}$ is not possible (for otherwise $\int\rho^{\rm SS} < N$ as discussed above). Uniqueness of the solution of the linearized problem thus precludes the possibility that $r^{\rm SS} < \sqrt{2N/B}$. We conclude that the support of $\rho^{\rm SS}$ (as far as the $x_\perp$ direction is concerned) is *exactly* the cylinder $|x_\perp| \le \sqrt{2N/B}$. For each $x_\perp$ in this cylinder, the bound (2.2) is saturated. It is remarkable that this holds for all $N \le N_c^{\rm SS}$ and B. (For $N \ge N_c^{\rm SS}$ the radius is, of course, $\sqrt{2N_c^{\rm SS}/B}$.) The atom has a sharp surface; there is no "exponential decay" in the $x_\perp$ direction as might have been expected.

Proof: For δ positive and small, define $\rho^\delta = (1-\delta)\rho^{\rm SS} + \delta\widehat{\rho}$, where $\widehat{\rho}$ is the minimizer for the linear problem. We wish to compute the energy $\mathcal{E}^{\rm SS}[\rho^\delta]$ to leading order in δ. The two potential energy terms are trivial. The attraction is linear in δ while the repulsion is quadratic. The kinetic energy $T[\rho^\delta]$ is more problematic. Note, by convexity of $\rho \mapsto T[\rho]$, that $T[\rho^\delta] \le (1-\delta)T[\rho^{\rm SS}] + \delta T[\widehat{\rho}]$. Hence we have

$$\mathcal{E}^{\rm SS}[\rho^\delta] \le E^{\rm SS}(N,Z,B) + \delta\Big(\mathcal{E}_{\rm lin}^{\rm SS}[\widehat{\rho}] - \mathcal{E}_{\rm lin}^{\rm SS}[\rho^{\rm SS}]\Big) + O(\delta^2).$$

If $\rho^{\rm SS}$ is not a minimizer for $\mathcal{E}^{\rm SS}_{\rm lin}$ we would be able to lower $E^{\rm SS}$ by using ρ^δ in place of $\rho^{\rm SS}$, for some small δ. This is a contradiction. ■

2.5. COROLLARY. *The derivative of the function $E^{\rm SS}(N,Z,B)$ with respect to N is equal to the value of $-\mu_1^{\rm SS}(x_\perp)$ at the edge of the atom, i.e., if $|x_\perp| = R^{\rm SS}$ then*

$$\frac{\partial E^{\rm SS}(N,Z,B)}{\partial N} = -\mu_1^{\rm SS}(x_\perp) =: -\mu_1^{\rm SS}(R^{\rm SS}).$$

Proof: Choose two numbers $N_\pm$ satisfying $0 < N_- < N < N_+$. In the proof of Theorem 2.4 replace $\widehat{\rho}$ by the two functions $\rho_\pm$ that minimize $\mathcal{E}^{\rm SS}_{\rm lin}$ under the modified constraints $\int \rho_\pm \le N_\pm$. Note that the Schrödinger equation (2.13) is not changed; the potential remains $\phi^{\rm SS}_{x_\perp}$.

Defining $\rho^\delta_\pm = (1-\delta)\rho^{\rm SS} + \delta\rho_\pm$, we have $\int \rho^\delta_\pm \le N + \delta(N - N_\pm)$ and

$$E^{\rm SS}(N+\delta(N-N_\pm),Z,B) \le \mathcal{E}^{\rm SS}[\rho^\delta_\pm] = E(N,Z,B) + \delta\Big(\mathcal{E}^{\rm SS}_{\rm lin}[\rho_\pm] - \mathcal{E}^{\rm SS}_{\rm lin}[\rho^{\rm SS}]\Big) + O(\delta^2).$$

Since $E^{\rm SS}(N+\delta(N-N_\pm),Z,B)$ is a convex function we obtain

$$\frac{\mathcal{E}^{\rm SS}_{\rm lin}[\rho_-] - \mathcal{E}^{\rm SS}_{\rm lin}[\rho^{\rm SS}]}{N - N_-} \le \frac{dE^{\rm SS}}{dN}(N,Z,B) \le \frac{\mathcal{E}^{\rm SS}_{\rm lin}[\rho_+] - \mathcal{E}^{\rm SS}_{\rm lin}[\rho^{\rm SS}]}{N_+ - N}.$$

The analogue of (2.21) still holds, i.e., with $R^{\rm SS}_\pm$ denoting the respective radii,

$$\mathcal{E}^{\rm SS}_{\rm lin}[\rho_\pm] = -\int\limits_{|x_\perp|\le R^{\rm SS}_\pm} \mu_1^{\rm SS}(x_\perp)dx_\perp$$

The corollary is proved by letting $N_\pm$ approach N and using the fact that $\mu_1^{\rm SS}$ is continuous away from $x_\perp = 0$. ■

We turn next to the **virial theorem** for the functional $\mathcal{E}^{\rm SS}$ – more precisely a virial inequality. For an atom without magnetic field, there is the well known virial theorem $2K = A - R$, where K is the kinetic energy, A is the attractive energy and R is the Coulomb repulsion energy. In the TF theory of such an atom there is an additional virial *inequality*, $\frac{5}{3}K \le A - 2R$, and with equality if and only if $N = N_c^{\rm TF} = Z$. This is proved by multiplying the TF equation by ρ and then integrating. When $B \ne 0$ there is no virial theorem at the original quantum mechanical level, but in the TF theory of the strong regime, $Z^{4/3} \ll B \ll Z^3$, in which the TF theory has a ρ^3/B^2 kinetic energy density, there is both a virial theorem, $6K = A - R$, and a virial inequality, $3K \le A - 2R$ (with equality at $N = N_c^{\rm STF} = Z$) within the context of that TF theory. This is proved in the same manner as for the usual TF theory with $\rho^{5/3}$ kinetic energy density. The super-strong regime has two virial *inequalities* within the context of the $\mathcal{E}^{\rm SS}[\rho]$ theory. Neither of them becomes an equality, even when $N = N_c^{\rm SS}$. They are stated in the following.

2.6. LEMMA (Virial inequalities). *Define*

$$T^{\rm SS}=\int\left(\frac{\partial}{\partial x_3}\sqrt{\rho^{\rm SS}(x)}\right)^2 dx,\ A^{\rm SS}=\int Z|x|^{-1}\rho^{\rm SS}(x)dx,\ R^{\rm SS}=D(\rho^{\rm SS},\rho^{\rm SS})$$

and let $E^{\rm SS}=T^{\rm SS}-A^{\rm SS}+R^{\rm SS}$ *be the corresponding total energy. The following inequalities hold:*

$$R^{\rm SS}\le A^{\rm SS}-2T^{\rm SS}, \tag{2.23}$$

$$T^{\rm SS}\le A^{\rm SS}-2R^{\rm SS}. \tag{2.24}$$

In particular, these inequalities imply

$$A^{\rm SS}\le 3|E^{\rm SS}|,\quad T^{\rm SS}\le|E^{\rm SS}|\quad \textit{and}\quad R^{\rm SS}\le|E^{\rm SS}|. \tag{2.25}$$

Proof: Define $\rho_t(x)=t^{-3}\rho^{\rm SS}(t^{-1}x)$ with $t\ge 1$. The scaled density ρ_t satisfies (2.1) and (2.2) since $\rho^{\rm SS}$ does. (Note that $t\ge 1$ is important for (2.2).) Because $\rho^{\rm SS}$ is a minimizer, we have $\frac{d}{dt}\mathcal{E}^{\rm SS}[\rho_t]\big|_{t=1}\ge 0$. This gives (2.23). To prove (2.24) we multiply the variational equation (2.28) by $\sqrt{\rho^{\rm SS}}$ and integrate. Then (2.24) follows because $-\widehat{\mu}_N(x_\perp)\le 0$. Adding (2.23) and (2.24) we obtain $T^{\rm SS}+R^{\rm SS}\le\frac{2}{3}A^{\rm SS}$. Since $|E^{\rm SS}|+T^{\rm SS}+R^{\rm SS}=A^{\rm SS}$, this gives the first of (2.25). With (2.23) it also gives, $R^{\rm SS}\le|E^{\rm SS}|+R^{\rm SS}-T^{\rm SS}$, which is the second of (2.25). The third is analogous. ■

III. THE HYPER-STRONG MAGNETIC FIELD DENSITY FUNCTIONAL

We turn now to our next goal, which is to identify and to solve the $B/(2\pi Z^3)=\eta\to\infty$ limit of the super-strong theory. This we call the **hyper-strong theory** and it will turn out to be much simpler than the super-strong theory from which it arose.

The atom in the super-strong regime is very thin compared to its length. The radius in the $x_\perp$ direction is seen, from (2.20), to be $O(Z^{-1}\eta^{-1/2})$. From the bound on the eigenvalue $\widehat{\mu}_1$ in Lemma 2.1, with $a=Z^{-1}\eta^{-1/2}$, we surmise that the length is $O([Z\ln\eta]^{-1})$. This suggests that we first investigate the *one-dimensional* density $\overline{\rho}^{\rm SS}$ in the x_3 direction, which is obtained by integrating the density $\rho^{\rm SS}$ in the $x_\perp$ direction. Ultimately we shall prove that a suitably rescaled version of $\overline{\rho}^{\rm SS}$ has a nice limit, $\rho^{\rm HS}$, as $\eta\to\infty$, that $\rho^{\rm HS}$ satisfies a simple differential equation (which can be solved exactly), and that the energy can easily be computed in terms of $\rho^{\rm HS}$. Indeed, $\rho^{\rm HS}$ minimizes a simple energy functional. We begin this study with some preliminary remarks.

First, we note that if $\rho\in\mathcal{C}^{\rm SS}$ then the function $\overline{\rho}:\mathbf{R}\to\mathbf{R}^+$ defined by

$$\overline{\rho}(x)=\int_{\mathbf{R}^2}\rho(x_\perp,x)dx_\perp \tag{3.1}$$

is *a-priori* defined only for *almost* every $x \in \mathbf{R}$. In point of fact, $\overline{\rho}(x)$ is well defined for *every* $x \in \mathbf{R}$ because, as we shall show now, $\sqrt{\overline{\rho}} \in H^1(\mathbf{R})$ if $\rho \in \mathcal{C}^{\mathrm{SS}}$. Evidently $\int_{\mathbf{R}} \overline{\rho} < \infty$ so we have to prove that $T[\overline{\rho}] := \int_{\mathbf{R}} (d\sqrt{\overline{\rho}}/dx)^2 < \infty$. The map $f \to T[f] = \int_{\mathbf{R}} (d\sqrt{f}/dx)^2$ is convex (cf. [31] Theorem 7.1) and, since it is homogeneous of degree one, it is also sublinear. Thus, we have that

$$\begin{aligned} T[\overline{\rho}] = \int_{\mathbf{R}} \left(\frac{d}{dx} \sqrt{\overline{\rho}} \right)^2 &= \int_{\mathbf{R}} \left\{ \frac{d}{dx} \left[\int_{\mathbf{R}^2} \rho(x_\perp, x) dx_\perp \right]^{1/2} \right\}^2 dx \\ &\leq \int_{\mathbf{R}^2} \int_{\mathbf{R}} \left(\frac{d}{dx} \sqrt{\rho(x_\perp, x)} \right)^2 dx dx_\perp = T[\rho], \end{aligned} \tag{3.2}$$

which proves our claim.

Since functions in $H^1(\mathbf{R})$ are continuous, we have that $\overline{\rho}(x)$ is well defined and finite for every $\rho \in \mathcal{C}^{\mathrm{SS}}$ and every $x \in \mathbf{R}$. Indeed, $\overline{\rho}(x) \leq \left\{ \int \rho \right\}^{1/2} T[\rho]^{1/2}$ for every x.

We shall show below that as η approaches infinity the energy E^{SS} depends essentially only on the one-dimensional density $\overline{\rho}$. Indeed, we shall now introduce the limiting energy functional, the hyper-strong functional, which is defined for functions $\rho : \mathbf{R} \to \mathbf{R}^+$ in (1.26). The precise domain of definition of $\mathcal{E}^{\mathrm{HS}}$ is $\sqrt{\rho} \in H^1(\mathbf{R})$, i.e.,

$$\mathcal{C}^{\mathrm{HS}} = \{\rho : \ \rho \in L^1(\mathbf{R}), \ \ \rho \geq 0, \ \ d\sqrt{\rho}/dx \in L^2(\mathbf{R})\}. \tag{3.3}$$

Corresponding to $\mathcal{E}^{\mathrm{HS}}$ there is an energy

$$E^{\mathrm{HS}}(\lambda) := \inf\left\{\mathcal{E}^{\mathrm{HS}}[\rho] \, : \, \rho \in \mathcal{C}^{\mathrm{HS}}, \ \int_{\mathbf{R}} \rho \leq \lambda \right\}. \tag{3.4}$$

Clearly $\rho \mapsto \mathcal{E}^{\mathrm{HS}}[\rho]$ is strictly convex (because $\rho \mapsto \int \rho^2$ is strictly convex), and using Sobolev's inequality, it is easily seen to be bounded below (see the proof of Theorem 2.4). For the same reasons as before, $E^{\mathrm{HS}}(\lambda)$ is a convex and nonincreasing function of λ and we have

$$E^{\mathrm{HS}}(\lambda) = \inf\left\{\mathcal{E}^{\mathrm{HS}}[\rho] \, : \, \rho \in \mathcal{C}^{\mathrm{HS}}, \ \int_{\mathbf{R}} \rho = \lambda \right\}. \tag{3.5}$$

There is a critical λ_c, and $E^{\mathrm{HS}}(\lambda) = E^{\mathrm{HS}}(\lambda_c)$ for $\lambda > \lambda_c$.

3.1. THEOREM (Solution of the hyper-strong problem). *The hyper-strong problem (3.5) has a minimizer if and only if $\lambda \leq 2$. It is unique and given by $\rho^{\mathrm{HS}} = \psi^2$ with*

$$\begin{aligned} \psi(x) &= \frac{\sqrt{2}(2-\lambda)}{4 \sinh[\frac{1}{4}(2-\lambda)|x| + c]} && \textit{for } \lambda < 2 \\ \psi(x) &= \sqrt{2}(2+|x|)^{-1} && \textit{for } \lambda = 2, \end{aligned} \tag{3.6}$$

with $\tanh c = (2-\lambda)/2$. *The energy is*

$$E^{\rm HS}(\lambda) = \mathcal{E}^{\rm HS}[\psi^2] = -\tfrac{1}{4}\lambda + \tfrac{1}{8}\lambda^2 - \tfrac{1}{48}\lambda^3 \tag{3.7}$$

Proof: The existence of a minimizing ρ with $\int \rho \le \lambda$ is particularly simple. Since $\rho(x) \le 2\left\{\int \rho\right\}^{1/2}\{T[\rho]\}^{1/2} \le 2\sqrt{\lambda}T[\rho]^{1/2}$, we have that $\mathcal{E}^{\rm HS}[\rho] \ge T - 2\sqrt{\lambda}\sqrt{T}$ which is bounded below. This also shows that $T[\rho^{(n)}]$ is bounded for any minimizing sequence. Also, $\int(\rho^{(n)})^2$ remains bounded since $H^1(\mathbf{R}) \subset L^4(\mathbf{R})$. The lower semicontinuity of $\mathcal{E}^{\rm HS}[\rho]$ is trivial and we omit the proof. The uniqueness of the minimizer follows from the strict convexity of $\rho \mapsto \int \rho^2$.

The Euler-Lagrange equation is easy to derive (by replacing $\psi = \sqrt{\rho}$ by $\psi + \alpha f$ with $f \in C_0^\infty$ and α small). We omit the details. The distributional equation is

$$-\psi''(x) - \psi(0)\delta(x) + \psi(x)^3 = -\mu_\lambda \psi(x) \tag{3.8}$$

with $\delta(x)$ being Dirac's delta function at the origin. We want a solution to (3.8) with $\psi(x) \ge 0$ and $\int \psi^2 = \lambda$. Eq. (3.8) is equivalent to

$$-\psi''(x) + \psi(x)^3 = -\mu_\lambda \psi(x) \tag{3.9}$$

with the boundary condition $\psi'(0)/\psi(0) = -1/2$. By standard ordinary differential equation methods, we can note that the solution to (3.9) is unique once the three numbers $\psi'(0)$, $\psi(0)$ and μ_λ are specified. Thus, if we find a three parameter family of solutions, it must contain the correct one. We also note that a solution, ψ, to (3.8) which is in $H^1(\mathbf{R})$ must be a minimizer for $\mathcal{E}^{\rm HS}[\rho]$. This is so because ψ is then a critical point for $\mathcal{E}^{\rm HS}$, and a critical point of a convex function must be a minimizer.

Equation (3.9) is integrable in the form $(\psi')^2 = \frac{1}{2}\psi^4 + \mu_\lambda\psi^2$. The solution has the form

$$\psi(x) = \frac{a}{\sinh(b|x| + c)}$$

with $a, b, c > 0$. Then (3.9) and the delta-function condition at the origin are satisfied if

$$a^2 = 2b^2, \quad \mu_\lambda = b^2 \quad \text{and} \quad 2b = \tanh c,$$

the latter being the delta function condition at the origin. Thus b can range over the interval $\left(0, \frac{1}{2}\right)$. We find that

$$\lambda = \frac{2a}{b}\int_0^\infty [\sinh(x+c)]^{-2}dx = 2(1 - \tanh c)$$

This is the solution for $\lambda < 2$. The energy is given by

$$E^{\rm HS}(\lambda) = -\mu_\lambda \lambda - \tfrac{1}{2}\int_{-\infty}^{\infty} \psi^4(x)dx. \tag{3.10}$$

This yields (3.7) since $\int_c^\infty [\sinh x]^{-4}dx = [2 - 3\coth c + (\coth c)^3]/3$.

When $\lambda = \lambda_c = 2$ there is also a solution, obtained by taking the limit $b \to \infty$. This is given in (3.6).

We have obtained a minimizer for $0 \le \lambda \le 2$. Because (3.9) is integrable, we have found all $H^1(\mathbf{R})$ solutions to (3.8) and hence there can be no solution for $\lambda > 2$. There is also an indirect proof of this fact. Were there a solution for $\lambda > 2$, it would mean that $\mathcal{E}^{\rm HS}[\rho]$ has a minimizing ρ with $\lambda > 2$. But $E^{\rm HS}(\lambda)$ is seen to have a zero derivative at $\lambda = 2$ and we know that $E^{\rm HS}(\lambda)$ is convex and nonincreasing. Therefore, any minimizer with $\int \rho > 2$ would have to obey $\mathcal{E}^{\rm HS}[\rho] = E^{\rm HS}(2)$. But such a minimizer cannot exist because $\rho \mapsto \mathcal{E}^{\rm HS}[\rho]$ is *strictly* convex. ■

3.2. COROLLARY (Virial inequalities). *In analogy with Lemma 2.6, define the three components of the energy to be*

$$T^{\rm HS} = \int_{\mathbf{R}} \left(\frac{\partial}{\partial x}\sqrt{\rho^{\rm HS}(x)}\right)^2 dx, \quad A^{\rm HS} = \rho^{\rm HS}(0), \quad R^{\rm HS} = \tfrac{1}{2}\int_{\mathbf{R}} \rho^{\rm HS}(x)^2 dx,$$

where $\rho^{\rm HS}$ is the minimizer. Then

$$\begin{aligned} T^{\rm HS} &= |E^{\rm HS}| = \tfrac{1}{4}\lambda^2 - \tfrac{1}{8}\lambda^2 + \tfrac{1}{48}\lambda^2 \\ A^{\rm HS} &= \tfrac{1}{2}\lambda - \tfrac{1}{8}\lambda^2 \le 3|E^{\rm HS}| \quad \textit{and} \quad R^{\rm HS} = \tfrac{1}{8}\lambda^2 - \tfrac{1}{24}\lambda^3 \le |E^{\rm HS}|. \end{aligned}$$

In particular, $R^{\rm HS} = T^{\rm HS} = |E^{\rm HS}|$ and $A^{\rm HS} = 3|E^{\rm HS}|$ when $\lambda = \lambda_c = 2$.

We turn to the relationship between $E^{\rm SS}$ and $E^{\rm HS}$ as $\eta \to \infty$. First, we have to introduce the appropriate scaling for the functions $\rho \in \mathcal{C}^{\rm SS}$.

Scaling. If $\rho \in \mathcal{C}^{\rm SS}$, $x = (x_\perp, x_3)$, we define ρ_η by

$$\rho(x) = Z^4\eta\ln(\eta)\rho_\eta(Z\eta^{1/2}x_\perp, Z\ln(\eta)x_3). \tag{3.11}$$

We then have

$$\mathcal{E}^{\rm SS}[\rho] := Z^3[\ln\eta]^2\mathcal{E}_\eta^{\rm SS}[\rho_\eta] \tag{3.12}$$

where the function $\mathcal{E}_\eta^{\rm SS}$ is defined as follows:

$$\mathcal{E}_\eta^{\rm SS}[\rho_\eta] := \int \left(\frac{\partial\sqrt{\rho_\eta}}{\partial x_3}\right)^2 dx - \int \rho_\eta(x)V_\eta(x)dx + \tfrac{1}{2}\int\int \rho_\eta(x)V_\eta(x-y)\rho_\eta(y)dxdy \tag{3.13}$$

with

$$V_\eta(x) := \frac{1}{|\ln\eta|}(x_3^2 + \eta^{-1}|\ln\eta|^2 x_\perp^2)^{-1/2}, \tag{3.14}$$

The conditions (2.1) and (2.2) become

$$\int_{\mathbf{R}^3} \rho_\eta(x)dx = \lambda = N/Z \tag{3.15}$$

and

$$\int_{\mathbf{R}} \rho_\eta(x_\perp, x_3)dx_3 \le 1. \tag{3.16}$$

Corresponding to $\mathcal{E}_\eta^{\mathrm{SS}}$ there is an energy

$$E_\eta^{\mathrm{SS}}(\lambda) := \inf\{\mathcal{E}_\eta^{\mathrm{SS}}(\rho_\eta) \;:\; \rho_\eta \in \mathcal{C}^{\mathrm{SS}}, \int \rho_\eta \le \lambda,\ \rho_\eta \text{ satisfies (3.16)}\}.$$

This energy is related to E^{SS} by the scaling given in (3.12), i.e.,

$$E^{\mathrm{SS}}(N, Z, B) = Z^3[\ln\eta]^2 E_\eta^{\mathrm{SS}}(\lambda).$$

We shall denote the minimizing density by ρ_η^{SS}. It is obtained from the unscaled minimizer ρ^{SS} by the scaling in (3.11).

We have, by Corollary 2.5, that

$$-\mu_1^{\mathrm{SS}}(R^{\mathrm{SS}}) = \frac{\partial E^{\mathrm{SS}}}{\partial N} = Z^2[\ln\eta]^2 \frac{\partial E_\eta^{\mathrm{SS}}(\lambda)}{\partial\lambda}. \tag{3.17}$$

We shall now prove that $E_\eta^{\mathrm{SS}}(\lambda) \to E^{\mathrm{HS}}(\lambda)$ as $\eta \to \infty$. First we need the following estimate.

3.3. PROPOSITION. *For any choice of λ, T and $R > 0$ there is a constant $C(\lambda, T, R)$ such that if $\eta > 3$*

$$\left|\overline{\rho}(0) - \int_{\mathbf{R}^3} V_\eta \rho\right| \le C(\lambda, T, R)\left(\frac{1 + |\ln|\ln\eta||}{|\ln\eta|}\right) \tag{3.18}$$

when $\rho \in \mathcal{C}^{\mathrm{SS}}, \int\rho \le \lambda, \int \rho(x_\perp, x_3)dx_3 \le 1$, $T[\rho] \le T$ and $\rho(x_\perp, x_3) = 0$ for $|x_\perp| > R$. We can take $C(\lambda, T, R) = \lambda + 8\sqrt{2}\lambda^{1/4}T^{3/4} + (\mathrm{const.})TR(1 + |\ln R|)$.

Remark: If ρ satisfies the first four of the conditions above then the function $\rho_y(x) = \rho(x + y)$ also does so for all $y \in \mathbf{R}^3$. However, $\int V_\eta \rho_y \to 0$ as $|y| \to \infty$ while $\overline{\rho}_y(0)$ is independent of y provided $y_3 = 0$. Therefore $C(\lambda, T, R)$ cannot be independent of R.

Proof: We write the difference on the left side of (3.18) as $A_1 + A_2 + A_3$ with

$$A_1 = -\int_{|x_3|\ge 1} V_\eta(x)\rho(x)dx, \qquad A_2 = \int_{|x_3|\le 1} V_\eta(x)[\rho(x_\perp, 0) - \rho(x)]dx,$$

$$A_3 = \int_{\mathbf{R}^2}\left\{1 - \int_{|x_3|\le 1} V_\eta(x_\perp, x_3)dx_3\right\}\rho(x_\perp, 0)dx_\perp. \tag{3.19}$$

Since $|V_\eta(x)| \le 1/|\ln\eta|$ for $|x_3| \ge 1$, we have $|A_1| \le \lambda/|\ln\eta|$. To estimate A_2 we first note the following inequality for $\psi(x) := \sqrt{\rho(x)}$.

$$\psi(x_\perp, x_3) \le \left\{ \int_{-\infty}^{x_3} (\partial\psi^2/\partial x_3) dx_3 \right\}^{1/2} \le \sqrt{2}\lambda(x_\perp)^{1/4} T(x_\perp)^{1/4} \tag{3.20}$$

where $T(x_\perp) = \int_{\mathbf{R}} (\partial\psi/\partial x_3)^2 dx_3$ and $\lambda(x_\perp) = \int_{\mathbf{R}} \psi^2 dx_3$. Combining this with (2.4) we obtain

$$|\rho(x_\perp, x_3) - \rho(x_\perp, 0)| \le 2\sqrt{2}\sqrt{x_3}\lambda(x_\perp)^{1/4} T(x_\perp)^{3/4} \tag{3.21}$$

and hence

$$\begin{aligned} |A_2| &\le 2\sqrt{2} \int\limits_{|x_3|\le 1} V_\eta(x)\sqrt{x_3}\lambda(x_\perp)^{1/4} T(x_\perp)^{3/4} dx \\ &\le \frac{2\sqrt{2}}{|\ln\eta|} \left(\int\limits_{|x_3|\le 1} \frac{dx_3}{\sqrt{x_3}} \right) \int \lambda(x_\perp)^{1/4} T(x_\perp)^{3/4} dx_\perp \le \frac{8\sqrt{2}}{|\ln\eta|}\lambda^{1/4} T^{3/4}. \end{aligned}$$

Finally, we carry out the x_3- integration in (3.19) and obtain, using (3.20) and $\lambda(x_\perp) \le 1$:

$$\begin{aligned} |A_3| &= \left| \int \left[\frac{2}{|\ln\eta|} \sinh^{-1}\Big(\eta^{1/2}/(|\ln\eta||x_\perp|)\Big) - 1 \right] \rho(x_\perp, 0) dx_\perp \right| \\ &\le 2T \left\{ \int\limits_{|x_\perp|\le R} \left[\frac{2}{|\ln\eta|} \sinh^{-1}\Big(\eta^{1/2}/(|\ln\eta||x_\perp|)\Big) - 1 \right]^2 dx_\perp \right\}^{1/2} \\ &\le (\text{const.}) \frac{T}{|\ln\eta|} \left\{ \int_{|x_\perp|\le R} \Big[(\ln|x_\perp|)^2 + (\ln|\ln\eta|)^2 \Big] dx_\perp \right\}^{1/2}. \end{aligned}$$

The last inequality follows from

$$\sinh^{-1}(1/\varepsilon|x_\perp|) = \ln(1/\varepsilon) + \ln(1/|x_\perp|) + \ln(1 + \sqrt{1 + \varepsilon^2|x_\perp|^2}).$$

Moreover, $\ln(\eta^{-1/2}|\ln\eta|) = -\frac{1}{2}|\ln\eta| + O(\ln|\ln\eta|)$, so that

$$\begin{aligned} &\left[\frac{2}{|\ln\eta|} \sinh^{-1}\Big(\eta^{1/2}/(|\ln\eta||x_\perp|)\Big) - 1 \right]^2 \\ &= \frac{4}{|\ln\eta|^2} \left[\ln(1/|x_\perp|) + O(\ln|\ln\eta|) + \ln(1 + \sqrt{1 + \eta^{-1}|\ln\eta|^2|x_\perp|^2}) \right]^2 \\ &\le (\text{const.}) \frac{1}{|\ln\eta|^2} \Big[(\ln|x_\perp|)^2 + (\ln|\ln\eta|)^2 \Big]. \qquad \blacksquare \end{aligned}$$

As a corollary of Proposition 3.3 we obtain

3.4. PROPOSITION: *For $C(\lambda, T, R)$ and ρ as in Proposition 3.2 one has*

$$\left| \int_{\mathbf{R}^3} \int_{\mathbf{R}^3} \rho(x) V_\eta(x-y)\rho(y) dx dy - \int_{\mathbf{R}} \overline{\rho}(x)^2 dx \right| \leq \lambda C(\lambda, T, 2R) \left(\frac{1 + |\ln|\ln\eta||}{|\ln\eta|} \right).$$

Proof: Write $y = x - \xi$ and apply (3.18) to the ξ- integration for fixed x. ■

3.5. THEOREM (E^{HS} is the limit of E_η^{SS}). *For all $\lambda \geq 0$*

$$\lim_{\eta\to\infty} Z^{-3}[\ln(B/Z^3)]^{-2} E^{\mathrm{SS}}(N, Z, B) = \lim_{\eta\to\infty} E_\eta^{\mathrm{SS}}(\lambda) = E^{\mathrm{HS}}(\lambda).$$

Furthermore, if ρ_η^{SS} and ρ^{HS} denote the super-strong and hyper-strong minimizers respectively, we have for all $\lambda \geq 0$

$$\overline{\rho}_\eta^{\mathrm{SS}} \to \rho^{\mathrm{HS}} \quad in\ L^1_{\mathrm{loc}}(\mathbf{R}).$$

If $\lambda \leq 2$ we get

$$\sqrt{\overline{\rho}_\eta^{\mathrm{SS}}} \to \sqrt{\rho^{\mathrm{HS}}} \quad in\ H^1(\mathbf{R}).$$

Proof: Let $\chi_\lambda : \mathbf{R}^2 \to \mathbf{R}^+$ be given by $\chi_\lambda(x_\perp) = 1/\lambda$ for $|x_\perp| \leq \sqrt{\lambda/\pi}$ (which is the rescaled version of the upper bound $\sqrt{2N/B}$ on the cylindrical radius of the atom) and $\chi_\lambda(x_\perp) = 0$ otherwise. For each function $\widehat{\rho} \in \mathcal{C}^{\mathrm{HS}}$ with $\int_{\mathbf{R}} \widehat{\rho} \leq \lambda$ we define $\rho \in \mathcal{C}^{\mathrm{SS}}$ by $\rho(x_\perp, x_3) = \chi_\lambda(x_\perp)\widehat{\rho}(x_3)$. In terms of (3.1), $\overline{\rho} = \widehat{\rho}$. Also, $\int_{\mathbf{R}^3} \rho \leq \lambda$ and $\int_{\mathbf{R}} \rho dx_3 \leq 1$. Furthermore, $T[\rho] = \int_{\mathbf{R}} (d\sqrt{\widehat{\rho}}/dx)^2$. Using Propositions 3.3 and 3.4 we have $\mathcal{E}_\eta^{\mathrm{SS}}[\rho] \leq \mathcal{E}^{\mathrm{HS}}[\widehat{\rho}] + (1+\lambda)C(\lambda, T, 2R)(1 + |\ln|\ln\eta||)/|\ln\eta|$. Therefore, $\limsup_{\eta\to\infty} E_\eta^{\mathrm{SS}}(\lambda) \leq E^{\mathrm{HS}}(\lambda)$.

To derive the inequality $\liminf_{\eta\to\infty} E_\eta(\lambda) \geq E^{\mathrm{HS}}(\lambda)$ we can take any $\rho \in \mathcal{C}^{\mathrm{SS}}$ and define $\overline{\rho} \in \mathcal{C}^{\mathrm{HS}}$ by (3.1). Evidently $\overline{\rho}$ satisfies all the requisite conditions for the $\mathcal{E}^{\mathrm{HS}}$ minimization problem. The rest follows as in the preceding paragraph, but with the additional information provided by (3.2) that $T[\rho] \geq T[\overline{\rho}]$.

To prove the convergence of the densities we first notice that the convergence of the energies and Propositions 3.3 and 3.4 imply that $\mathcal{E}^{\mathrm{HS}}[\overline{\rho}_\eta^{\mathrm{SS}}] \to E^{\mathrm{HS}}(\lambda)$ as $\eta \to \infty$. This fact, together with the uniqueness of the minimizer for $\mathcal{E}^{\mathrm{HS}}$, implies that our theorem will be established if we prove that for any *minimizing* sequence ρ_n, with $\int \rho_n = \lambda$, there is a subsequence ρ_{n_k} such that $\sqrt{\rho_{n_k}} \to \sqrt{\rho^{\mathrm{HS}}}$ in $L^2_{\mathrm{loc}}(\mathbf{R})$ and in $H^1(\mathbf{R})$ if $\lambda \leq 2$ as $k \to \infty$.

Since $T[\rho_n] = \int (d\sqrt{\rho_n}/dx)^2$ is bounded (see the proof of Theorem 3.1), the sequence $\sqrt{\rho_n}$ is bounded in $H^1(\mathbf{R})$. Thus, by passing to a subsequence (that we again denote ρ_n) we can assume, by the Banach-Alaoglu theorem, that $\sqrt{\rho_n}$ converges weakly in $H^1(\mathbf{R})$ to some function $\sqrt{\rho_\eta}$ which, by lower semicontinuity, minimizes $\mathcal{E}_{\mathrm{HS}}$, i.e., $\rho_\eta = \rho^{\mathrm{HS}}$. Weak convergence in $H^1(\mathbf{R})$ implies that we can find a subsequence that converges strongly in $L^2_{\mathrm{loc}}(\mathbf{R})$. To show strong convergence in

$H^1(\mathbf{R})$ we only have to conclude that the $H^1(\mathbf{R})$ norm of $\sqrt{\rho_n}$ converges to the $H^1(\mathbf{R})$ norm of $\sqrt{\rho^{\rm HS}}$. Since $\int \rho_n = \lambda$ and $\int \rho^{\rm HS} = \lambda \leq 2$, we have that $\sqrt{\rho_n}$ converges strongly to $\sqrt{\rho^{\rm HS}}$ in $L^2(\mathbf{R})$. It is therefore enough to prove that $T[\rho_n]$ converges to $T[\rho]$.

Because of the strong $L^2(\mathbf{R})$ convergence we can pass to a subsequence such that $\rho_n(x)$ converges to $\rho^{\rm HS}(x)$ for almost every $x \in \mathbf{R}$. But since $T[\rho_n]$ is bounded, this convergence must, in fact, occur for *every* $x \in \mathbf{R}$. Thus $\rho_n(0) \to \rho^{\rm HS}(0)$. Also, lower semicontinuity in the $H^1(\mathbf{R})$ topology (which we also used in the beginning of Theorem 3.1) means that

$$\liminf_{n\to\infty} \int (d\sqrt{\rho_n}/dx)^2 dx \geq \int (d\sqrt{\rho^{\rm HS}}/dx)^2 dx \tag{3.22}$$

and

$$\liminf_{n\to\infty} \int \rho_n(x)^2 dx \geq \int \rho^{\rm HS}(x)^2 dx. \tag{3.23}$$

(Note that (3.23) is also a consequence of Fatou's Lemma.) Since $\mathcal{E}^{\rm HS}[\rho_n]$ converges to $E^{\rm HS}(\lambda)$, we see that both (3.22) and (3.23) must be equalities. But (3.22) (with equality) is precisely what was needed to complete the proof. ■

Since $\lambda \mapsto E^{\rm HS}(\lambda)$ is strictly decreasing for $\lambda \leq 2$ we immediately conclude from Theorem 3.5 that the following version of Theorem 1.5 holds in the SS theory.

3.6. COROLLARY. *As $B/Z^3 \to \infty$ we get for the critical electron number $N_c^{\rm SS}$ the lower bound* $\liminf_{B/Z^3\to\infty} N_c^{\rm SS}/Z \geq 2$.

IV. THE DENSITY MATRIX FUNCTIONAL

In this section we present a third functional which is more complicated than the functionals $\mathcal{E}^{\rm SS}$ and $\mathcal{E}^{\rm HS}$. It is not a functional of a density ρ, but depends on a density matrix of a new type that we shall now describe. Each density matrix we shall consider is a *one-dimensional*, single-particle density matrix that is defined for each value of $x_\perp \in \mathbf{R}^2$. It will be denoted by $\Gamma_{x_\perp}$ or, if we need to include the one-dimensional coordinates explicitly, as $\Gamma_{x_\perp}(x_3, x_3')$.

Our new functional is defined on the convex set $\mathcal{G}_B^{\rm DM}$ of $L^2(\mathbf{R})$-operator valued functions $\Gamma : \mathbf{R}^2 \ni x_\perp \mapsto \Gamma_{x_\perp}$ that satisfy the conditions

$$\begin{aligned}
&\text{(a)}\quad x_\perp \mapsto (f, \Gamma_{x_\perp} f) \text{ is measurable for all } f \in L^2(\mathbf{R})\\
&\text{(b)}\quad \Gamma_{x_\perp} \text{ is a positive semidefinite trace class operator on } L^2(\mathbf{R}) \text{ for almost all } x_\perp \in \mathbf{R}^2\\
&\text{(c)}\quad 0 \leq \Gamma_{x_\perp} \leq (B/2\pi) I \text{ for almost all } x_\perp \in \mathbf{R}^2\\
&\text{(d)}\quad \int_{\mathbf{R}^2} {\rm Tr}_{L^2(\mathbf{R})}[(1 - \partial^2/\partial x_3^2)\Gamma_{x_\perp}] dx_\perp < \infty.
\end{aligned} \tag{4.1}$$

Conditon (d) requires some explanation. The expression $T(x_\perp) := \mathrm{Tr}_{L^2(\mathbf{R})}[-\partial_3^2 \Gamma_{x_\perp}]$ is *defined* to be $\sum_n \alpha_n \int_{\mathbf{R}} |df_n(x_3)/dx_3|^2 dx_3$ where $0 \le \alpha_n \le B/2\pi$ and f_n are the eigenvalues and normalized eigenvectors of $\Gamma_{x_\perp}$. Our notation suppresses the dependence of α_n and f_n on $x_\perp$ and we neither assume nor prove here that these quantities are $x_\perp$-measurable. It is important, however, and easy to prove, that $T(x_\perp)$ is a measurable function; condition (d) then requires it to be in $L^1(\mathbf{R}^2)$. First of all, it is easy to check (by Fubini's Theorem for sums) that

$$T(x_\perp) = \sum\nolimits_k \left(\frac{d\phi_k}{dx_3}, \Gamma_{x_\perp} \frac{d\phi_k}{dx_3} \right) \tag{4.2}$$

where $\phi_1, \phi_2, \ldots$ are $C_0^\infty(\mathbf{R})$ functions that form an orthonormal basis for $L^2(\mathbf{R})$. From (4.2) and condition (a), $x_\perp \mapsto T(x_\perp)$ is evidently measurable.

Since $\Gamma_{x_\perp}$ is trace class we can define the map $\mathcal{G}_B^{\mathrm{DM}} \ni \Gamma \mapsto \rho_\Gamma \in L^1(\mathbf{R}^3)$ by

$$\rho_\Gamma(x) := \Gamma_{x_\perp}(x_3, x_3) = \sum_n \alpha_n |f_n(x_3)|^2. \tag{4.3}$$

Remark: To show that ρ_Γ is a measurable function on $\mathbf{R}^3$ it is enough to show that

$$\rho_\Gamma(x_\perp, x_3) = \lim_{k\to\infty} (\zeta_k^{(x_3)}, \Gamma_{x_\perp} \zeta_k^{(x_3)}), \tag{4.4}$$

where $\zeta_k^{(x_3)} = \frac{k}{2}\chi_{[x_3-k^{-1}, x_3+k^{-1}]}$ (χ_A denotes the characteristic function of the set A). The reason (4.4) suffices is that $(\rho_k^{(x_3)}, \Gamma_{x_\perp}\rho_k^{(x_3)}) = \sum_{m,n} (\rho_k^{(x_3)}, \phi_m)(\phi_m, \Gamma_{x_\perp}\phi_n)(\phi_n, \rho_k^{(x_3)})$, where $\phi_1, \phi_2, \ldots$ are an ($x_\perp$ independent) orthonormal basis as before. The first and last factors are measurable functions of x_3, while the middle factor is a measurable function of $x_\perp$. The product is then a measurable function on $\mathbf{R}^3$. Finally, we note that the pointwise limit (i.e., $k \to \infty$) of measurable functions is measurable.

Now we turn to the proof of (4.4). Using the $x_\perp$ dependent eigenfunctions f_n, we can write

$$(\zeta_k^{(x_3)}, \Gamma_{x_\perp} \zeta_k^{(x_3)}) = \sum_n \alpha_n |(f_n, \zeta_k^{(x_3)})|^2.$$

Introducing the maximal function M_{f_n} of f_n we have (by definition) that $|(f_n, \zeta_k^{(x_3)})| \le M_{f_n}(x_3)$ and the maximal inequality $\int M_{f_n}(x_3)^2 \le \|f_n\|^2 = 1$. Since $(f_n, \zeta_k^{(x_3)}) \to f_n(x_3)$ for almost every x_3 as $k \to \infty$ by Lebesgue's Theorem, we can use dominated convergence to conclude that

$$\lim_{k\to\infty} \sum_n \alpha_n |(f_n, \zeta_k^{(x_3)})|^2 = \sum_n \alpha_n |f_n(x_3)|^2 = \rho_\Gamma(x).$$

The density ρ_Γ is a non-negative function with the properties

$$\begin{aligned}&\text{(a)}\quad \int \rho_\Gamma(x)dx = \int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}\left[\Gamma_{x_\perp}\right] dx_\perp \\ &\text{(b)}\quad \int_{\mathbf{R}} \left(\frac{\partial\sqrt{\rho_\Gamma(x)}}{\partial x_3}\right)^2 dx_3 \le \mathrm{Tr}_{L^2(\mathbf{R})}\left[-\tfrac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right] \text{ for almost all } x_\perp \in \mathbf{R}^2.\end{aligned} \tag{4.5}$$

Property (b) is easily seen by again writing $\Gamma_{x_\perp} = \sum_n \alpha_n f_n \otimes \overline{f}_n$. Then by a standard argument in the theory of distributions, and using the fact that the f_n's are in $H^1(\mathbf{R})$, we have that for almost every $x_\perp$

$$\left|\frac{\partial\sqrt{\rho_\Gamma(x)}}{\partial x_3}\right| = (\sqrt{\rho_\Gamma})^{-1}\left|\frac{\partial\rho_\Gamma}{\partial x_3}\right| \le (\sqrt{\rho_\Gamma})^{-1}\sum_n \alpha_n|f_n|\left|\frac{\partial f_n}{\partial x_3}\right|,$$

with the understanding that the right side is zero where $\rho_\Gamma = 0$. Since $\rho_\Gamma = \sum_n \alpha_n|f_n|^2$, property (b) in (4.5) follows by estimating the sum above by the Cauchy-Schwarz inequality.

We point out that the set $\mathcal{C}^{\mathrm{SS}}$ defined in the previous section can be thought of as a subset of $\bigcup_{B>0}\mathcal{G}_B^{\mathrm{DM}}$. In fact, if $\rho \in \mathcal{C}^{\mathrm{SS}}$ we can define $\Gamma^\rho_{x_\perp}$ by the integral kernel $\Gamma^\rho_{x_\perp}(x_3, x_3') = \sqrt{\rho(x_\perp, x_3)\rho(x_\perp, x_3')}$. The conditions (2.3) (with $C = B/2\pi$) on ρ translate into the conditions (4.1) on Γ^ρ.

Notice that in general ρ_Γ does not satisfy condition (b) of (2.3) with $C = B/2\pi$. This property would follow if we knew that $\Gamma_{x_\perp}$ is of rank one for almost all $x_\perp$, i.e., we can make the following identification

$$\mathcal{C}^{\mathrm{SS}} = \bigcup_{B>0}\{\Gamma \in \mathcal{G}_B^{\mathrm{DM}} \,:\, \Gamma_{x_\perp} \text{ has rank at most one for almost all } x_\perp\}.$$

To motivate the definition $\mathcal{G}_B^{\mathrm{DM}}$ we consider an antisymmetric many-body wave function Ψ in the lowest Landau band in the sense that $\Pi_0^N\Psi = \Psi$, where Π_0^N is the projection of the physical Hilbert space $\bigwedge_1^N L^2(\mathbf{R}^3)$ onto the subspace where all the electrons are in the lowest Landau band. For such a function Ψ we define

$$\Gamma^\Psi_{x_\perp}(x_3, x_3') = N\int \Psi(x_\perp, x_3; x^2, \ldots, x^N)\overline{\Psi(x_\perp, x_3'; x^2, \ldots, x^N)}dx^2\ldots dx^N. \tag{4.6}$$

4.1 LEMMA. *If the normalized many-body wave function Ψ satisfies $\Pi_0^N\Psi = \Psi$ and $(\Psi, \sum_i H^i_{\mathbf{A}}\Psi) < \infty$ then Γ^Ψ defined in (4.6) is in $\mathcal{G}_B^{\mathrm{DM}}$.*

Proof: Consider the kernel of the usual one-particle density matrix K_Ψ for Ψ given in (1.19). Then K_Ψ is an operator in $L^2(\mathbf{R}^3)$ satisfying $0 \le K_\Psi \le I$ and $\Pi_0 K_\Psi \Pi_0 = K_\Psi$ and we have $\Gamma^\Psi_{x_\perp}(x_3, x_3') = K_\Psi(x_\perp, x_3; x_\perp, x_3')$. Conditions (b) and (d) of (4.1) are now clearly satisfied by Γ^Ψ.

In order to prove (c) we first notice that for all $x_\perp \in \mathbf{R}^2$ we can find a sequence (u_n) in $L^2(\mathbf{R}^2)$ converging in the sense of distributions to the Dirac delta function $\delta_{x_\perp}$ at $x_\perp \in \mathbf{R}^2$ such that for all $f \in L^2(\mathbf{R})$ the sequence $\Pi_0(u_n \otimes f)$ converges in $L^2(\mathbf{R}^3)$. This follows from the expression (1.14) for Π_0. Furthermore, $(u_n \otimes f, \Pi_0(u_n \otimes f)) \to (B/2\pi)\|f\|^2_{L^2(\mathbf{R})}$ as $n \to \infty$. Then condition (c) indeed follows from

$$(u_n \otimes f, K_\Psi(u_n \otimes f)) = (u_n \otimes f, \Pi_0 K_\Psi \Pi_0(u_n \otimes f)) \leq (u_n \otimes f, \Pi_0(u_n \otimes f))$$

for all $x_\perp \in \mathbf{R}^2$ in the limit as $n \to \infty$. ∎

We now define our density matrix functional on the set $\mathcal{G}_B^{\mathrm{DM}}$ by (1.22) Because of the convexity of the kernel $|x-y|^{-1}$, this is a convex functional on the (convex) set $\mathcal{G}_B^{\mathrm{DM}}$. Since two different density matrices might have the same density the functional is not strictly convex.

The energy for this density matrix functional is, as usual, defined to be

$$E^{\mathrm{DM}}(N,Z,B) = \inf\{\mathcal{E}^{\mathrm{DM}}[\Gamma] \,:\, \Gamma \in \mathcal{G}_B^{\mathrm{DM}},\ \int \rho_\Gamma \leq N\}. \tag{4.7}$$

Notice that the dependence of the energy on B is only through the set $\mathcal{G}_B^{\mathrm{DM}}$.

That the energy is bounded below, i.e., $E^{\mathrm{DM}}(N,Z,B) > -\infty$, follows from the following lemma by ignoring the positive repulsive term, i.e., the last term in (1.22).

4.2 LEMMA. *If $\Gamma \in \mathcal{G}_B^{\mathrm{DM}}$ we have for almost every $x_\perp$*

$$\int_{\mathbf{R}} \rho_\Gamma(x)^3 dx_3 \leq \left(\frac{3}{\pi^2}\right) B^2 \mathrm{Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right]. \tag{4.8}$$

If, furthermore, $\int \rho_\Gamma \leq N$ and $\hat{h}_{Z,x_\perp}$ is the one-dimensional operator on $L^2(\mathbf{R})$ given in Lemma 2.1, i.e.,

$$\hat{h}_{Z,x_\perp} = -\frac{\partial^2}{\partial x_3^2} - \frac{Z}{|x|} = -\frac{\partial^2}{\partial x_3^2} - \frac{Z}{\sqrt{|x_\perp|^2 + x_3^2}}, \tag{4.9}$$

we have the bounds

$$\int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}\left[\hat{h}_{Z,x_\perp}\Gamma_{x_\perp}\right] dx_\perp \geq -\tfrac{5}{6}(\tfrac{\pi}{2})^{2/5} Z^{6/5} N^{3/5} B^{2/5} \tag{4.10}$$

and

$$\int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}\left[\hat{h}_{Z,x_\perp}\Gamma_{x_\perp}\right] dx_\perp \geq -2NZ^2\left[\ln(2^{-1/2}Z^{-1}N^{-1/2}B^{1/2} + \tfrac{1}{2})\right]^2 - NZ^2. \tag{4.11}$$

Proof: The bound (4.8) is a special case of the one-dimensional Lieb-Thirring inequality [40]. To prove (4.8) we notice that since $\Gamma_{x_\perp} \leq \frac{B}{2\pi} I$ we get for all $\alpha > 0$ that

$$\mathrm{Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right] - \alpha\int_{\mathbf{R}} \rho_\Gamma(x)^3 dx_3$$

is bounded below by the sum of the negative eigenvalues of the one-dimensional operator $-\frac{\partial^2}{\partial x_3^2} - \alpha\rho_\Gamma(x)^2$ multiplied by $B/2\pi$. The Lieb-Thirring inequality implies that the sum of the negative eigenvalues is in turn bounded below by $-\frac{4}{3}\int_{\mathbf{R}}\left(\alpha\rho_\Gamma(x)^2\right)^{3/2}dx_3$. Thus by optimizing over α

$$\begin{aligned}\mathrm{Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right] &\geq \left(\alpha - \frac{2}{3\pi}B\alpha^{3/2}\right)\int_{\mathbf{R}}\rho_\Gamma(x)^3 dx_3 \\ &\geq \frac{\pi^2}{3}B^{-2}\int_{\mathbf{R}}\rho_\Gamma(x)^3 dx_3.\end{aligned}$$

The second bound (4.10) also follows from the Lieb-Thirring inequality. In fact, for all $R > 0$ we get by using the Lieb-Thirring inequality for $|x_\perp| < R$ that

$$\int_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}\left[\hat{h}_{Z,x_\perp}\Gamma_{x_\perp}\right]dx_\perp \geq -\frac{2}{3\pi}B\int_{|x_\perp|\leq R}\left(\frac{Z}{|x|}\right)^{3/2}dx - \frac{NZ}{R}. \tag{4.12}$$

The last term which is the estimate for $|x_\perp| > R$ follows from

$$\int_{|x_\perp|>R}\mathrm{Tr}_{L^2(\mathbf{R})}\left[\hat{h}_{Z,x_\perp}\Gamma_{x_\perp}\right]dx_\perp \geq -\frac{Z}{R}\int\rho_\Gamma(x)dx \geq -\frac{NZ}{R}.$$

Optimizing (4.12) over R gives (4.10).

Although the estimate (4.10) is always correct it is only interesting when $B \lesssim NZ^2$. When $B \gtrsim NZ^2$ the last estimate (4.11) is better than (4.10). To prove (4.12) we appeal to Lemma 2.1 on the one- dimensional Coulomb problem. Let the first two eigenvalues of $\hat{h}_{Z,x_\perp}$ be denoted by $-\hat{\mu}_1(|x_\perp|)$, $-\hat{\mu}_2(|x_\perp|)$. Then since $\hat{\mu}_1$ is a monotone decreasing function of $|x_\perp|$, we see that the optimal (in the sense of minimizing the left side of (4.11)) density matrix Γ is obtained by concentrating as many particles as possible in the lowest eigenstate of $\hat{h}_{Z,x_\perp}$ in a disk $|x_\perp| < R$. Since $\Gamma \in \mathcal{G}_B^{\mathrm{DM}}$ implies $0 \leq \Gamma_{x_\perp} \leq (B/2\pi)I$, which means that the two-dimensional density in each state is less than $B/2\pi$, we conclude that R must be less than $\sqrt{2N/B}$. Indeed, $R = \sqrt{2N/B}$ if we never have to occupy the second eigenstate of $\hat{h}_{Z,x_\perp}$, that is if $-\widehat{\mu}_1(R) \leq \inf_{x_\perp}(-\mu_2(|x_\perp|)$. Although this inequality does not hold in general it is satisfied for the lower bounds on $-\hat{\mu}_1$ and $-\hat{\mu}_2$ given in Lemma 2.1. Replacing $\hat{h}_{Z,x_\perp}$ by the smaller operator having the same eigenfunctions as $\widehat{h}_{Z,x_\perp}$ and having these bounds as the exact eigenvalues, we obtain

$$\int_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}\left[\hat{h}_{Z,x_\perp}\Gamma_{x_\perp}\right]dx_\perp \geq -\frac{B}{2\pi}Z^2\int_{|x_\perp|^2<2NB^{-1}}\left(1 + \left[\sinh^{-1}\left(\frac{1}{Z|x_\perp|}\right)\right]^2\right)dx_\perp.$$

Using $\sinh^{-1}t = \ln(t + \sqrt{1+t^2})$ we easily arrive at the bound (4.12).■

The energy E^{DM} obeys the scaling relation (1.24). Indeed, if $\Gamma \in \mathcal{G}_B^{\mathrm{DM}}$ then, defining $\widetilde{\Gamma}$ by the following relation between the integral kernels

$$\widetilde{\Gamma}_{x_\perp}(x_3, x_3') = Z^{-4}\Gamma_{Z^{-1}x_\perp}(Z^{-1}x_3, Z^{-1}x_3'),$$

we get $\widetilde{\Gamma} \in \mathcal{G}^{\rm DM}_{B/Z^3}$, since if $f \in L^2(\mathbf{R})$ with $\|f\| = 1$, then

$$
\begin{aligned}
(f, \widetilde{\Gamma}_{x_\perp} f) &= Z^{-2} \int_{\mathbf{R}} \int_{\mathbf{R}} \overline{f(Zx_3)} \widetilde{\Gamma}_{Z^{-1}x_\perp}(x_3, x_3') f(Zx_3') dx_3 dx_3' \\
&\leq Z^{-2} \frac{B}{2\pi} \int_{\mathbf{R}} |f(Zx_3)|^2 dx_3 = \frac{B}{2\pi Z^3},
\end{aligned}
$$

by (4.1), and thus $\widetilde{\Gamma}_{x_\perp} \leq B/(2\pi Z^3) I$. Furthermore, $\int \rho_{\widetilde{\Gamma}} = N/Z$ and $\mathcal{E}^{\rm DM}[\widetilde{\Gamma}] = Z^{-3}\mathcal{E}^{\rm DM}[\Gamma]$.

We are now prepared to show the existence of a unique minimizer in (4.7). This result is significantly more difficult than the corresponding result, Theorem 2.2, for the super-strong functional.

4.3 THEOREM (Unique minimizer for $\mathcal{E}^{\rm DM}$). *For each $N \geq 0$ there is a unique minimizer $\Gamma^{\rm DM} \in \mathcal{G}^{\rm DM}_B$ for $\mathcal{E}^{\rm DM}$ with $\int \rho_{\Gamma^{\rm DM}} \leq N$, i.e., $E^{\rm DM}(N, Z, B) = \mathcal{E}^{\rm DM}[\Gamma^{\rm DM}]$. The energy $E^{\rm DM}(N, Z, B)$ is a monotonically non-increasing, convex function of N and a non-increasing function of B.*

Proof of existence of a minimizer: Let $\Gamma^{(n)}$ be a minimizing sequence for $\mathcal{E}^{\rm DM}$ with $\int \rho_{\Gamma^{(n)}} \leq N$, i.e., $\mathcal{E}^{\rm DM}[\Gamma^{(n)}] \to E^{\rm DM}(N, Z, B)$ as $n \to \infty$. We can conclude from (4.8) that $\rho^{(n)} := \rho_{\Gamma^{(n)}}$ is a bounded sequence in $L^3(\mathbf{R}^3)$. As in the proof of Theorem 2.2 we can use the convexity of the functional $\mathcal{E}^{\rm DM}$ to find a new minimizing sequence, which we still denote $\Gamma^{(n)}$, and a non-negative function $\rho^\infty \in L^3(\mathbf{R}^3)$ with $\int \rho^\infty \leq N$ such that

(i) $\lim_{n\to\infty} \rho^{(n)}(x) = \rho^\infty(x)$ for almost every x.
(ii) There is a function $G \in L^3(\mathbf{R}^3) \cap L^{6/5}(\mathbf{R}^3)$ such that $\rho^{(n)}(x) \leq G(x)$ for all x and n.

It follows from this by dominated convergence that $D(\rho^{(n)} - \rho^\infty, \rho^{(n)} - \rho^\infty) \to 0$, as $n \to \infty$. In fact, if, as in the super-strong case, we write $\mathcal{E}^{\rm DM}[\Gamma]$ as a sum of three terms, $T[\Gamma] + A[\rho_\Gamma] + R[\rho_\Gamma]$, we have

$$\lim_{n\to\infty} A[\rho^{(n)}] = A[\rho^\infty]$$

and

$$\lim_{n\to\infty} R[\rho^{(n)}] = R[\rho^\infty].$$

To conclude the proof of the existence part of the theorem we have to find a $\Gamma^{\rm DM} \in \mathcal{G}^{\rm DM}_B$ having the following two properties.

$$T[\Gamma^{\rm DM}] \leq \liminf_{n\to\infty} T[\Gamma^{(n)}], \tag{4.13}$$

and

$$\rho_{\Gamma^{\rm DM}} = \rho^\infty. \qquad (4.14).$$

To show the existence of such a $\Gamma^{\rm DM}$ we again choose functions $\phi_1, \phi_2, \ldots$ in $C_0^\infty(\mathbf{R})$ that form an orthonormal basis for $L^2(\mathbf{R})$. From condition (c) of (4.1) we conclude that the functions on $\mathbf{R}^2$, given by $m_{k\ell}^{(n)}(x_\perp) = (\phi_k, \Gamma_{x_\perp}^{(n)} \phi_\ell)$, are bounded by $B/2\pi$.

We shall now argue that by taking a subsequence of convex combinations of the $\Gamma^{(n)}$'s we can construct a new minimizing sequence for $\mathcal{E}^{\rm DM}$ in $\mathcal{G}_B^{\rm DM}$, which we again denote $\Gamma^{(n)}$, for which the sequences $m_{k\ell}^{(n)}(x_\perp)$ converge pointwise almost everywhere and for which the limit $\rho^{(n)} \to \rho^\infty$ is unchanged. For each sequence, i.e., for each fixed k and ℓ, this claim follows by a slight modification of the argument using Mazur's Theorem that we used above and in Theorem 2.1. Indeed, since the function $x_\perp \mapsto m_{k\ell}^{(n)}(x_\perp)$ is bounded, we can pick a bounded set $A \subset \mathbf{R}^2$ and, by Banach-Alaoglu, pass to a subsequence such that we also get weak $L^2(A)$ convergence. By using Mazur's Theorem again (as in Theorem 2.1), we can convert this into strong convergence in $L^2(A)$, and then, by passing, to a further subsequence, obtain pointwise convergence almost everywhere. By doing this for countably many A's that cover $\mathbf{R}^2$, and using Cantor's "diagonal" argument, we can finally obtain a minimizing sequence $\Gamma^{(n)}$ such that $m_{k\ell}^{(n)}$ converges pointwise almost everywhere in $\mathbf{R}^2$. We have thus proved the claim for every one of the countably many pairs k, ℓ. Using a "diagonal" argument once more we obtain a sequence such that $m_{k\ell}^{(n)}$ converges almost everywhere for all pairs.

Since $\Gamma_{x_\perp}^{(n)}$ is bounded in norm by $B/2\pi$ we have now that there is a subset of $\mathbf{R}^2$ of measure zero such that the sequence $(f, \Gamma_{x_\perp}^{(n)} g)$ converges pointwise for $x_\perp$ outside this set for all pairs of functions $f, g \in L^2(\mathbf{R})$. This limit defines bounded quadratic forms on $L^2(\mathbf{R})$ for almost every $x_\perp$. These quadratic forms in turn define operators $\Gamma_{x_\perp}^{\rm DM}$ for which we have

$$\Gamma_{x_\perp}^{(n)} \rightharpoonup \Gamma_{x_\perp}^{\rm DM}, \tag{4.15}$$

weakly as operators on $L^2(\mathbf{R})$ for almost every $x_\perp$. It is clear that the density matrix valued function defined by $\Gamma^{\rm DM} : x_\perp \mapsto \Gamma_{x_\perp}^{\rm DM}$ has properties (a) and (c) of (4.1).

To prove that $\Gamma^{\rm DM}$ has property (b) of (4.1) we appeal to Fatou's Lemma for sequences. In fact, using (4.15) we have

$$\mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma_{x_\perp}^{\rm DM}] = \sum_j (\phi_j, \Gamma_{x_\perp}^{\rm DM} \phi_j) \le \liminf_{n\to\infty} \mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma_{x_\perp}^{(n)}],$$

and then by Fatou again

$$\int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma_{x_\perp}^{\rm DM}] dx_\perp \le \liminf_{n\to\infty} \int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma_{x_\perp}^{(n)}] dx_\perp = N.$$

In exactly the same fashion we prove that condition (d) of (4.1) holds. In fact, we prove the stronger assertion (4.13):

$$T[\Gamma^{\mathrm{DM}}] = \int_{\mathbf{R}^2} \sum_j (\frac{d\phi_j}{dx_3}, \Gamma^{\mathrm{DM}}_{x_\perp} \frac{d\phi_j}{dx_3}) dx_\perp \le \liminf_{n\to\infty} T[\Gamma^{(n)}].$$

We are left with proving (4.14). We already know that $\rho^{(n)}(x)$ converges to $\rho^\infty(x)$ almost everywhere in $\mathbf{R}^3$. It is then enough to show that for almost every $x_\perp$ there is a subsequence of the functions $\rho^{(n)}(x_\perp, \cdot)$ which converges to $\rho_{\Gamma^{\mathrm{DM}}}(x_\perp, \cdot)$ in the sense of distributions on $\mathbf{R}$; this will prove that $\rho_{\Gamma^{\mathrm{DM}}}(x) = \rho^\infty(x)$ for almost every $x \in \mathbf{R}^3$.

Since $T[\Gamma^{(n)}]$ is bounded we have that

$$\int_{\mathbf{R}^2} \liminf_{n\to\infty} \mathrm{Tr}_{L^2(\mathbf{R})}[(1 - \partial^2/\partial x_3^2)\Gamma^{(n)}_{x_\perp}] dx_\perp \le N + \liminf_{n\to\infty} T[\Gamma^{(n)}] < \infty,$$

and thus for for almost every $x_\perp$ we can find a subsequence n_ℓ (depending on $x_\perp$) such that

$$\sup_\ell \mathrm{Tr}_{L^2(\mathbf{R})}[(1 - \partial^2/\partial x_3^2)\Gamma^{(n_\ell)}_{x_\perp}] < \infty \quad . \tag{4.16}$$

It follows from the weak convergence in (4.15) that

$$\left(1 - \partial^2/\partial x_3^2\right)^{1/2} \Gamma^{(n_\ell)}_{x_\perp} \left(1 - \partial^2/\partial x_3^2\right)^{1/2} \rightharpoonup \left(1 - \partial^2/\partial x_3^2\right)^{1/2} \Gamma^{\mathrm{DM}}_{x_\perp} \left(1 - \partial^2/\partial x_3^2\right)^{1/2}, \tag{4.17}$$

on the dense set of $C_0^\infty(\mathbf{R})$ functions. Since the operators are bounded in norm by (4.16), we conclude that (4.17) holds for all functions in $L^2(\mathbf{R})$, i.e., it holds weakly.

Given a test function $\theta \in C_0^\infty(\mathbf{R})$ we can consider it as a multiplication operator on $L^2(\mathbf{R})$. The operator $(1 - \frac{\partial^2}{\partial x_3^2})^{-1/2}\theta(1 - \frac{\partial^2}{\partial x_3^2})^{-1/2}$ is then easily seen to be compact; indeed, it is Hilbert-Schmidt. Since a compact operator can be approximated in norm by a finite rank operator we conclude from the uniform boundedness of the sequence in (4.16) and the weak limit in (4.17) that

$$\int_{\mathbf{R}} \rho^{(n_\ell)}(x)\theta(x_3) dx_3 = \mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma^{(n_\ell)}_{x_\perp}\theta] \to \mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma^{\mathrm{DM}}_{x_\perp}\theta] = \int_{\mathbf{R}} \rho_{\Gamma^{\mathrm{DM}}}(x)\theta(x_3) dx_3,$$

as $\ell \to \infty$ which is exactly what we needed in order to conclude (4.14). That the energy E^{DM} is convex follows as usual from the convexity of the functional $\mathcal{E}^{\mathrm{DM}}$. That the energy is non-increasing in the variables N and B is obvious. We have thus proved the statements of Theorem 4.3 except for the uniqueness. $\square$

Remark: As for the functionals $\mathcal{E}^{\mathrm{SS}}$ and $\mathcal{E}^{\mathrm{HS}}$, there exists an N_c^{DM} such that the energy curve $N \mapsto E^{\mathrm{DM}}(N, Z, B)$ is strictly decreasing for $N < N_c^{\mathrm{DM}}$ and constant for $N \ge N_c^{\mathrm{DM}}$.

Although we have not yet proved the uniqueness of $\Gamma^{\rm DM}$ stated in Theorem 4.3 we can conclude that the density $\rho^{\rm DM} := \rho_{\Gamma^{\rm DM}}$ is unique, i.e., if there were two different minimizers they must have the same density. This follows from the strict convexity (as a function of the density) of the last term, $R[\rho_\Gamma]$, in the energy functional. We can therefore define a linearized energy functional using the density $\rho^{\rm DM}$ in the following way:

$$\mathcal{E}^{\rm DM}_{\rm lin}[\Gamma] = \int_{\mathbf{R}^2} {\rm Tr}_{L^2(\mathbf{R})}[h^{\rm DM}_{x_\perp}\Gamma_{x_\perp}]dx_\perp, \tag{4.18}$$

where $h^{\rm DM}_{x_\perp}$ is the one-dimensional Schrödinger operator

$$h^{\rm DM}_{x_\perp} = -\frac{\partial^2}{\partial x_3^2} - \phi^{\rm DM}_{x_\perp}(x_3), \tag{4.19}$$

with potential as in (2.10)

$$\phi^{\rm DM}_{x_\perp}(x_3) = Z|x|^{-1} - |x|^{-1} * \rho^{\rm DM}. \tag{4.20}$$

Since $\rho^{\rm DM} \in L^1(\mathbf{R}^3) \cap L^3(\mathbf{R}^3)$ it follows easily (see [30]) that $\phi^{\rm DM}$ is continuous in $x = (x_\perp, x_3)$ for $x \neq 0$ and $\phi^{\rm DM} \to 0$ as $|x| \to \infty$.

We shall now prove that $\Gamma^{\rm DM}$ is a minimizer for the linear functional $\mathcal{E}^{\rm DM}_{\rm lin}$ on the set of $\Gamma \in \mathcal{G}^{\rm DM}_B$ satisfying $\int \rho_\Gamma \leq N$. Indeed, for any $\Gamma \in \mathcal{G}^{\rm DM}_B$ we have

$$\mathcal{E}^{\rm DM}[\Gamma] = \mathcal{E}^{\rm DM}_{\rm lin}[\Gamma] + D(\rho_\Gamma - \rho^{\rm DM}, \rho_\Gamma - \rho^{\rm DM}) - D(\rho^{\rm DM}, \rho^{\rm DM}). \tag{4.21}$$

If $\Gamma_0 \in \mathcal{G}^{\rm DM}_B$ then, for all $\delta > 0$, we get from (1.22) and (4.18) that

$$\begin{aligned}\mathcal{E}^{\rm DM}[(1-\delta)\Gamma^{\rm DM} + \delta\Gamma_0] = (1-\delta)\mathcal{E}^{\rm DM}_{\rm lin}[\Gamma^{\rm DM}] + \delta\mathcal{E}^{\rm DM}_{\rm lin}[\Gamma_0] - D(\rho^{\rm DM}, \rho^{\rm DM})\\ + \delta^2 D(\rho_{\Gamma_0} - \rho^{\rm DM}, \rho_{\Gamma_0} - \rho^{\rm DM}).\end{aligned} \tag{4.22}$$

Hence if $\int \rho_{\Gamma_0} \leq N$ and $\mathcal{E}^{\rm DM}_{\rm lin}[\Gamma^{\rm DM}] > \mathcal{E}^{\rm DM}_{\rm lin}[\Gamma_0]$ we can choose δ small enough to conclude that

$$\mathcal{E}^{\rm DM}[(1-\delta)\Gamma^{\rm DM} + \delta\Gamma_0] < \mathcal{E}^{\rm DM}_{\rm lin}[\Gamma^{\rm DM}] - D(\rho^{\rm DM}, \rho^{\rm DM}) = \mathcal{E}^{\rm DM}[\Gamma^{\rm DM}].$$

This contradicts the fact that $\Gamma^{\rm DM}$ is a minimizer for $\mathcal{E}^{\rm DM}$. We thus conclude that $\Gamma^{\rm DM}$ is a minimizer for $\mathcal{E}^{\rm DM}_{\rm lin}$. We have proved:

4.4 THEOREM. *A minimizer $\Gamma^{\rm DM} \in \mathcal{G}^{\rm DM}_B$ for $\mathcal{E}^{\rm DM}$ under the constraint $\int \rho^{\rm DM} \leq N$ is also a minimizer for the linearized functional $\mathcal{E}^{\rm DM}_{\rm lin}$ (with the same constraint).*

We are now in a position to complete the proof of Theorem 4.3. In fact, we can use the characterization of $\Gamma^{\rm DM}$ as a minimizer for the linear functional to show that it is unique. It is essential here that we have already argued that the density $\rho^{\rm DM}$ is unique.

Proof of the uniqueness part of Theorem 4.3: It is easy to describe the minimizer for the linear problem in terms of eigenvalues and eigenvectors for the one-dimensional operator $h^{\rm DM}_{x_\perp}$.

Let $-\mu_1(x_\perp), -\mu_2(x_\perp), \ldots \le 0$ denote the eigenvalues of $h^{\rm DM}_{x_\perp}$ and let $e^{(1)}_{x_\perp}, e^{(2)}_{x_\perp}, \ldots \in L^2(\mathbf{R})$ be the corresponding normalized eigenvectors. Then the minimizer $\Gamma^{\rm DM}$ is given by filling levels, i.e., corresponding to N there is a $-\mu \le 0$, **the chemical potential**, such that if we denote $i_0(x_\perp) = \max\{i\,:\,\mu_i(x_\perp) > \mu\}$ we have

$$\Gamma^{\rm DM}_{x_\perp} = \frac{B}{2\pi}\sum_{i\le i_0} e^{(i)}_{x_\perp}\otimes\overline{e^{(i)}_{x_\perp}} + \lambda(x_\perp)e^{(i_0(x_\perp)+1)}_{x_\perp}\otimes\overline{e^{(i_0(x_\perp)+1)}_{x_\perp}}, \tag{4.23}$$

where $0 \le \lambda(x_\perp) \le \frac{B}{2\pi}$ gives the filling of the last level. It is only non-zero on the set where the eigenvalue of the last level is equal to the chemical potential, i.e., $\mu_{i_0(x_\perp)+1}(x_\perp) = \mu$. The uniqueness of $\Gamma^{\rm DM}$ follows if we can prove that the function λ is unique. This is true because λ is given from the unique density by the relation

$$\rho^{\rm DM}(x) = \frac{B}{2\pi}\sum_{i\le i_0}|e^{(i)}_{x_\perp}(x_3)|^2 + \lambda(x_\perp)|e^{(i_0(x_\perp)+1)}_{x_\perp}|^2. \tag{4.24}$$

■

The condition $\int \mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma^{\rm DM}_{x_\perp}]dx_\perp \le N$ implies that the rank of $\Gamma^{\rm DM}_{x_\perp}$ is finite for almost every $x_\perp$. Furthermore, there are some cases in which it is easy to establish that the rank has a finite bound independent of $x_\perp$. Since the potential $\phi^{\rm DM}_{x_\perp}(x_3)$ tends to zero as $|x_3|$ tends to infinity the eigenvalues $\mu_1, \mu_2, \ldots$ can accumulate only at zero and we see from (4.23) that the finiteness of the rank holds uniformly in $x_\perp$ if $\mu > 0$. Another case for which we can make the assertion is $N > Z$. Here, there is necessarily some radius R such that the potential $\phi^{\rm DM}_{x_\perp}(x_3)$ is bounded above by $-C/|x|$ for some $C > 0$ and for $|x| > R$. Then, by any one of a variety of arguments, the number of *negative* eigenvalues of $h^{\rm DM}_{x_\perp}$ is bounded by a constant depending only on R and C.

In exactly the same way as in Proposition 2.3 we have that $\mu_1(x_\perp)$ is a decreasing convex function of $|x_\perp|$. We can conclude from this that $\Gamma_{x_\perp}$ must vanish outside the ball $\{x_\perp\,:\,|x_\perp| < R\}$, where $\pi R^2(B/2\pi) = N$, i.e.,

$$R = \sqrt{2N/B}. \tag{4.25}$$

It also follows that the density $\rho^{\rm DM}$ is discontinuous at the boundary. It has a jump of at least $B/2\pi$.

The density matrix $\Gamma^{\rm DM}$ is non-zero everywhere inside this ball if and only if $\Gamma_{x_\perp}$ has rank at most one everywhere and $N \le N^{\rm DM}_c$. If the rank is greater than one for some $x_\perp$ the support is strictly smaller.

Since the eigenfunction $e^{(1)}_{x_\perp}$ corresponding to the lowest eigenvalue $-\mu_1(x_\perp)$ for $h^{\rm DM}_{x_\perp}$ is a strictly positive function of $x_3 \in \mathbf{R}$ we see that $\rho^{\rm DM}$ cannot have bounded support in the x_3 direction. We have proved the following theorem.

4.5. THEOREM. (Support of $\rho^{\rm DM}$). *The density $\rho^{\rm DM}$ for the minimizer $\Gamma^{\rm DM}$ of $\mathcal{E}^{\rm DM}$ is* **not** *spherically symmetric. Indeed, the support of $\rho^{\rm DM}$ is an infinite cylinder $\{x \in \mathbf{R}^3 : |x_\perp| \le R^{\rm DM}\}$ with $R^{\rm DM} \le \sqrt{2N/B}$.*

As usual, the chemical potential $-\mu$ is the derivative of the energy curve $N \mapsto E^{\rm DM}(N, Z, B)$,

$$-\mu = \frac{\partial E^{\rm DM}}{\partial N}. \tag{4.26}$$

The proof of this is similar to the proof of Corollary 2.5.

The final major topic of this section is the relationship between the energies $E^{\rm DM}$ and $E^{\rm SS}$. We have already seen that we can identify $\mathcal{C}^{\rm SS}$ with the subset of $\bigcup\limits_{B>0} \mathcal{G}^{\rm DM}_B$ consisting of density matrices of rank at most one. Furthermore, it is clear from the definitions (1.25) and (1.22) of the functionals $\mathcal{E}^{\rm SS}$ and $\mathcal{E}^{\rm DM}$ that $\Gamma \in \mathcal{C}^{\rm SS}$ implies

$$\mathcal{E}^{\rm DM}[\Gamma] = \mathcal{E}^{\rm SS}[\rho_\Gamma]. \tag{4.27}$$

In the proof of the following theorem we shall show that if the parameter $\eta = B/(2\pi Z^3)$ is large enough then the minimizer $\Gamma^{\rm DM}$ of $\mathcal{E}^{\rm DM}$ is, indeed, in the subset $\mathcal{C}^{\rm SS}$. It then follows from (4.27) that $E^{\rm DM}$ and $E^{\rm SS}$ are identical.

Heuristically, the reason that the minimizer Γ belongs to $\mathcal{C}^{\rm SS}$ is that if B/Z^3 is large we can without violating condition (b) of (4.1), allow all the particles to be in the lowest eigenstate of the one-dimensional operator $h^{\rm DM}_{x_\perp}$.

4.6. THEOREM. (Equality of $E^{\rm DM}$ and $E^{\rm SS}$ for large B). *There exists a universal constant $\eta_c > 0$ such that if $B/Z^3 \ge \eta_c$ then*

$$E^{\rm DM}(N, Z, B) = E^{\rm SS}(N, Z, B). \tag{4.28}$$

Furthermore, the minimizer $\Gamma^{\rm DM}$ has at most one eigenstate for each $x_\perp$ and

$$\Gamma^{\rm DM}_{x_\perp}(x_3, x_3') = \sqrt{\rho^{\rm SS}(x_\perp, x_3)\rho^{\rm SS}(x_\perp, x_3')}. \tag{4.29}$$

Proof: It is clear that $E^{\rm DM} \le E^{\rm SS}$ since we can use the density matrix on the right side of (4.29) as a trial density for $\mathcal{E}^{\rm DM}$ and use (4.27).

To prove the lower bound we write

$$\mathcal{E}^{\rm DM}[\Gamma] = \int_{\mathbf{R}^2} {\rm Tr}_{L^2(\mathbf{R})}[h^{\rm SS}_{x_\perp}\Gamma_{x_\perp}]dx_\perp - D(\rho^{\rm SS}, \rho^{\rm SS}) + D(\rho^{\rm SS} - \rho_\Gamma, \rho^{\rm SS} - \rho_\Gamma) \quad , \tag{4.30}$$

where

$$h_{x_\perp}^{\mathrm{SS}} = -\frac{\partial^2}{\partial x_3^2} - \phi_{x_\perp}^{\mathrm{SS}}(x_3), \tag{4.31}$$

and $\phi_{x_\perp}^{\mathrm{SS}}$ is given in (2.10). Using that $|x-y|^{-1}$ is a positive definite kernel we get

$$\mathcal{E}^{\mathrm{DM}}[\Gamma] \geq \int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}[h_{x_\perp}^{\mathrm{SS}} \Gamma_{x_\perp}] dx_\perp - D(\rho^{\mathrm{SS}}, \rho^{\mathrm{SS}}) \quad . \tag{4.32}$$

If we can prove that the minimizer on the set $\mathcal{G}_B^{\mathrm{DM}}$ of the following linear functional

$$\Gamma \mapsto \int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}[h_{x_\perp}^{\mathrm{SS}} \Gamma_{x_\perp}] dx_\perp \tag{4.33}$$

(supplemented by the constraint $\int \rho_\Gamma \leq N$) has rank at most one for all $x_\perp$, then we know from Theorem 2.4 that it must be given by $\sqrt{\rho^{\mathrm{SS}}(x_\perp, x_3)\rho^{\mathrm{SS}}(x_\perp, x_3')}$. Thus the right side of (4.32) would be bounded below by E^{SS} and the theorem follows.

To prove that the minimizer of (4.33) has rank one when B/Z^3 is large enough we shall treat small values of N and large values of N differently.

We first consider the case of small N. If $-\mu_1^{\mathrm{SS}}(x_\perp), -\mu_2^{\mathrm{SS}}(x_\perp)$ denote the first and second eigenvalue of $h_{x_\perp}^{\mathrm{SS}}$ we shall show that if $|y_\perp|, |x_\perp| \leq R^{\mathrm{SS}}$ (the cylindrical radius of the SS atom) then for B/Z^3 large enough

$$\mu_1^{\mathrm{SS}}(x_\perp) > \mu_2^{\mathrm{SS}}(y_\perp). \tag{4.34}$$

This will imply that the minimizer of (4.33) has rank one.

If we neglect the positive term $\rho^{\mathrm{SS}} * |x|^{-1}$ in $h_{x_\perp}^{\mathrm{SS}}$ we see from Lemma 2.1 on the energy of the one-dimensional Coulomb problem that

$$\mu_2^{\mathrm{SS}}(y_\perp) \leq Z^2/4. \tag{4.35}$$

However, from Proposition 2.3 we know that $\mu_1^{\mathrm{SS}}(x_\perp) \geq \mu_1^{\mathrm{SS}}(R^{\mathrm{SS}})$.

We have the scaling relation (3.17), namely $Z^{-2}[\ln\eta]^{-2}\mu_1^{\mathrm{SS}}(R^{\mathrm{SS}}) = -\frac{dE_\eta}{d\lambda}$, and thus we have

$$\frac{\mu_1^{\mathrm{SS}}(x_\perp)}{\mu_2^{\mathrm{SS}}(y_\perp)} \geq \frac{\mu_1^{\mathrm{SS}}(R^{\mathrm{SS}})}{Z^2/4} = -4[\ln\eta]^2 \frac{dE_\eta}{d\lambda}. \tag{4.36}$$

However, since $E_\eta(\lambda) \to E^{\mathrm{HS}}(\lambda)$ as $\eta \to \infty$ (see Theorem 3.5) and $\lambda \mapsto E_\eta(\lambda)$ is a convex function we conclude that

$$\frac{dE_\eta(\lambda)}{d\lambda} \to \frac{dE^{\mathrm{HS}}(\lambda)}{d\lambda} \text{ as } \eta \to \infty.$$

If λ is strictly smaller than 2 the derivative $\frac{dE^{\mathrm{HS}}(\lambda)}{d\lambda}$ is bounded away from zero. Indeed, from (3.7) $\frac{dE^{\mathrm{HS}}}{d\lambda} = -\frac{1}{16}\lambda^2 + \frac{1}{4}\lambda - \frac{1}{4}$. Thus (4.36) implies that if N/Z is strictly less than 2 and η is large enough then (4.34) holds.

We now turn to the case of large N, i.e. N/Z not strictly less than 2. We shall, in fact, consider N/Z strictly greater than 1. In this case we shall show that the operator $h_{x_\perp}^{\mathrm{SS}}$ has at most one negative eigenvalue for all $x_\perp \neq 0$ provided η is large enough. This will then again imply that the minimizer of (4.33) has rank one.

As we have argued in the proof of Lemma 2.1 the second eigenvalue $-\mu_2^{\mathrm{SS}}(x_\perp)$ of $h_{x_\perp}^{\mathrm{SS}}$ is identical to the lowest eigenvalue of the *three-dimensional* operator

$$H_{x_\perp} = -\Delta + V_{x_\perp}, \tag{4.37}$$

where

$$V_{x_\perp}(y) = -Z(|x_\perp|^2 + |y|^2)^{-1/2} + \int \rho^{\mathrm{SS}}(x')(|x_\perp - x'_\perp|^2 + |x'_3 - |y||^2)^{-1/2} dx', \tag{4.38}$$

is a spherically symmetric potential.

We shall show that if N/Z is strictly greater than one and if B/Z^3 is large enough then the operator $H_{x_\perp}$ has no negative eigenvalues. To do this we first observe that if $\lambda = N/Z = 1+\delta$ for some $\delta > 0$ we can find a constant $c_\delta > 0$ such that if B/Z^3 is large enough the inequality

$$\int_\Omega \rho^{\mathrm{SS}} > (1+\delta/2)Z \tag{4.39}$$

holds for the integral of ρ^{SS} on the set

$$\Omega = \{(x_\perp, x_3) \,:\, |x_\perp| < R^{\mathrm{SS}} \text{ and } |x_3| < c_\delta Z^{-1}[\ln\eta]^{-1}\}. \tag{4.40}$$

The estimate (4.39) follows from the scaling relation (3.11):

$$\rho^{\mathrm{SS}}(x) = Z^4 \eta \ln(\eta) \rho_\eta^{\mathrm{SS}}(Z\eta^{1/2}x_\perp, Z\ln(\eta)x_3) \tag{4.41}$$

and the fact proved in Theorem 3.5 that $\overline{\rho}_\eta^{\mathrm{SS}} \to \overline{\rho}^{\mathrm{HS}}$ in $L^1_{\mathrm{loc}}(\mathbf{R})$ as $\eta \to \infty$.

From (4.39) we get the following lower bound on the potential $V_{x_\perp}$

$$V_{x_\perp}(y) \geq -\frac{Z}{|y|} + \frac{Z(1+\delta/2)}{\sqrt{4(R^{\mathrm{SS}})^2 + (|y| + c_\delta Z^{-1}[\ln\eta]^{-1})^2}}.$$

Hence if $|y| > \frac{3}{\delta}c_\delta Z^{-1}[\ln\eta]^{-1}$ and η is large enough (depending only on δ) we get $V_{x_\perp}(y) \geq 0$. We thus have the following estimate for B/Z^3 large enough

$$V_{x_\perp}(y) \geq \begin{cases} -\frac{Z}{|y|}, & |y| < \frac{3}{\delta}c_\delta Z^{-1}[\ln\eta]^{-1} \\ 0 & \text{otherwise} \end{cases}. \tag{4.42}$$

We now estimate the number of negative eigenvalues of $H_{x_\perp}$ using the Cwikel, Lieb, Rosenbljum bound [47-49] and (4.42). The number of negative eigenvalues of $H_{x_\perp}$ is at most

$$0.1156 \int |V_{x_\perp}(y)|_-^{3/2} dy \leq 0.1156 \int_{|y|<3\delta^{-1}c_\delta Z^{-1}[\ln\eta]^{-1}} Z^{3/2}|y|^{-3/2} dy \leq c_\delta \frac{8\pi}{\delta}(\ln\eta)^{-3/2}.$$

Thus for η large enough we find that $H_{x_\perp}$ has no negative eigenvalues and the theorem follows. ■

Remark: We point out that in the above proof it is really $\ln(B/Z^3)$ that must be large. Since it is hard to estimate B/Z^3 from knowledge of its logarithm, it is very hard to give a reasonable estimate on the numerical value of η_c and we have not attempted to do so. The reason for the logarithm in the above proof is that we we use the functional $\mathcal{E}^{\rm HS}$, which only approximates $\mathcal{E}^{\rm SS}$ when $\ln\eta$ is large (see Proposition 3.3). However, it is reasonable to believe that $\mathcal{E}^{\rm SS}$ *is valid even for smaller* η.

We proceed to discuss the viral inequalities for the density matrix functional. These inequalities are identical to the corresponding inequalities for the super-strong functional given in Lemma 2.6. Since the proof is a simple generalization of the proof of Lemma 2.6 we shall leave it to the reader.

4.7. LEMMA (Virial inequalities). *Define* $T^{\rm DM} := \int_{\mathbf{R}^2} {\rm Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma^{\rm DM}_{x_\perp}\right] dx_\perp$,

$$A^{\rm DM} := \int Z|x|^{-1}\rho^{\rm DM}(x)dx, R^{\rm DM} := \tfrac{1}{2}\int\int \rho^{\rm DM}(x)|x-y|^{-1}\rho^{\rm DM}(y)dxdy,$$

where $\rho^{\rm DM} = \rho_{\Gamma^{\rm DM}}$. *Then* $E^{\rm DM} = T^{\rm DM} - A^{\rm DM} + R^{\rm DM}$ *and the following inequalities hold:*

$$R^{\rm DM} \leq A^{\rm DM} - 2T^{\rm DM} \quad \textit{and} \quad T^{\rm DM} \leq A^{\rm DM} - 2R^{\rm DM}. \tag{4.43}$$

These inequalities imply

$$A^{\rm DM} \leq 3|E^{\rm DM}|, \quad T^{\rm DM} \leq |E^{\rm DM}| \quad \textit{and} \quad R^{\rm DM} \leq |E^{\rm DM}|. \tag{4.44}$$

4.8. THEOREM. *We have the following estimates on the energy* $E^{\rm DM}$

$$E^{\rm DM}(N,Z,B) \geq -\frac{5}{12}\left(\frac{\pi}{2}\right)^{2/5} Z^{6/5}N^{3/5}B^{2/5} \tag{4.45}$$

and

$$E^{\rm DM}(N,Z,B) \geq -NZ^2\left[\ln\left(2^{-1/2}Z^{-1}N^{-1/2}B^{1/2}+\tfrac{1}{2}\right)\right]^2 - NZ^2. \tag{4.46}$$

Proof: According to (4.43) $R^{\rm DM} \geq -\frac{1}{2}(T^{\rm DM} - A^{\rm DM})$. Hence $E^{\rm DM} \geq \frac{1}{2}(T^{\rm DM} - A^{\rm DM})$. The estimates (4.45) and (4.46) then follow from (4.10) and (4.11). ■

Combining the estimates (4.45–46) we get with $\lambda = N/Z$

$$E^{\rm DM}(N,Z,B) \geq -C_\lambda \begin{cases} Z^{9/5}B^{2/5} & \text{if } B/Z^3 \leq 1 \\ Z^3(1+[\ln(BZ^{-3})]^2) & \text{if } B/Z^3 \geq 1 \end{cases} . \tag{4.47}$$

We know from (1.24) that $E^{\rm DM}(N,Z,B) = Z^3 E^{\rm DM}(N/Z,1,B/Z^3)$ (notice that the bound (4.47) respects this scaling). Since $E^{\rm DM}(N/Z,1,B/Z^3) = E^{\rm SS}(N/Z,1,B/Z^3)$ for large B/Z^3 we get from Theorem 3.5 the asymptotic relation

$$E^{\rm DM}(\lambda,1,2\pi\eta) \approx [\ln\eta]^2 E^{\rm HS}(\lambda) \tag{4.48}$$

for large η. Or stated differently,

$$E^{\rm DM}(N,Z,B)/Z^3[\ln(B/Z^3)]^2 E^{\rm HS}(N/Z) \to 1, \tag{4.49}$$

as $B/Z^3 \to \infty$. Recall that according to (3.7) the function $E^{\rm HS}(\lambda)$ is a third degree polynomial for $0 \leq \lambda \leq 2$.

We conclude this section with an estimate on the density $\rho^{\rm DM} = \rho_{\Gamma^{\rm DM}}$. This estimate will be needed in Sect. V to give an upper bound on the true quantum energy.

4.9. PROPOSITION (Bound on $\rho^{\rm DM}$). *The density $\rho^{\rm DM}$ satisfies the bound*

$$\begin{aligned}\int_{\mathbf{R}} \left(\frac{\partial}{\partial x_3}\sqrt{\rho^{\rm DM}}(x)\right)^2 dx_3 &\leq \left(\frac{2B}{\pi}\right) Z^2 \left\{1 + \frac{\pi^2}{12} + [\sinh^{-1}(\frac{1}{2Z|x_\perp|})]^2\right\} \\ &\leq (\text{const.}) BZ^2\{1+[\ln(Z|x_\perp|)]^2\}.\end{aligned} \tag{4.50}$$

Proof: To simplify the notation we write ρ and Γ instead of $\rho^{\rm DM}$ and $\Gamma^{\rm DM}$.

We recall the estimate (4.5b)

$$\int_{\mathbf{R}} \left(\frac{\partial}{\partial x_3}\sqrt{\rho(x)}\right)^2 dx_3 \leq {\rm Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right].$$

We are thus left with estimating ${\rm Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right]$. Since Γ minimizes the linear functional $\mathcal{E}_L$ (see Theorem 4.4) we conclude that for all $x_\perp$

$${\rm Tr}_{L^2(\mathbf{R})}\left[\left(-\frac{\partial^2}{\partial x_3^2} - \phi_{x_\perp}\right)\Gamma_{x_\perp}\right] \leq 0$$

where $\phi_{x_\perp}$ was defined in (4.20). Thus

$$\begin{aligned}\tfrac{1}{2}{\rm Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right] &\leq -{\rm Tr}_{L^2(\mathbf{R})}\left[\left(-\tfrac{1}{2}\frac{\partial^2}{\partial x_3^2} - \phi_{x_\perp}\right)\Gamma_{x_\perp}\right] \\ &\leq -{\rm Tr}_{L^2(\mathbf{R})}\left[\left(-\tfrac{1}{2}\frac{\partial^2}{\partial x_3^2} - Z(|x_\perp|^2+x_3^2)^{-1/2}\right)\Gamma_{x_\perp}\right] \\ &\leq -\frac{B}{2\pi}\left(\text{sum of negative eigenvalues of } -\tfrac{1}{2}\frac{\partial^2}{\partial x_3^2} - Z(|x_\perp|^2+x_3^2)^{-1/2}\right),\end{aligned}$$

where we have used that $0 \le \Gamma_{x_\perp} \le \frac{B}{2\pi} I$.

We now again appeal to Lemma 2.1 on the one-dimensional Coulomb problem to estimate the sum of the negative eigenvalues of $\frac{1}{2}\widehat{h}_{2Z,x_\perp} = -\frac{1}{2}\frac{d^2}{dx_3^2} - Z(|x_\perp|^2 + x_3^2)^{-1/2}$. We obtain

$$\begin{aligned}\mathrm{Tr}_{L^1(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right] &\le \frac{B}{2\pi}(2Z)^2\left\{1 + \left[\sinh^{-1}\left(\frac{1}{2Z|x_\perp|}\right)\right]^2 + 2\sum_{n=1}^{\infty}\frac{1}{4n^2}\right\} \\ &= \frac{2B}{\pi}Z^2\left\{1 + \frac{\pi^2}{12} + \left[\sinh^{-1}\left(\frac{1}{2Z|x_\perp|}\right)\right]^2\right\}.\end{aligned}$$

We have here used the formula $\sum_{n=1}^{\infty} n^{-2} = \pi^2/6$. ■

V. UPPER BOUND TO THE QUANTUM ENERGY

This section begins the study of the quantum mechanical many-body problem with the goal — achieved in Sect. VIII — of showing that the functionals studied in the earlier sections do, indeed, give the correct asymptotics as $Z \to \infty$ and $B/Z^{4/3} \to \infty$. There are N electrons with the atomic Hamiltonian H_N given in (1.1).

The first goal is a variational upper bound to the ground state energy (1.2). Although the bound is valid for all B and Z, it is only in the asymptotic regime $Z \to \infty$ and $B/Z^{4/3} \to \infty$ that it agrees with the true energy to leading order. This bound is far from the best obtainable with our methods; little effort will be made here to optimize constants. We emphasize, however, that our bound is a little more than just a bound on $E^{\mathrm{Q}}(N,Z,B)$; it is, in fact, a bound on $E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)$. In other words, our variational (or comparison) functions have the property that all the electrons are in the lowest Landau band.

Our final conclusion is stated in Theorem 5.1 in which our bound is related to the density matrix energy E^{DM} plus correction terms. To show that the corrections are of lower order than E^{Q}, we need a simple-minded, independent upper bound to E^{Q}. This is provided in Theorem 5.3. This theorem also bounds E^{Q} in terms of the energy of the independent electron model (without repulsion). In Theorem 5.2, we show that there is a simple modification of the density matrix functional with the property that it gives an upper bound to the energy without the need for correction terms. This modified functional (the smeared density matrix functional $\mathcal{E}^{\mathrm{SDM}}$) has the defect, however, of not being easily related to a lower bound for E^{Q}. Thus, E^{SDM} may be computationally useful, but only after an independent proof (via E^{DM}) shows that E^{SDM} is asymptotically exact.

We shall use the variational principle of Lieb [50] which asserts that the true quantum-mechanical ground state energy, E^{Q}, satisfies

$$E^{\mathrm{Q}} \leq \mathrm{Tr}\big[(H_{\mathbf{A}} - Z|x|^{-1})K\big] + \tfrac{1}{2}\int\int k(x,x)k(y,y)|x-y|^{-1}dxdy \tag{5.1}$$

Here, $H_{\mathbf{A}} = [\boldsymbol{\sigma}\cdot(\mathbf{p}+\mathbf{A})]^2$ and $K = K(x,s;x's')$ is any density matrix (a nonnegative, self-adjoint, trace class operator on $L^2(\mathbf{R}^3;\mathbf{C}^2)$) satisfying

(i) $K \leq \mathrm{I}$.

(ii) $\mathrm{Tr}K \leq N$. (5.2)

In other words, K is a 2×2 matrix of operators on $L^2(\mathbf{R}^3)$ and k, which appears in (5.1), denotes the kernel of the operator obtained from the trace of this 2×2 matrix, i.e., $k(x,x') = \sum_s K(x,s;x',s)$. The "diagonal", $k(x,x)$ is well defined as an $L^1(\mathbf{R}^3)$ function because k is the kernel of a trace class operator. The symbol Tr denotes the trace on $L^2(\mathbf{R}^3,\mathbf{C}^2)$, i.e., the matrix trace as well as the $L^2(\mathbf{R}^3)$ trace. Note that in [50] there is another contribution to the integrand in (5.1). It is the "exchange term" and it is omitted here because it is negative.

We shall choose K to have all spins "down", i.e. $K(x,s;x',s') = \delta(s=-\tfrac{1}{2})\delta(s'=-\tfrac{1}{2})k(x,x')$, and (5.2) becomes

$$\text{(i}'\text{)}\quad 0 \leq \int\int \overline{f(x)}f(x')k(x,x')dxdx' \leq \int |f(x)|^2dx \quad \text{for all } f\in L^2(\mathbf{R}^3)$$
$$\text{(ii}'\text{)}\quad \int k(x,x)dx \leq N. \tag{5.3}$$

Our choice of the kernel k is

$$k(x,x') = \frac{2\pi}{B}\int \Pi_0^{\perp}(x_\perp,y_\perp)\Gamma^{\mathrm{DM}}_{y_\perp}(x_3,x_3')\Pi_0^{\perp}(y_\perp,x_\perp')dy_\perp. \tag{5.4}$$

Here $\Pi_0^{\perp}$ is the kernel of the projection onto the lowest Landau level in $L^2(\mathbf{R}^2;dx_\perp)$ (i.e. the kernel in (1.14) with the δ-function and $P^{\downarrow}$ omitted). It is given by

$$\Pi_0^{\perp}(x_\perp,y_\perp) = \frac{B}{2\pi}\exp\big\{\frac{i}{2}(x_\perp\times y_\perp)\cdot\mathbf{B} - \tfrac{1}{4}(x_\perp - y_\perp)^2B\big\}. \tag{5.5}$$

We have constructed K such that $\Pi_0K = K$. If we look at the proof [50] of the variational principle, we see trivially that the right side of (5.1) is a bound to the energy in which the condition $\Pi_0^N\Psi = \Psi$ is added as a constraint, i.e., it is a bound on $E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)$. The function Γ^{DM} in (5.4) is the integral kernel for the minimizer of the density matrix energy functional (1.22) on the set $\mathcal{G}_B^{\mathrm{DM}}$

satisfying $\int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}[\Gamma^{\mathrm{DM}}_{x_\perp}]dx_\perp \leq N$. One easily checks that (i′) and (ii′) of (5.3) are satisfied. Indeed, since $0 \leq \Gamma^{\mathrm{DM}}_{y_\perp} \leq (B/2\pi)\, I$ we find

$$\begin{aligned} \int\int \overline{f(x)} k(x,x') f(x') dx dx' &\leq \int\limits_{\mathbf{R}^2} \left(\int\limits_{\mathbf{R}} \left| \int\limits_{\mathbf{R}^2} \Pi_0^\perp(y_\perp, x_\perp) f(x) dx_\perp \right|^2 dx_3 \right) dy_\perp \\ &\leq \int |f(x)|^2 dx. \end{aligned}$$

In the last inequality we have used the fact that $\Pi_0^\perp$ is the kernel of a projection. Moreover, recalling the definition of the density $\rho^{\mathrm{DM}}(x) := \Gamma^{\mathrm{DM}}_{x_\perp}(x_3, x_3)$, we have

$$\begin{aligned} k(x,x) &= \int \left|\Pi_0^\perp(x_\perp, y_\perp)\right|^2 \rho^{\mathrm{DM}}(y_\perp, x_3) dy_\perp \\ &= \int m(x_\perp - y_\perp) \rho^{\mathrm{DM}}(y_\perp, x_3) dy_\perp =: m *_\perp \rho^{\mathrm{DM}}(x), \end{aligned} \tag{5.6}$$

with m being the Gaussian

$$m(x_\perp) = \frac{B}{2\pi} \exp(-\tfrac{1}{2}|x_\perp|^2 B), \tag{5.7}$$

with normalization $\int m = 1$. Equation (5.3 (ii′)) follows immediately from (5.6) and $\int \rho^{\mathrm{DM}} \leq N$. Note the introduction of the *convolution operator* $*_\perp$ in (5.6), which is convolution over the $x_\perp$ variables *only*.

Let us now consider the various terms in (5.1). Writing $H_{\mathbf{A}} = -\partial_3^2 + H_{\mathbf{A}}^\perp$ and using that $H_{\mathbf{A}}^\perp \Pi_0^\perp = 0$ we obtain

$$\mathrm{Tr}[H_{\mathbf{A}} k] = \int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}[-\partial_3^2 \Gamma^{\mathrm{DM}}_{x_\perp}] dx_\perp. \tag{5.8}$$

In the term

$$\mathrm{Tr}(-Z|x|^{-1}k) = -Z \int k(x,x)|x|^{-1} dx \tag{5.9}$$

and in the last term of (5.1) we would like to replace $k(x,x)$ by $\rho^{\mathrm{DM}}(x)$, since, with that replacement, the right side of (5.1) is precisely the energy $\mathcal{E}^{\mathrm{DM}}[\Gamma^{\mathrm{DM}}]$.

In other words,

$$\begin{aligned} E^{\mathrm{Q}} \leq \text{Right side of (5.1) } &= E^{\mathrm{DM}} + a - b, \\ a &= Z \int |x|^{-1} [\rho^{\mathrm{DM}}(x) - k(x,x)] dx, \\ b &= \int\int |x-y|^{-1} [\rho^{\mathrm{DM}}(x)\rho^{\mathrm{DM}}(y) - k(x,x)k(y,y)] dx dy. \end{aligned} \tag{5.10}$$

We claim that $b \geq 0$, and hence that it can be omitted from further consideration. To see this, we can note (by a simple change of variables of integration) that $b = (\rho^{\rm DM}, Q\rho^{\rm DM})$ where Q is the quadratic form whose kernel is $|x-x'|^{-1} - (m *_\perp |x|^{-1} *_\perp m)(x-x')$, i.e.,

$$Q(x,x') = |x-x'|^{-1} - \int\limits_{\mathbf{R}^2}\int\limits_{\mathbf{R}^2} m(x_\perp - y_\perp)m(x'_\perp - y'_\perp)\left[(x_3-x'_3)^2 + (y_\perp - y'_\perp)^2\right]^{-1/2} dy'_\perp dy_\perp .$$

Since Q is a function only of $x - x'$, we can evaluate b in terms of the three-dimensional Fourier transform $\widehat{\rho^{\rm DM}}$ and the two-dimensional Fourier transform $\widehat{m}$. A simple calculation shows that up to a constant that depends on normalization convention,

$$b = \int |\widehat{\rho^{\rm DM}}(p)|^2 |p|^{-2}[1 - |\widehat{m}(p_\perp)|^2]dp.$$

(Note that the reality of $\rho^{\rm DM}$ and m implies that $\widehat{\rho^{\rm DM}}(p) = \overline{\widehat{\rho^{\rm DM}}(-p)}$ and $\widehat{m}(p_\perp) = \overline{\widehat{m}(-p_\perp)}$.) Now m is a nonnegative function (a Gaussian, in fact) and $\int m = 1$; hence $|\widehat{m}(p)| \leq 1$ for all p, and we conclude that $b \geq 0$.

Next, we turn our attention to bounding a from above. We pick an $r > 0$ and write $a = a_1 + a_2$ with

$$a_1 = Z \int\limits_{|x|\leq r} |x|^{-1}(\rho^{\rm DM}(x) - k(x,x))dx$$

and

$$a_2 = Z \int\limits_{|x|\geq r} |x|^{-1}(\rho^{\rm DM}(x) - k(x,x))dx.$$

We use two methods to estimate a_1. The first uses the Lieb- Thirring inequality in one dimension [40] and it is accurate and useful when $B \ll Z^2N^2$. If we recall that $0 \leq \Gamma^{\rm DM}_{x_\perp} \leq (B/2\pi)I$, this inequality can be stated as (see (4.8)) $T^{\rm DM} \geq (\pi^2/3)B^{-2}\int(\rho^{\rm DM})^3$. Therefore

$$\begin{aligned} a_1 &\leq Z \int\limits_{|x|\leq r} |x|^{-1}\rho^{\rm DM}(x)dx \leq ZB^{2/3}\left(\int \rho^3 B^{-2}dx\right)^{1/3}\left(\int\limits_{|x|\leq r}|x|^{-3/2}dx\right)^{2/3} \\ &\leq 4\cdot 3^{-1/3}ZB^{2/3}T^{1/3}r \leq 4\cdot 3^{-1/3}ZB^{2/3}r|E^{\rm DM}|^{1/3}, \end{aligned} \tag{5.11}$$

where we have used the virial inequality $T^{\rm DM} \leq |E^{\rm DM}|$ from (4.44).

The other estimate, that gives small errors for $B \gg Z^2N^{1/6}$, uses the inequality $\rho \leq 2\int_{\mathbf{R}} \sqrt{\rho}|\partial\sqrt{\rho}/\partial x_3|dx_3$ combined with the bound (4.50)

$$\int\limits_{\mathbf{R}} (\partial\sqrt{\rho^{\rm DM}}/\partial x_3)^2 dx_3 \leq ({\rm const.})BZ^2\{1 + [\ln(Z|x_\perp|)]^2\}.$$

This gives

$$
\begin{aligned}
a_1 &\leq Z \int\limits_{|x|\leq r} |x|^{-1}\rho^{\rm DM}(x)dx \\
&\leq Z \int\limits_{|x_\perp|\leq r} \left(\int\limits_{|x_3|\leq r} |x|^{-1}dx_3 \right) \left(2\int \sqrt{\rho^{\rm DM}(x)}\ \left|\partial\sqrt{\rho^{\rm DM}(x)}/\partial x_3\right| dx_3 \right) dx_\perp \\
&\leq 4Z\left(\int \rho^{\rm DM}(x)dx\right)^{1/2} \left\{ \int\limits_{|x_\perp|\leq r} [\sinh^{-1}(|x_\perp|r^{-1})]^2 \int\limits_{\mathbf{R}} \left(\partial\sqrt{\rho^{\rm DM}(x)}/\partial x_3\right)^2 dx_3 dx_\perp \right\}^{1/2} \\
&\leq ({\rm const.})B^{1/2}Z^2N^{1/2}r\{1+[\ln(Zr)]^2\}^{1/2}. \qquad (5.12)
\end{aligned}
$$

To bound a_2 we write it as

$$a_2 = \int\limits_{|x|\geq r} \rho^{\rm DM}(x)\phi(x)dx$$

with

$$\phi(x) = Z\int_{\mathbf{R}^2} m(y_\perp)\left[|x|^{-1} - \tfrac{1}{2}(|x|^2+|y_\perp|^2-2x_\perp\cdot y_\perp)^{-1/2} - \tfrac{1}{2}(|x|^2+|y_\perp|^2+2x_\perp\cdot y_\perp)^{-1/2}\right]dy_\perp,$$

where we have used $m(y_\perp) = m(-y_\perp)$. Since the function $t\mapsto t^{-1/2}$ is convex, and $(1+s)^{-1/2}\geq 1-\frac{1}{2}s$, we have

$$
\begin{aligned}
&\tfrac{1}{2}(|x|^2+|y_\perp|^2-2x_\perp\cdot y_\perp)^{-1/2} + \tfrac{1}{2}(|x|^2+|y_\perp|^2+2x_\perp\cdot y_\perp)^{-1/2} \\
&\quad \geq (|x|^2+|y_\perp|^2)^{-1/2} \geq |x|^{-1}(1-\tfrac{1}{2}|y_\perp|^2|x|^{-2}).
\end{aligned}
$$

Hence,

$$\phi(x) \leq \tfrac{1}{2}Z|x|^{-3}\int\limits_{\mathbf{R}^2} m(y_\perp)y_\perp^2 dy_\perp = ZB^{-1}|x|^{-3},$$

and we obtain the desired bound for a_2 by using the virial inequality (4.44):

$$
\begin{aligned}
a_2 &\leq ZB^{-1}\int\limits_{|x|\geq r} \rho^{\rm DM}(x)|x|^{-3}dx \\
&\leq B^{-1}\left(\int \rho^{\rm DM}(x)Z|x|^{-1}dx\right)\sup_{|x|\geq r}|x|^{-2} \\
&\leq r^{-2}B^{-1}|E^{\rm DM}|. \qquad (5.13)
\end{aligned}
$$

We now add (5.11) and (5.13) and optimize the bound with respect to r. This gives

$$\begin{aligned} a_1 + a_2 &\le (2^{5/3}3^{-1/9} + 2^{2/3}3^{-2/9}) Z^{2/3} B^{1/9} |E^{\rm DM}|^{5/9} \\ &\le (2^{5/3}3^{-1/9} + 2^{2/3}3^{-2/9})(5/12)^{5/9}(\pi/2)^{2/9} Z^{4/3} N^{1/3} B^{1/3} \\ &= 2.76 Z^{4/3} N^{1/3} B^{1/3} \end{aligned} \tag{5.14}$$

where we have used the estimate (4.45). This bound is of lower order than $|E^{\rm DM}|$ provided $B \ll Z^2 N^2$. We can also add (5.12) and (5.13) and choose $r = B^{-1/2} E^{1/3} Z^{-2/3} N^{-1/6}$ (this is not optimal). In this case we obtain, this time using (4.46):

$$\begin{aligned} a_1 + a_2 &\le ({\rm const.}) Z^{4/3} N^{1/3} |E^{\rm DM}|^{1/3} \big\{1 + ({\rm const.})[\ln(B|E^{\rm DM}|^{-2/3} Z^{-2/3} N^{1/3})]^2\big\}^{1/2} \\ &\le ({\rm const.}) Z^2 N^{2/3} \big\{1 + |\ln N|^2 + [\ln(B/NZ^2)]^2\big\}^{5/6} \end{aligned} \tag{5.15}$$

which we shall show is small compared to $|E^{\rm Q}|$ if $B \gg Z^2 N^{1/16}$ (see Theorem 5.3 and (5.24)).

The conclusion we have reached is that $E^{\rm Q} \le E^{\rm DM}$ plus corrections (which we shall show below to be of lower order by a power of Z for large Z). It can be stated as follows.

5.1. THEOREM (Upper bound in terms of $E^{\rm DM}$). *For all N, B and Z the true quantum ground state energy $E^{\rm Q}$ and the confined energy $E^{\rm Q}_{\rm conf}$ are related to the energy $E^{\rm DM}$ by*

$$E^{\rm Q}(N,Z,B) \le E^{\rm Q}_{\rm conf}(N,Z,B) \le E^{\rm DM}(N,Z,B) + R_{\rm U}(N,Z,B).$$

where $R_{\rm U}(N,Z,B)$ is the lesser of the following two quantities:

$$2.76 Z^{4/3} N^{1/3} B^{1/3} \quad \textit{and} \quad ({\rm const.}) Z^2 N^{2/3} \big\{1 + |\ln N|^2 + [\ln(B/NZ^2)]^2\big\}^{5/6}. \tag{5.16}$$

In fact, our calculation here shows more than Theorem 5.1. Let us define a **smeared density matrix functional** by means of (1.22), but with the Coulomb attraction (not the repulsion) changed from $-Z|x|^{-1}$ to the function

$$-Zm *_\perp |x|^{-1} = -Z \int_{\mathbf{R}^2} m(x_\perp - y_\perp)[x_3^2 + (x_\perp - y_\perp)^2]^{-1/2} dx_\perp .$$

We denote the corresponding energy, as in (4.7) by $E^{\rm SDM}(N,Z,B)$.

5.2. THEOREM (Upper bound in terms of $E^{\rm SDM}$). *For all N, B and Z, the three energies satisfy*

$$E^{\rm Q}(N,Z,B) \le E^{\rm SDM}(N,Z,B) \le E^{\rm DM} + R_{\rm U}(N,Z,B) \tag{5.17}$$

$$E^{\rm DM}(N,Z,B) \le E^{\rm SDM}(N,Z,B) \tag{5.18}$$

with $R_{\mathrm{U}}(N,Z,B)$ *as in Theorem 5.1.*

Proof: (5.17) is simply a transcription of our calculations above.

Inequality (5.18) follows from the definitions of E^{SDM} and E^{DM} as infima. For each $y_\perp \in \mathbf{R}^2$ define $\Gamma^{y_\perp}$ by $\Gamma^{y_\perp}_{x_\perp} = \Gamma^{\mathrm{SDM}}_{x_\perp - y_\perp}$. (Here Γ^{SDM} is the minimizer for $E^{\mathrm{SDM}}(N,Z,B)$. If none exists then we have to use a minimizing sequence in an obvious way.) Then $E^{\mathrm{DM}}(N,Z,B) \leq \mathcal{E}^{\mathrm{DM}}[\Gamma^{y_\perp}]$. However, a simple calculation shows that

$$\int_{\mathbf{R}^2} m(y_\perp)\mathcal{E}^{\mathrm{DM}}[\Gamma^{y_\perp}]dy_\perp = \mathcal{E}^{\mathrm{SDM}}[\Gamma^{\mathrm{SDM}}]. \qquad \blacksquare$$

The next theorem gives a simple bound for $E^{\mathrm{Q}}(N,Z,B)$ in terms of the independent particle model.

5.3 THEOREM (Simple upper bounds). *Let* $E^{\mathrm{Q}}_{(1)}(N,Z,B)$ *be the ground state energy for the Hamiltonian (1.1) without the last (repulsion) term, i.e., for* $H^{(1)}_N := \sum_1^N \left[H^i_{\mathbf{A}} - Z/|x^i|\right]$. *Then, if* $n \leq N$,

$$E^{\mathrm{Q}}(N,Z,B) \leq E^{\mathrm{Q}}_{(1)}(n, Z - \tfrac{1}{2}n, B). \tag{5.19}$$

A bound for $E^{\mathrm{Q}}_{(1)}$ *is given by*

$$E^{\mathrm{Q}}_{(1)}(N,Z,B) \leq -(\text{const.})\begin{cases} n^{3/5}Z^{6/5}B^{2/5}, & \textit{for } B \leq nZ^2 \\ nZ^2, & \textit{for } B \geq nZ^2 \end{cases}, \tag{5.20}$$

with $n = \min\{N,Z\}$.

Proof: Let $K_{(1)}$ denote the one-particle reduced density matrix for the ground state of $H^{(1)}_n$. [Note: n and not N. Note also that if there are several ground states, then choose any one. If there is none, then our proof can easily be carried out with a minimizing sequence, $K^\varepsilon_{(1)}$ with $\varepsilon \to 0$, in place of $K_{(1)}$.]. This operator satisfies $0 \leq K_{(1)} \leq I$ and $\mathrm{Tr} K_{(1)} = n$. Let $\rho_{(1)}(x) = K_{(1)}(x,x)$ as usual. A very important fact is that $\Phi(x) := \int |x-y|^{-1}\rho_{(1)}(y)dy$ has its maximum at $x = 0$ (because otherwise we could lower the energy of our state by moving the nucleus from $x = 0$ to another point $x \in \mathbf{R}^3$ at which $\Phi(x) < \Phi(0)$; this argument is used again later in the N-body context just before (6.10), where a lengthier discussion is given). Thus, we have $\mathrm{Tr}\left[|x|^{-1}K_{(1)}\right] = \Phi(0) \geq \int f(x)\Phi(x)dx$ for any $f : \mathbf{R}^3 \to \mathbf{R}^+$ with $\int f \leq 1$. We now have, by the variational principle (5.1) and with $f := \frac{1}{2}\rho_{(1)}$,

$$\begin{aligned} E^{\mathrm{Q}}(N,Z,B) &\leq E^{\mathrm{Q}}f(n,Z,B) \leq \mathrm{Tr}\left[H_{\mathbf{A}}K_{(1)}\right] - Z\Phi(0) + \int f\Phi \\ &\leq \mathrm{Tr}\left[\left(H_{\mathbf{A}} - (Z - \tfrac{1}{2}n)|x|^{-1}\right)K_{(1)}\right] = E^{\mathrm{Q}}_{(1)}(n, Z - \tfrac{1}{2}n, B) \quad . \end{aligned} \tag{5.21}$$

The first inequality states simply that $E^{\rm Q}(N,Z,B)$ is monotone in N (because we can always remove particles to "infinity"). Inequality (5.21) proves (5.19).

To bound $E^{\rm Q}_{(1)}(N,Z,B)$ we use the same variational principle (5.1) (without the repulsion term) and choose, as before, a variational density matrix $K = k\otimes$ (all spins down) with $k(x,y) = g(x)g(y)\Pi_0^\perp(x_\perp,y_\perp)h(x_3-y_3)$, where $\Pi_0^\perp$ is in (5.5), $g:\mathbf{R}^3\mapsto\mathbf{R}^+$ and $h(x)=\int_{-\mu}^{\mu}\exp[2\pi ipx]dp$ for some number $\mu>0$. We demand that g satisfies the condition: $\int g^2\le \pi N/\mu B$. Since $\Pi_0^\perp(x_\perp,x_\perp)=B/2\pi$ and $h(0)=2\mu$, this condition states that $n:=\mathrm{Tr}K=(2\mu)(B/2\pi)\int g^2\le N$, which means that we are computing an upper bound for $E^{\rm Q}_{(1)}(n,Z,B)$. Since $E^{\rm Q}_{(1)}(N,Z,B)$ is a decreasing function of N the fact that $n\le N$ is acceptable.

We have to check that $K\le I$ as an operator. Since $\Pi_0^\perp\le I$ on $L^2(\mathbf{R}^2)$ and $h(x_3-y_3)\le I$ as an operator on $L^2(\mathbf{R})$ (Plancherel) we will, indeed, have $K\le I$ if $0\le g(x)\le 1$ for all $x\in\mathbf{R}^3$. Now we can compute the right side of (5.1) $=\mathrm{Tr}\,[(H_{\mathbf A}-Z/|x|)K]$. Using $H_{\mathbf A}\Pi_0^\perp=0$, we find that

$$E^{\rm Q}_{(1)}(N,Z,B)\le \frac{B}{2\pi}\int_{-\mu}^{\mu}p^2dp\int g^2+\frac{B\mu}{\pi}\int|\nabla g|^2-Z\frac{B\mu}{\pi}\int|x|^{-1}g(x)^2dx. \tag{5.22}$$

Now we fix $R>0$ and choose g to be a smooth, radial function with $g(x)=1$ for $|x|<R$, $g(x)=0$ for $|x|>2R$ and $g(x)\le 1$ everywhere. The condition on $\int g^2$, is $\mu BR^3=(\mathrm{const.})n$. We then obtain

$$E^{\rm Q}_{(1)}(N,Z,B)\le(\mathrm{const.})\left[\mu^2+R^{-2}-(\mathrm{const.})Z/R\right]\le(\mathrm{const.})n[n^2R^{-6}B^{-2}+R^{-2}-(\mathrm{const.})Z/R].$$

We now choose $n=\min\{N,Z\}$ and $R=(\mathrm{const.})\max\{Z^{-1/5}n^{2/5}B^{-2/5},Z^{-1}\}$. ■

Remarks: (i). By omitting the repulsion term in H_N, we have the trivial *lower bound* $E^{\rm Q}(N,Z,B)\ge E^{\rm Q}_{(1)}(N,Z,B)$. Since $E^{\rm Q}_{(1)}(N,Z,B)$ is trivially convex in N (because it is the sum

of the N lowest eigenvalues), we have $E^{\rm Q}_{(1)}(N,Z,B)\ge(N/n)E^{\rm Q}_{(1)}(n,Z,B)$ with $n=\min\{N,Z\}$. Thus

$$\max\{1,N/Z\}E^{\rm Q}_{(1)}(n,Z,B)\le E^{\rm Q}(N,Z,B)\le E^{\rm Q}_{(1)}(n,Z-\tfrac12 n,B). \tag{5.23}$$

(ii). In the next section, eq. (6.6), we will encounter the operator $H_{\mathbf A}-\delta Z/|x|$ with $\delta>1$. However, we will need a *lower bound* only for $h(\delta):=\Pi_0(H_{\mathbf A}-\delta Z/|x|)\Pi_0=\Pi_0(p_3^2-\delta Z/|x|)\Pi_0$. This can easily be achieved as follows. By a scaling $x_3\to\delta^{-1}x_3$ we find that $h(\delta)$ is unitarily equivalent to $\delta^2\Pi_0[p_3^2-Z(x_3^2+\delta^2x_\perp^2)^{-1/2}]\Pi_0$ and this operator is greater than $\delta^2h(1)$.

(iii). The upper bound in (5.20) for $B\le nZ^2$ is, in fact, optimal (*cf.* the lower bound (4.45) to $E^{\rm DM}$). It has the correct asymptotic dependence — as we prove in this paper. The bound for $B\ge nZ^2$ is not optimal. It misses a logarithmic factor. It is easy to get an upper bound on $E^{\rm DM}$

(and thus, by Theorem 5.1, on E^{Q} as well) with the correct logarithmic factor in the following way. Recall that $E^{\mathrm{DM}}(N,Z,B)=Z^3E^{\mathrm{DM}}(\lambda,1,B/Z^3)$ and that $E^{\mathrm{DM}}(\lambda,1,2\pi\eta)$ is a decreasing function of η with the asymptotic form (4.48) or (4.49). This immediately implies that for $B/Z^3\geq 1$

$$E^{\mathrm{DM}}(N,Z,B)\leq -C_\lambda Z^3(1+[\ln(B/Z^3)]^2). \tag{5.24}$$

(iv). A **corollary** of Theorem 5.3 and (5.24) is that R_{U} is really of lower order than E^{Q} as $Z\to\infty$ with N/Z held fixed; this follows from (5.16). It is important to note here that any upper bound to E^{Q} also gives a *lower* bound to $|E^{\mathrm{Q}}|$. Furthermore, once we have established that $E^{\mathrm{DM}}/E^{\mathrm{Q}}\to 1$ as $Z\to\infty$ and $B/Z^{4/3}\to\infty$ (see Theorem 1.3 and (8.6)) we will also know that R_{U} is of lower order than E^{DM}. Theorem 5.3 and (5.24) will be needed again in (8.7) to show that R_{L} is also lower order.

VI. PROOF OF CONCENTRATION IN THE LOWEST LANDAU BAND

It is often asserted that electrons in a large, constant magnetic field are confined to the lowest Landau band, but this is *not* true in the parameter regions 1 and 2, even if B is large. It is also not true under the weaker assumption $Z^{-2}N^{2/3}B\ll 1$. We expect the confinement to occur, however, when $Z^{-2}N^{2/3}B\gg 1$ and that assertion is the content of Theorem 1.2, which we shall prove now.

Proof of Theorem 1.2 (Confinement to lowest Landau band): Part 1. Let Π_0^i be the projection onto the subspace of $\mathcal{H}=\bigotimes^N L^2(\mathbf{R}^3;\mathbf{C}^2)$ in which electron i is in the lowest Landau band. Note $\bigotimes^N$ and not $\bigwedge^N$; at this point we are temporarily dropping symmetry constraints. The integral kernel for Π_0^i is given in (1.14) (with (x,y) replaced by (x^i,y^i)) and multiplied by the identity operator in the other variables. We let $\Pi_>^i:=I-\Pi_0^i$ be the projection onto all the other bands.

If α is any subset of the integers $\{1,2,\ldots,N\}$ we now define the projection

$$\Pi^\alpha=\prod_{i\in\alpha}\Pi_0^i\prod_{j\notin\alpha}\Pi_>^j, \tag{6.1}$$

i.e., Π^α is the projection in $\mathcal{H}$ onto the subspace in which particles $i\in\alpha$ are in the lowest Landau band while the remaining particles are in orthogonal bands. Clearly, $\sum_\alpha\Pi^\alpha=I$. Note that $\Pi_0^N=\Pi^\alpha$ when $\alpha=\{1,2,\ldots,N\}$.

We claim that for any $\varepsilon>0$

$$H_N\geq\sum_\alpha\Pi^\alpha H^\alpha\Pi^\alpha, \tag{6.2}$$

where H^α is the modified Hamiltonian defined by

$$
\begin{aligned}
H^\alpha = \sum_{i=1}^{N} H^i_{\mathbf{A}} - (1+\varepsilon)Z\sum_{i\in\alpha}|x^i|^{-1} - (1+\varepsilon^{-1})Z\sum_{i\notin\alpha}|x^i|^{-1} + (1-3\varepsilon)\sum_{\substack{i<j\\ i,j\in\alpha}}|x^i-x^j|^{-1} \\
-(3\varepsilon^{-1}-1)\sum_{\substack{i<j\\ i,j\notin\alpha}}|x^i-x^j|^{-1} - (\tfrac{3}{2}\varepsilon^{-1}+\tfrac{3}{2}\varepsilon-1)\sum_{i\in\alpha, j\notin\alpha}|x^i-x^j|^{-1}.
\end{aligned}
\tag{6.3}
$$

To prove this, consider the three kinds of terms in (1.1). For the first, $\sum_i H^i_{\mathbf{A}}$, the decomposition (6.2) is evidently an identity since each $H^i_{\mathbf{A}}$ commutes with each Π^α. For the second term, we can write

$$
|x^i|^{-1} = (\Pi^i_0 + \Pi^i_>)|x^i|^{-1}(\Pi^i_0+\Pi^i_>).
\tag{6.4}
$$

The "diagonal" terms, i.e., $\Pi^i_0|x^i|^{-1}\Pi^i_0$ and $\Pi^i_>|x^i|^{-1}\Pi^i_>$, yield, without further ado, the terms in (6.3) proportional to Z. The term in (6.3) proportional to εZ and $\varepsilon^{-1}Z$ come from the "off-diagonal" terms in (6.4) by using the Schwarz inequality as follows:

$$
-\Pi^i_>|x^i|^{-1}\Pi^i_0 - \Pi^i_0|x^i|^{-1}\Pi^i_> \ge -\varepsilon\Pi^i_0|x^i|^{-1}\Pi^i_0 - \varepsilon^{-1}\Pi^i_>|x^i|^{-1}\Pi^i_>.
\tag{6.5}
$$

Thus we have proved (6.2) as far as the single particle potential, $-Z/|x|$, is concerned.

The two-body terms $|x^i-x^j|^{-1}$ are only slightly more complicated. We can write $|x^i-x^j|^{-1}$ in a manner similar to (6.4) using $\Pi^i_0, \Pi^i_> \Pi^j_0$ and $\Pi^j_>$. Now there will be 16 terms instead of 4 as in (6.4). Again, we bound the "off-diagonal" terms by the Schwarz inequality; the result is (6.3).

Our next goal is to bound H^α on functions Ψ that are antisymmetric in the α variables (we denote the number of these by $0\le n_\alpha \le N$) and also antisymmetric in the remaining $n_{\sim\alpha} = N - n_\alpha$ variables. Additionally, we require that the $n_{\sim\alpha}$ variables are in the second or higher Landau band, i.e., $\Pi^i_0\Psi = 0$ for $i\notin\alpha$. Conversely, $\Pi^i_0\Psi=\Psi$ for $i\in\alpha$.

Part 2. First we study the three terms in (6.3) that involve *only* the α variables. These are the first, second and fourth terms in (6.3) and (after relabelling the particles) they are equal to

$$
\widehat{H}^\alpha := (1-3\varepsilon)H_{n_\alpha} + \varepsilon\sum_{i=1}^{n_\alpha}\{3H^i_{\mathbf{A}} - 4Z|x^i|^{-1}\},
\tag{6.6}
$$

where H_{n_α} is given by (1.1) with $N = n_\alpha$ there. The last sum in (6.6), when restricted to the lowest Landau band, can be bounded below by the true ground state energy $E^{\mathrm{Q}}(n_\alpha, Z, B)$ multiplied by a universal constant. In fact, from the remark (ii) following Theorem 5.3, eq. (5.19) (with $\delta = 8/3$ there), we can estimate the sum (when restricted to the lowest Landau band) below by $3(8.2)^2E^{\mathrm{Q}}_{(1)}(n_\alpha, Z/2, B)$. From Theorem 5.3 the energy $E^{\mathrm{Q}}_{(1)}(n_\alpha, Z/2, B)$ is bounded below by $E^{\mathrm{Q}}(n_\alpha, Z, B)$.

Thus, we reach the following conclusion about $\widehat{H}^\alpha$:

$$\Pi^\alpha \widehat{H}^\alpha \Pi^\alpha \geq \Pi^\alpha \{(1-3\varepsilon) E^{\mathrm{Q}}_{\mathrm{conf}}(n_\alpha, Z, B) + (\mathrm{const.})\varepsilon E^{\mathrm{Q}}(n_\alpha, Z, B)\} \Pi^\alpha. \tag{6.7}$$

Note the distinction between $E^{\mathrm{Q}}_{\mathrm{conf}}$ and E^{Q} in (6.7).

Part 3. The remaining four terms in H^α can be bounded below by

$$\widetilde{H}^\alpha = T^{\sim\alpha} - (1+\varepsilon^{-1})Z \sum_{i\notin\alpha} |x^i|^{-1} - 3\varepsilon^{-1} \sum_{i\notin\alpha} \left\{ \sum_{j\in\alpha} |x^i - x^j|^{-1} \right\} - 3\varepsilon^{-1} \sum_{\substack{i<j \\ i,j\notin\alpha}} |x^i - x^j|^{-1}, \tag{6.8}$$

where $T^{\sim\alpha}$ is the kinetic energy operator (the sum of the $H^i_{\mathbf{A}}$'s) for the electrons *not in* α. Let us note that for one particle $2B\Pi_> \leq \Pi_> H_{\mathbf{A}} \Pi_> = \Pi_>[(\mathbf{p}+\mathbf{A})^2 + \boldsymbol{\sigma}\cdot\mathbf{B}]\Pi_>$. Thus, $\Pi_>(\mathbf{p}+\mathbf{A})^2\Pi_> \geq \Pi_>(2B - \boldsymbol{\sigma}\cdot\mathbf{B})\Pi_>$. Hence, since $B \geq \pm\boldsymbol{\sigma}\cdot\mathbf{B}$

$$\Pi_> H_{\mathbf{A}} \Pi_> \geq \Pi_>[\tfrac{1}{2}(\mathbf{p}+\mathbf{A})^2 + \tfrac{1}{2}(2B - \boldsymbol{\sigma}\cdot\mathbf{B}) + \boldsymbol{\sigma}\cdot\mathbf{B}]\Pi_> \geq \tfrac{1}{2}\Pi_>[(\mathbf{p}+\mathbf{A})^2 + B]\Pi_>. \tag{6.9}$$

Because there are no kinetic energy operators in (6.8) for the α particles, the x^j's for $j \in \alpha$ appearing in (6.8) can be taken to be *fixed points* in $\mathbf{R}^3$ whose value is adjusted to give the lowest possible energy for $\Pi^\alpha \widetilde{H}^\alpha \Pi^\alpha$. Given any admissible antisymmetric function $\Psi(x_{n_\alpha+1}, \ldots, x_N)$, and corresponding density $\rho_\Psi(x)$ (as given in (1.3)) with $x \in \mathbf{R}^3$, we can always translate Ψ (i.e., $x \mapsto x+y$) so that the maximum of $\int \rho_\Psi(x+z)|x|^{-1}dx$ occurs at $z=0$. Such a translation will minimize $-(\Psi, \sum_i |x^i|^{-1}\Psi)$. This, in turn, implies that the maximum of $\int \rho_\Psi(x)|x-x^j|^{-1}dx$ occurs at $x^j = 0$. This observation, together with (6.9), means that inf spec $(\Pi^\alpha \widetilde{H}^\alpha \Pi^\alpha) \geq$ inf spec$(\Pi^\alpha \overline{H}^\alpha \Pi^\alpha)$, where

$$\overline{H}^\alpha = nB/2 + \frac{1}{2}\sum_{i=1}^n [\mathbf{p}^i + \mathbf{A}(x^i)]^2 - [(1+\varepsilon^{-1})Z + 3\varepsilon^{-1}n_\alpha] \sum_{i=1}^n |x^i|^{-1} - 3\varepsilon^{-1} \sum_{1\leq i<j\leq n} |x^i - x^j|^{-1}. \tag{6.10}$$

Here $n := n_{\sim\alpha} = N - n_\alpha$.

To obtain a lower bound to $\overline{H}^\alpha$ we start by using the decomposition in Lévy-Leblond's paper [51] for $n \geq 2$:

$$\overline{H}^\alpha = nB/2 + \frac{1}{(n-1)} \sum_{i=1}^n \left\{ \sum_{\substack{j=1 \\ j\neq i}}^n \tfrac{1}{2}[\mathbf{p}^j + \mathbf{A}(x^j)]^2 - [(1+\varepsilon^{-1})Z + 3\varepsilon^{-1}n_\alpha]|x^j|^{-1} - \frac{3(n-1)}{2\varepsilon}|x^j - x^i|^{-1} \right\}. \tag{6.11}$$

To bound the operator in braces $\{\ \}$, we can set $x^i = 0$ (for the reason given in the preceding paragraph). We also introduce a cutoff $R > 0$ and note that $-|x|^{-1} \geq -v - R^{-1}$ where the potential v is given by $v(x) = |x|^{-1} - R^{-1}$ for $|x| \leq R$ and $v = 0$ if $|x| \geq R$. Finally, we use the

Lieb-Thirring inequality† to bound the energy of $\sum\{\frac{1}{2}[\mathbf{p}+\mathbf{A}]^2 - V\}$ by $0.114\int V^{5/2}$. Here, the potential V is

$$V = ((1+\varepsilon^{-1})Z + 3\varepsilon^{-1}(n_\alpha + (n-1)/2))v \le \varepsilon^{-1}[2Z+3N]v.$$

We find that the operator in { } in (6.11) is bounded below by $-8\pi(0.114)R^{1/2}\varepsilon^{-5/2}[2Z+3N]^{5/2} - \varepsilon^{-1}[2Z+3N]n/R$. We minimize this expression with respect to R. The result for all $n = N - n_\alpha > 0$ is (after replacing $n/(n-1)$ by 2)

$$\overline{H}^\alpha \ge (N-n_\alpha)B/2 - 24\varepsilon^{-2}(0.114\pi/2)^{2/3}(N-n_\alpha)^{1/3}[2Z+3N]^2. \tag{6.12}$$

Our final lower bound on $\Pi^\alpha H^\alpha \Pi^\alpha$ is $K^\alpha \Pi^\alpha$, where K^α is the number given by the sum of the right sides of (6.7) and (6.12) for $\widehat{H}^\alpha$ and $\overline{H}^\alpha$ respectively.

Part 4. Our goal now is to show that the ε in the previous inequalities can be chosen to depend (only) on $\lambda^{2/3}\beta = Z^{-2}N^{2/3}B$ and Λ in such a way that

$$K^\alpha \ge E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B) + \delta(\lambda^{2/3}\beta,\Lambda)E^{\mathrm{Q}}(N,Z,B), \tag{6.13}$$

for every α, and where $\delta(\lambda^{2/3}\beta,\Lambda) \to 0$ as $\lambda^{2/3}\beta \to \infty$ for each fixed Λ. Equation (1.16) is an immediate consequence of this because $E^{\mathrm{Q}}(N,Z,B) = \inf\{(\Psi, H_N\Psi) : (\Psi,\Psi) = 1\}$, but

$$(\Psi, H_N\Psi) \ge \sum_\alpha K^\alpha(\Psi, \Pi^\alpha\Psi) \quad \text{and} \quad (\Psi,\Psi) = \sum_\alpha (\Psi, \Pi^\alpha\Psi). \tag{6.14}$$

To prove (6.13) we first note that $E^{\mathrm{Q}}_{\mathrm{conf}}$ and E^{Q} are both monotone nonincreasing in N (because we can always move particles away to spatial infinity if we wish). Therefore we can replace n_α by N in (6.7).

The contribution of the right side of (6.7) is exactly of the correct form (provided we can let $\varepsilon \to 0$ as $\lambda^{2/3}\beta \to \infty$).

In case $B \le Z^3$ (and $\lambda^{2/3}\beta \ge 1$) the contribution of the right side of (6.12) can be usefully bounded below by omitting the B term. The rest is bounded below (replacing $N - n_\alpha$ by N) by

$$-(\text{const.})(1+\tfrac{3}{2}\Lambda)^2\varepsilon^{-2}(\lambda^{2/3}\beta)^{-2/5}Z^{6/5}N^{3/5}B^{2/5} \ge (\text{const.})(1+\tfrac{3}{2}\Lambda)^2\varepsilon^{-2}(\lambda^{2/3}\beta)^{-2/5}E^{\mathrm{Q}}(N,Z,B)$$

The last inequality follows from the upper bound on $E^{\mathrm{Q}}(N,Z,B)$ given in Theorem 5.3.

† In [52] the Lieb-Thirring inequality was originally proved for $-\Delta - V$. Because of the diamagnetic inequality, the proof also works when $-\Delta = \mathbf{p}^2$ is replaced by $(\mathbf{p}+\mathbf{A})^2$, as remarked by several authors.

In case $B \geq Z^3$ we retain the B term in (6.12) and we see (since $(N - n_\alpha) \geq (N - n_\alpha)^{1/3}$) that (6.12) is actually positive (and hence can be neglected) if Z and ε are not too small. Recall that $Z \geq N/\Lambda \geq 1/\Lambda$, so Z is never small. We can easily let $\varepsilon \to 0$ as $\lambda^{2/3}\beta \to \infty$. ■

VII. REDUCTION TO A ONE-BODY PROBLEM

Our goal here is to replace the two-body Coulomb repulsion $\sum_{i<j} |x^i - x^j|^{-1}$ and attraction $-Z\sum_i |x^i|^{-1}$ by the following one-body potential plus a constant:

$$\Phi^{\mathrm{DM}} = -\sum_{i=1}^{N} \phi^{\mathrm{DM}}(x^i) - D(\rho^{\mathrm{DM}}, \rho^{\mathrm{DM}}), \tag{7.1}$$

where ρ^{DM} is the density for the minimizer of $\mathcal{E}^{\mathrm{DM}}$.

$$\phi^{\mathrm{DM}}(x) := \phi^{\mathrm{DM}}_{x_\perp}(x_3) = Z|x|^{-1} - |x|^{-1} * \rho^{\mathrm{DM}}(x), \tag{7.2}$$

and with a relative error that vanishes as $Z \to \infty$.

Such a reduction is much more difficult in the $B \gg Z^3$ case than it is in the $B \ll Z^3$ case treated in our companion paper [28]. In the latter case, spherical symmetry is not broken, and it is sufficient to use a bound of the form (with Ψ being the ground state of H_N, or an approximate ground state)

$$(\Psi, \sum\nolimits_{i<j} |x^i - x^j|^{-1}\Psi) \geq D(\rho_\Psi, \rho_\Psi) - (1.68)\int \rho_\Psi^{4/3}(x)dx \tag{7.3}$$

as in [46] or else the easier bound [52]

$$(\Psi, \sum\nolimits_{i<j} |x^i - x^j|^{-1}\Psi) \geq D(\rho_\Psi, \rho_\Psi) - (\mathrm{const.})\left\{N\int \rho_\Psi^{5/3}(x)dx\right\}^{1/2}. \tag{7.4}$$

Here ρ_Ψ is the one-particle density of Ψ. This inequality is then followed by

$$D(\rho_\Psi, \rho_\Psi) \geq 2D(\rho_\Psi, \widehat{\rho}) - D(\widehat{\rho}, \widehat{\rho}) \tag{7.5}$$

for any fixed function $\widehat{\rho}$ (which is conveniently taken to be the solution to the TF problem). The term $2D(\rho_\Psi, \widehat{\rho})$ is $\int \rho_\Psi\{|x|^{-1} * \widehat{\rho}\}$, and this is the expectation value in the state Ψ of the one-body potential $\sum_{i=1}^N (|x|^{-1} * \widehat{\rho})(x^i)$.

In the case, $B \gg Z^3$, no bound that does not somehow take the broken spherical symmetry into account will suffice for all values $B \gg Z^3$. (It turns out, mysteriously, that (7.3) or (7.4) suffices when $Z^5 \gg B \gg Z^3$, but not when $B \geq Z^5$.) The reason is that any bound that does not break symmetry will yield a bound for the error (called the "exchange energy") of the form $N \cdot (\mathrm{length})^{-1}$, and the length in question will necessarily be the shortest, i.e. the diameter of the cylinder rather than its height. This diameter is, as we saw in Sect. 2, proportional to $Z^{1/2}B^{-1/2}$. Thus, we should incorrectly estimate the exchange energy to be $NB^{1/2}Z^{-1/2} \sim Z^{1/2}B^{1/2}$. This has to be compared with the total energy $Z^3[\ln(B/Z^3)]^2$. The two energies are equal roughly when $Z^{1/2}B^{1/2} = Z^3$, or $B = Z^5$.

The exchange energy is roughly the self energy of a charge distribution corresponding to an electron smeared over the region of space occupied by the electron, the exchange hole. In the small field case, $B \ll Z^3$, this hole is a little ball. In the present case the exchange hole is rather like a cylinder with base radius $\sim B^{-1/2}$ and length $Z^{-1}[\ln(B/Z^3)]^{-1}$. The self energy in this case would be of the order of $Z\ln(B/Z^3)\ln(B/Z^2)$. Thus the total exchange energy is anticipated to be of the order $Z^2\ln(B/Z^3)\ln(B/Z^2)$, which is small compared to the total energy. Our bound on the exchange energy is slightly worse. In fact we shall prove the following theorem.

7.1. THEOREM (Bound on the exchange energy). *For the atomic Hamiltonian H_N defined in (1.1) we have the following lower bound when $N = \lambda Z$.*

$$H_N \geq \sum_{i=1}^{N}\Big((1 - Z^{-1/3})H_{\mathbf{A}}^i - \phi^{\mathrm{DM}}(x^i)\Big) - D(\rho^{\mathrm{DM}}, \rho^{\mathrm{DM}}) - C_\lambda(1+\lambda^5)(1+Z^{8/3})(1+[\ln(B/Z^3)]^2). \tag{7.6}$$

Proof: The main idea in the proof is to introduce ultraviolet cut-offs in the Coulomb kernel. The cut-offs are different in the directions along the magnetic field and perpendicular to it, thereby reflecting the different length-scales of the problem. The cut-off parallel to the field will be smaller than the cut-off perpendicular to the field. The real difficulty in the proof lies in controlling the error entailed by the small cut-off parallel to the field. We estimate this error in terms of the kinetic energy of the motion along the field.

We draw the reader's attention to the fact that the kinetic energy is involved, which means that our error estimate in (7.6) really involves Planck's constant. This situation is different from the bound given in (7.3), which does not depend on derivatives of the many-body function Ψ.

For $\delta > 0$ define the regularized Coulomb potential

$$V(x) = |x|^{-1}[1 - \exp(-|x|/\delta)]. \tag{7.7}$$

Our notation suppresses the dependence of V on δ. Even though this regularization is spherically symmetric, the parameter δ^{-1} will essentially be the ultraviolet cut-off perpendicular to the field. Indeed, we now introduce an additional cut-off parallel to the field. This additional cut-off is most conveniently done on the Fourier transform of V,

$$\widehat{V}(p) = \int \exp[-ip\cdot x]V(x)dx = 4\pi(|p|^{-2} - (|p|^2 + \delta^{-2})^{-1}). \tag{7.8}$$

For $a > 0$ we define the cut-off potential

$$\widehat{V}_<(p) = \begin{cases} \widehat{V}(p) & , \text{ if } |p_3| \le a^{-1} \\ 0 & , \text{ if } |p_3| > a^{-1} \end{cases} . \tag{7.9}$$

Additionally, let $\widehat{V}_>(p) = \widehat{V}(p) - \widehat{V}_<(p)$. We shall prove that the main part of the repulsive energy comes from $\widehat{V}_<(p)$.

Since $\widehat{V}_<(p) \ge 0$, its inverse Fourier transform $V_<(x)$ defines a positive semidefinite kernel, i.e., $\int\int \overline{f}(x)V_<(x-y)f(y)dxdy \ge 0$ for all functions f. As a consequence the following holds for any $\rho \in L^1(\mathbf{R}^3)$ (see [53]).

$$\sum_{i<j} V_<(x^i - x^j) \ge \sum_i \int \rho(y)V_<(x^i - y)dy - \tfrac{1}{2}NV_<(0) - \tfrac{1}{2}\int\int \rho(x)\rho(y)V_<(x-y)dxdy. \tag{7.10}$$

This inequality can be seen by the following computation which is easily made rigorous by approximating the delta function by a sequence of smooth compactly supported functions.

$$\begin{aligned}
\textstyle\sum_{i<j} V_<(x^i - x^j) &= \sum_{i<j} \int\int \delta(x - x^i)V_<(x-y)\delta(y - x^j)dxdy \\
&= \tfrac{1}{2}\int\int \left(\sum_i \delta(x - x^i) - \rho(x)\right) V_<(x-y) \left(\sum_i \delta(y - x^i) - \rho(y)\right) dxdy \\
&\quad - \frac{N}{2}V(0) + \sum_i \int V_<(x^i - y)\rho(y)dy - \tfrac{1}{2}\int\int \rho(x)\rho(y)V_<(x-y)dxdy.
\end{aligned}$$

Inequality (7.10) follows from the positivity of the kernel of $V_<$. In our application of (7.10) we shall take $\rho = \rho^{\mathrm{DM}}$.

We must estimate $V_<(0)$ which, according to (7.10), is essentially the exchange energy per particle. From the formula for the inverse Fourier transform we get

$$\begin{aligned}
V_<(0) &= (2\pi)^{-3}\int \widehat{V}_<(p)dp = (2\pi)^{-3}\int_{|p_3|\le 1/a} \widehat{V}(p)dp \\
&= (2\pi)^{-1}\int_{-1/a}^{1/a} \ln(1 + |p_3|^{-2}\delta^{-2})dp_3 \le (2\pi)^{-1}\int_{-1/a}^{1/a} \left[\ln(1 + a^2\delta^{-2}) - 2\ln(a|p_3|)\right]dp_3 \\
&= \pi^{-1}a^{-1}(2 + \ln(1 + a^2\delta^{-2})).
\end{aligned} \tag{7.11}$$

We turn now to $V_>$, the inverse Fourier transform of $\widehat{V}_>$. It follows from (7.7), (7.11) and the definition of $\widehat{V}_>$ that $V_>(0)$ is of order δ^{-1}. We can therefore not use (7.10) with $V_>$ in place of $V_<$, since this would yield an estimate of the exchange energy per particle that is too large. Indeed, δ will be chosen smaller than the perpendicular radius, $\sim Z^{1/2}B^{-1/2}$, of the atom. Thus, an exchange bound of the form $N\delta^{-1}$ will be larger than the total energy when B is large enough, i.e., when $B \gg Z^5$. The moral of this is that if our error terms are to be useful the parameter δ must appear inside a logarithm. Hence the $V_>$ part of the kernel has to be treated differently from $V_<$. Our main estimate on $V_>$ is as follows.

7.2. LEMMA. *If* $\psi \in L^2(\mathbf{R})$ *with* $\int |\psi|^2 = 1$ *then*

$$\sup_{x_\perp} \left| \int_{\mathbf{R}} V_>(x)|\psi(x_3)|^2 dx_3 \right| \leq (8\pi^{-1}a)^{1/2} \ln(1+a^2\delta^{-2}) \left(\int_{\mathbf{R}} \left(\frac{d\psi(x_3)}{dx_3} \right)^2 dx_3 \right)^{3/4} . \tag{7.12}$$

Proof of Lemma 7.2: The supremum norm of the function $x_\perp \mapsto \int_{\mathbf{R}} V_>(x)|\psi(x_3)|^2 dx_3$ can be estimated by the L^1 norm of its Fourier transform which is the function $p_\perp \mapsto (2\pi)^{-1} \int_{\mathbf{R}} \widehat{V}_>(p)\widehat{|\psi|^2}(p_3)dp_3$. Thus

$$\begin{aligned} \sup_{x_\perp} \left| \int_{\mathbf{R}} \widehat{V}_>(x)|\psi(x_3)|^2 dx_3 \right| &\leq (2\pi)^{-3} \int_{\mathbf{R}^2} \left| \int_{\mathbf{R}} \widehat{V}_>(p)\widehat{|\psi|^2}(p_3)dp_3 \right| dp_\perp \\ &\leq (2\pi)^{-3} \int_{\mathbf{R}^2} \widehat{V}(p_\perp, a^{-1})dp_\perp \int_{|p_3|\geq 1/a} |\widehat{|\psi|^2}(p_3)|dp_3, \end{aligned} \tag{7.13}$$

where we have used that $\widehat{V}$ is positive and monotonically decreasing in p_3 for each fixed value of $p_\perp$. The first integral in (7.13) is easy to calculate:

$$\int_{\mathbf{R}^2} \widehat{V}(p_\perp, a^{-1})dp_\perp = (2\pi)^2 \ln(1+a^2\delta^{-2}). \tag{7.14}$$

The second integral in (7.13) can be estimated by the Cauchy- Schwarz inequality.

$$\begin{aligned} \int_{|p_3|\geq 1/a} \left| \widehat{|\psi|^2}(p_3) \right| dp_3 &\leq \left(\int_{|p_3|\geq 1/a} |p_3|^{-2} dp_3 \right)^{1/2} \left(\int_{\mathbf{R}} |p_3|^2 \left| \widehat{|\psi|^2}(p_3) \right|^2 dp_3 \right)^{1/2} \\ &= (4\pi a)^{1/2} \left(\int_{\mathbf{R}} \left(\frac{d}{dx_3}|\psi|^2 \right)^2 dx_3 \right)^{1/2} . \end{aligned}$$

Using $\sup_x |\psi(x)| \leq \sqrt{2} \left(\int \left| \frac{d}{dx_3}\psi \right|^2 dx_3 \right)^{1/4}$ we find

$$\int_{|p_3|\geq 1/a} \left| \widehat{|\psi|^2}(p_3) \right| dp_3 \leq (32\pi a)^{1/2} \left(\int \left| \frac{d\psi}{dx_3} \right|^2 dx_3 \right)^{3/4} . \tag{7.15}$$

Inserting (7.14) and (7.15) into (7.13) gives (7.12). This finishes the proof of Lemma 7.2. ■

Continuation of the proof of Theorem 7.1. We are now prepared to estimate the many-body Hamiltonian H_N. Using $|x|^{-1} \geq V(x)$ we get, for all $0 < \alpha < 1$,

$$\begin{aligned} H_N &\geq \sum_{i=1}^N (H^i_{\mathbf{A}} - Z|x^i|^{-1}) + \sum_{1\leq i<j\leq N} V(x^i - x^j) \\ &\geq \sum_{i=1}^N ((1-\alpha)H^i_{\mathbf{A}} - Z|x^i|^{-1}) + \sum_{1\leq i<j\leq N} V_<(x^i - x^j) \\ &\quad + \sum_{i=1}^N \left[\alpha H^i_{\mathbf{A}} + \tfrac{1}{2}\sum_{j\neq i} V_>(x^i - x^j)\right]. \end{aligned} \tag{7.16}$$

We can estimate the operator

$$\alpha H^i_{\mathbf{A}} + \tfrac{1}{2}\sum_{j\neq i} V_>(x^i - x^j)$$

with the $N-1$ points $x^j, j \neq i$ fixed, in which case it is a one-body operator. Since $H_{\mathbf{A}} \geq -(\partial/\partial x_3)^2$ we find from Lemma 7.2 the following lower bound independent of $x^j, j \neq i$

$$\begin{aligned} \alpha H^i_{\mathbf{A}} + \tfrac{1}{2}\sum_{j\neq i} V_>(x^i - x^j) &\geq \inf_T \left\{\alpha T - \tfrac{1}{2}(N-1)(8\pi^{-1}a)^{1/2}\ln(1+a^2\delta^{-2})T^{3/4}\right\} \\ &\geq -\tfrac{1}{3}\left(\tfrac{3}{8}\right)^4\alpha^{-3}(8\pi^{-1}a)^2(N-1)^4[\ln(1+a^2\delta^{-2})]^4. \end{aligned} \tag{7.17}$$

Combining (7.10) (with $\rho = \rho^{\mathrm{DM}}$), (7.11), (7.16) and (7.17) we find for all $0 < \alpha < 1$ and all a and $\delta > 0$

$$\begin{aligned} H_N \geq &\sum_{i=1}^N \left((1-\alpha)H^i_{\mathbf{A}} - Z|x^i|^{-1} + \int \rho^{\mathrm{DM}}(y)V_<(x^i - y)dy\right) \\ &- \tfrac{1}{2}\int\int \rho^{\mathrm{DM}}(x)\rho^{\mathrm{DM}}(y)V_<(x-y)dxdy - \tfrac{1}{2}N\pi^{-1}a^{-1}(2+\ln(1+a^2\delta^{-2})) \\ &- \tfrac{1}{3}\left(\tfrac{3}{8}\right)^4\alpha^{-3}N(N-1)^4(8\pi^{-1}a)^2[\ln(1+a^2\delta^{-2})]^4. \end{aligned} \tag{7.18}$$

To arrive at the final estimate (7.6) we should like to replace $V_<$ in (7.18) by $|x|^{-1}$. We shall first replace $V_<$ by V and then V by $|x|^{-1}$. The error in the first replacement can be estimated with the aid of Lemma 7.2. Indeed,

$$\begin{aligned} \left|\int \rho^{\mathrm{DM}}(y)[V(x-y) - V_<(x-y)]dy\right| &= \int \rho^{\mathrm{DM}}(y)V_>(x-y)dy \\ \leq (8\pi^{-1}a)^{1/2}\ln(1+a^2\delta^{-2}) &\int_{\mathbf{R}^2}\left(\int_{\mathbf{R}}(\partial\sqrt{\rho^{\mathrm{DM}}(x)}/\partial x_3)^2 dx_3\right)^{3/4}\left(\int_{\mathbf{R}}\rho^{\mathrm{DM}}(x)dx_3\right)^{1/4} dx_\perp. \end{aligned}$$

The integral $\left(\int\limits_{\mathbf{R}} \rho^{\rm DM}\right)^{1/4}$ appears because of the normalization. Now, using Hölder's inequality, the estimate (4.5) and the virial inequality (4.44),

$$\begin{aligned}\int \rho^{\rm DM}(y) V_>(x-y)dy &\le (8\pi^{-1}a)^{1/2}\ln(1+a^2\delta^{-2})N^{1/4}\left(\int (\partial\sqrt{\rho^{\rm DM}}/\partial x_3)^2 dx\right)^{3/4} \\ &\le (8\pi^{-1}a)^{1/2}\ln(1+a^2\delta^{-2})N^{1/4}|E^{\rm DM}|^{3/4}. \end{aligned} \tag{7.19}$$

Finally we control the replacement of V by $|x|^{-1}$ this time using (4.8) and (4.44)

$$\begin{aligned}\int \rho^{\rm DM}(y)[v(x-y)-|x-y|^{-1}]dy &= \int \rho^{\rm DM}(y)\exp(-|x-y|\delta^{-1})|x-y|^{-1}dy \\ &\le \left(\int \rho^{\rm DM}(y)^3 dy\right)^{1/3}\left(\int \exp\left(-\tfrac{3}{2}|y|\delta^{-1}\right)|y|^{-3/2}dy\right)^{2/3} \\ &\le ({\rm const.})B^{2/3}|E^{\rm DM}|^{1/3}\delta. \end{aligned} \tag{7.20}$$

Using (7.19) and (7.20) together with the estimate (4.46) on $E^{\rm DM}$ we get the following lower bound instead on (7.18).

$$\begin{aligned} H_N \ge &\sum_{i=1}^{N}((1-\alpha)H^i_{\mathbf{A}} - \phi^{\rm DM}(x^i)) - \tfrac{1}{2}\int\int \rho^{\rm DM}(x)\rho^{\rm DM}(y)|x-y|^{-1}dxdy \\ &- ({\rm const.})\Big[Na^{-1}(2+\ln(1+a^2\delta^{-2})) + \alpha^{-3}N^5a^2(\ln(1+a^2\delta^{-2}))^4 \\ &+ N^{5/4}a^{1/2}Z^{9/4}\ln(1+a^2\delta^{-2})(1+[\ln(BZ^{-3})]^2)^{3/4} \\ &+ \delta B^{2/3}NZ(1+[\ln(BZ^{-3})]^2)^{1/3}\Big]. \end{aligned} \tag{7.21}$$

We now make the choices $\delta = B^{-2/3}Z^{1/3}$, $a = Z^{-5/3}[1+\ln(1+BZ^{-3})]^{-1}$ and $\alpha = Z^{-1/3}$. Recalling that $N = \lambda Z$ we arrive at (7.6). This finishes the proof of Theorem 7.1. ■

VIII. LIMIT OF QUANTUM MECHANICS

In this section we shall complete the proof of the main result that the quantum energy $E^{\rm Q}(N,Z,B)$ can be approximated by the energy $E^{\rm DM}(N,Z,B)$. Unlike the semi-classical Thomas-Fermi approximation studied in our companion paper [28] the approximation of $E^{\rm Q}$ by $E^{\rm DM}$ is quite simple after having made the reduction to a one-body problem.

Proof of Theorem 1.3 (Energy asymptotics for regions 3, 4, 5): Since Theorem 5.1 contains the appropriate upper bound on E^Q we here only have to address the question of a lower bound. Furthermore it follows from Theorem 1.2 on the confinement to the lowest Landau band that we can replace $E^{\rm Q}$ by the ground state energy $E^{\rm Q}f_{\rm conf}$ of the confined Hamiltonian $\Pi_0^N H_N \Pi_0^N$.

If $\Pi_0^N\Psi=\Psi$ we know from Lemma 4.1 that $\Gamma^\Psi\in\mathcal{G}_B^{\mathrm{DM}}$. From Theorem 7.1 we also know that for such a normalized function Ψ

$$(\Psi,H_N\Psi)\geq(1-Z^{-1/3})\int\limits_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}^\Psi\right]dx_\perp-\int\phi^{\mathrm{DM}}(x)\rho_\Psi(x)dx-D(\rho^{\mathrm{DM}},\rho^{\mathrm{DM}})-R_{\mathrm{L}} \tag{8.1}$$

where $R_{\mathrm{L}}=(\mathrm{const.})(1+\lambda^5)(1+Z^{8/3})(1+[\ln(B/Z^3)]^2)$.

It is clear that if $(\Psi,H_N\Psi)\leq 0$ (which we can of course assume) then $\int\limits_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}[\hat{h}_{Z,x_\perp}\Gamma_{x_\perp}^\Psi]\,dx_\perp\leq 0$ where $\widehat{h}_{Z,x_\perp}$ was defined in (4.9). Hence

$$\begin{aligned}\tfrac{1}{2}\int\limits_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial}{\partial x_3^2}\Gamma_{x_\perp}^\Psi\right]dx_\perp&=\int\limits_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}\big[(\widehat{h}_{Z,x_\perp}-\tfrac{1}{2}\widehat{h}_{2Z_1x_\perp})\Gamma_{x_\perp}^\Psi\big]dx_\perp\\&\leq-\tfrac{1}{2}\int\limits_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}[\widehat{h}_{2Z,x_\perp}\Gamma_{x_\perp}^\Psi]dx_\perp\\&\leq c_\lambda Z^3(1+[\ln(B/Z^3)]^2),\end{aligned} \tag{8.2}$$

where the last inequality follows from (4.11).

Thus from (8.1) we get the estimate

$$\begin{aligned}(\Psi,H_N\Psi)&\geq\int\limits_{\mathbf{R}^2}\mathrm{Tr}_{L^2(\mathbf{R})}\left[\left(-\frac{\partial^2}{\partial x_3^2}-\phi^{\mathrm{DM}}\right)\Gamma_{x_\perp}^\Psi\right]dx_\perp-D(\rho^{\mathrm{DM}},\rho^{\mathrm{DM}})-(\mathrm{const.})R_{\mathrm{L}}\\&=\mathcal{E}_{\mathrm{L}}^{\mathrm{DM}}[\Gamma^\Psi]-D(\rho^{\mathrm{DM}},\rho^{\mathrm{DM}})-(\mathrm{const.})R_{\mathrm{L}}\\&\geq E^{\mathrm{DM}}-(\mathrm{const.})R_{\mathrm{L}}.\end{aligned} \tag{8.3}$$

The last inequality in (8.3) is a consequence of Theorem 4.4 since it follows from there that

$$\mathcal{E}_{\mathrm{L}}^{\mathrm{DM}}[\Gamma^\Psi]\geq\mathcal{E}_{\mathrm{L}}^{\mathrm{DM}}[\Gamma^{\mathrm{DM}}]=\mathcal{E}^{\mathrm{DM}}[\Gamma^{\mathrm{DM}}]+D(\rho^{\mathrm{DM}},\rho^{\mathrm{DM}}).$$

Since (8.3) holds for all normalized Ψ satisfying $\Pi_0^N\Psi=\Psi$ we can take the infimum. We obtain

$$E_{\mathrm{conf}}^{\mathrm{Q}}(N,Z,B)\geq E^{\mathrm{DM}}(N,Z,B)-(\mathrm{const.})R_{\mathrm{L}}. \tag{8.4}$$

In Theorem 5.3 we proved that $E^{\mathrm{Q}}(N,Z,B)\leq -c_\lambda(Z^{9/5}B^{2/5}+1)$ and, indeed this bound is of the correct order if $B\leq Z^3$. If we compare this bound with the error R_{L} in (8.4) we see that only when $B\gg Z^{13/6}$ can R_{L} be negligible. When the magnetic field is in the range $Z^{4/3}\ll B\lesssim Z^{13/6}$ we must use the standard exchange estimate (7.3) rather than (7.6).

If Ψ is a normalized wave function with $\Pi_0^N\Psi = \Psi$ we can easily estimate the error in (7.3). In fact, from the Lieb-Thirring inequality (4.8)

$$\int \rho_\Psi^{4/3}(x)dx \le \left(\int \rho_\Psi^3(x)dx\right)^{1/6} \left(\int \rho_\Psi(x)dx\right)^{5/6} \le \left(\frac{3}{\pi^2}B^2 \int \mathrm{Tr}_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}^\Psi\right]dx_\perp\right)^{1/6} N^{5/6}.$$

If we now proceed as in (8.2) but using the estimate (4.10) instead of (4.11) we get if $(\Psi, H_N\Psi) \le 0$ that

$$\int \rho_\Psi^{4/3}(x)dx \le c_\lambda Z^{17/15}B^{2/5}. \tag{8.5}$$

As explained in the beginning of Sect. VII we combine (7.3) with the inequality $D(\rho_\Psi,\rho_\Psi) \ge 2D(\rho_\Psi,\rho^{\mathrm{DM}}) - D(\rho^{\mathrm{DM}},\rho^{\mathrm{DM}})$ and arrive at

$$\begin{aligned}(\Psi, H_N\Psi) \ge &\int_{\mathbf{R}^2} \mathrm{Tr}_{L^2(\mathbf{R})}\left[\left(-\frac{\partial^2}{\partial x_3^2} - \phi^{\mathrm{DM}}\right)\Gamma_{x_\perp}^\Psi\right]dx_\perp \\ &- D(\rho^{\mathrm{DM}},\rho^{\mathrm{DM}}) - c_\lambda Z^{17/15}B^{2/5} \\ &\ge E^{\mathrm{DM}} - c_\lambda Z^{17/15}B^{2/5}.\end{aligned}$$

We can thus conclude that (8.4) holds with R_{L} being the lesser of the two quantities

$$c_\lambda(Z^{17/15}B^{2/5}+1) \quad \text{and} \quad c_\lambda(1+Z^{8/3})(1+[\ln(B/Z^3)]^2). \tag{8.6}$$

To complete the proof of Theorem 1.3 we have to show that both R_{U} from (5.16) and R_{L} from (8.6) are negligible compared to E^{Q}. This immediately follows from Theorem 5.3 and (5.24). ∎

We can now summarize the relations between the true quantum energy E^{Q} and our three approximating energies $E^{\mathrm{DM}}, E^{\mathrm{SS}}$ and E^{HS} as follows

1) If $N/Z = \lambda$ and $B/(2\pi Z^3) = \eta$ are held fixed as $Z \to \infty$ then (the symbol $\approx$ here means that the ratio of the left side to the right side converges to one)

$$E^{\mathrm{Q}}(N,Z,B) \approx Z^3 E^{\mathrm{DM}}(\lambda, 1, 2\pi\eta). \tag{8.7}$$

2) If $N/Z = \lambda$ and $B/(2\pi Z^3) = \eta \ge \eta_c$ as $Z \to \infty$ then, from Theorem 4.6,

$$E^{\mathrm{Q}}(N,Z,B) \approx Z^3 E^{\mathrm{SS}}(\lambda, 1, 2\pi\eta). \tag{8.8}$$

3) If $N/Z = \lambda$ and $B/Z^3 \to \infty$ as $Z \to \infty$ then, from Theorem 3.5,

$$E^{\mathrm{Q}}(N,Z,B) \approx Z^3[\ln(B/(2\pi Z^3))]^2 E^{\mathrm{HS}}(\lambda), \tag{8.9}$$

which, when combined with (3.7), gives Theorem 1.4.

If we appeal to the strong Thomas-Fermi energy $E^{\rm STF}$ defined in [7] and [28] we can also give the asymptotics for small values of B/Z^3.

4) If $N/Z = \lambda, B/Z^3 \to 0$ but $B/Z^{4/3} \to \infty$ as $Z \to \infty$ then

$$E^{\rm Q}(N,Z,B) \approx Z^3(B/Z^3)^{2/5} E^{\rm STF}(\lambda,1,1), \tag{8.10}$$

which is just another way of writing (1.9). Because of Theorem 1.3 this last formula also holds for $E^{\rm DM}$:

$$E^{\rm DM}(\lambda,1,2\pi\eta) \approx (2\pi\eta)^{2/5} E^{\rm STF}(\lambda,1,1), \tag{8.11}$$

as $\eta \to 0$.

A simple modification of the proof of Theorem 1.3 can be used in a standard way to prove that the quantum density in the large Z limit can be approximated by the density of the minimizer for the density matrix functional.

8.1. THEOREM. *Let $\rho^{\rm DM}(x) = \rho^{\rm DM}(x;N,Z,B)$ denote the density for the minimizer $\Gamma^{\rm DM}$ described in Theorem 4.3. We then have the following limit for the quantum density $\rho^{\rm Q}$ as $Z \to \infty$ with $N/Z = \lambda$ and $B/(2\pi Z^3) = \eta$ held fixed*

$$Z^{-4}\rho^{\rm Q}(Z^{-1}x) \rightharpoonup \rho^{\rm DM}(x;\lambda,1,2\pi\eta), \tag{8.12}$$

weakly in $L^1_{\rm loc}(\mathbf{R}^3)$. If $N \le N_c^{\rm DM}$ the convergence is weakly in $L^1(\mathbf{R}^3)$.

While the convergence in (8.12) is not uniform in η, neither for large nor small η, we can find a limit that is uniform for large η by introducing

$$x_\eta := \left(\eta^{-1/2}x_\perp, [\ln(\eta)]^{-1}x_3\right).$$

The weak $L^1_{\rm loc}(\mathbf{R}^3)$ limit that is uniform in η for large η is

$$Z^{-4}\eta^{-1}[\ln(\eta)]^{-1}\rho^{\rm Q}(Z^{-1}x_\eta) \rightharpoonup \eta^{-1}[\ln(\eta)]^{-1}\rho^{\rm DM}(x_\eta;\lambda,1,2\pi\eta). \tag{8.13}$$

Proof: The precise meaning of the limit in weak $L^1_{\rm loc}$ is that for each $W \in L^\infty(\mathbf{R}^3)$ with compact support

$$Z^{-4}\eta^{-1}[\ln(\eta)]^{-1}\int \rho^{\rm Q}(Z^{-1}x_\eta)W(x)dx \to \eta^{-1}[\ln(\eta)]^{-1}\int \rho^{\rm DM}(x_\eta;\lambda,1,2\pi\eta)W(x)dx. \tag{8.14}$$

as $Z \to \infty$.

To prove (8.14) it is enough to consider $W \in C_0^\infty(\mathbf{R}^3)$. To arrive at this conclusion we first notice that it is clearly enough (see also Lemma III.4 in [30]) to consider test functions W that are characteristic functions of measurable sets. By outer regularity of the Lebesgue measure we can restrict our attention to open sets. However, let $f_n \in L^1_{\text{loc}}(\mathbf{R}^3)$ be non-negative functions satisfying $\int f_n \widetilde{W} \to \int f \widetilde{W}$ for all functions $\widetilde{W} \in C_0^\infty(\mathbf{R}^3)$ only. If now W is a characteristic function of an open set we can choose functions $W_\pm \in C_0^\infty(\mathbf{R}^3)$ such that $W_- \le W \le W_+$ and such that $\int f W_\pm$ are as close to $\int f W$ as we please. Then for all $\delta > 0$ we can choose n so large that

$$\int f W_- - \delta \le \int f_n W_- \le \int f_n W \le \int f_n W_+ \le \int f W_+ + \delta,$$

and the convergence weakly in L^1_{loc} follows. It is important that the functions f_n are non-negative for otherwise the conclusion would be wrong!

Weak convergence in $L^1(\mathbf{R}^3)$, which means that we consider all $W \in L^\infty(\mathbf{R}^3)$ without restriction on the support, follows (see again Lemma III.4 in [30]) if we have both weak convergence in L^1_{loc} and convergence for the constant function $W = 1$. This last condition simply means that $\lambda = N/Z$ (which is held fixed) converges to $\int \rho(x; \lambda, 1, 2\pi\eta) dx$. This is of course true if $N \le N_c^{\text{DM}}$.

The standard method [30] of proving (8.14) is to introduce the following perturbed Hamiltonian

$$H_N(\alpha) = H_N + \alpha \sum_{i=1} W_{Z,\eta}(x_i),$$

where the perturbing potential has the following scaling

$$W_{Z,\eta}(x) := Z^2 (\ln \eta)^2 W\left(Z\eta^{1/2} x_\perp, Z(\ln \eta) x_3\right),$$

and the corresponding perturbed density matrix functional is

$$\mathcal{E}_\alpha^{\text{DM}}[\Gamma] = \mathcal{E}^{\text{DM}}[\Gamma] + \alpha \int W_{Z,\eta}(x) \rho_\Gamma(x) dx.$$

In terms of these we define energy functions

$$E_\alpha^{\text{Q}}(N, Z, B) = \inf\ \text{spec}\ H_N(\alpha)$$

and

$$E_\alpha^{\text{DM}}(N, Z, B) = \inf\{\mathcal{E}_\alpha^{\text{DM}}[\Gamma] \big| \Gamma \in \mathcal{G}_B^{\text{DM}}, \int_{\mathbf{R}^2} \text{Tr}_{L^2(\mathbf{R})}[\Gamma_{x_\perp}] dx_\perp \le N\}.$$

Since we are assuming that $W \in C_0^\infty(\mathbf{R}^3)$ the proof of Theorem 4.3 is applicable also in the case of the perturbed functional $\mathcal{E}_\alpha^{\text{DM}}$ and shows the existence of a unique minimizer.

It is clear that E_α^{DM} satisfies the same scaling property as E^{DM}, i.e., $E_\alpha^{\text{DM}}(N, Z, B) = Z^3 E_\alpha^{\text{DM}}(\lambda, 1, 2\pi\eta)$. It is also easy to see that for large values of η the energy $E_\alpha^{\text{DM}}(N, Z, B)$ can be estimated above and below by expressions of the form (const.)$Z^3(\ln\eta)^2$, where the constants depend on W.

We would like now to show that the proof of Theorem 1.3 extends to include the statement that the energies E_α^{Q} and E_α^{DM} satisfy

$$\frac{E^{\mathrm{Q}}f_\alpha(N,Z,B)}{E_\alpha^{\mathrm{DM}}(N,Z,B)} \to 1 \tag{8.15}$$

as $Z\to\infty$ uniformly in η for large η. To do this we only need to argue that the unique minimizer for $\mathcal{E}_\alpha^{\mathrm{DM}}$ satisfies bounds similar to (4.50) and to the virial inequalities (4.44). These bounds were used in Sects. V and VII and were essential in the proof of Theorem 1.3.

1. *The estimate* (4.50): As in the proof of (4.50) we need to estimate

$$\begin{aligned}
&-\frac{B}{2\pi}\left(\text{sum of negative eigenvalues of } -\tfrac{1}{2}\frac{\partial^2}{\partial x_3^2}-Z|x|^{-1}+\alpha W_{Z,\eta}(x)\right)\le\\
&-\frac{B}{2\pi}\left(\text{sum of negative eigenvalues of } -\tfrac{1}{4}\frac{\partial^2}{\partial x_3^2}-Z|x|^{-1}\right)\\
&-\frac{B}{2\pi}\left(\text{sum of negative eigenvalues of } -\tfrac{1}{4}\frac{\partial^2}{\partial x_3^2}+\alpha W_{Z,\eta}(x)\right)
\end{aligned}.$$

The first term above was estimated in Proposition 4.9 the second can be estimated by the one-dimensional Lieb-Thirring inequality to be less than

$$\frac{B}{2\pi}\alpha^{3/2}\int|W_{Z,\eta}(x)|^{3/2}\le Z^2(\ln\eta)^2\int_{\mathbf{R}}|W(Z\eta^{1/2}x_\perp,x_3)|^{3/2}dx_3.$$

Since W has compact support the right side is bounded by the expression on the right side of (4.50) with a constant that now depends on W.

2. *The virial inequalities* (4.44): For the functional $\mathcal{E}_\alpha^{\mathrm{DM}}$ we can repeat the scaling argument that lead to the virial inequalities. Compared to the original virial inequalities we now get an extra term which depends on $W_{Z,\eta}$. By scaling, this term is of the form $Z^3(\ln\eta)^2$ multiplied by a constant which depends only on W. Hence we arrive at virial inequalities with constants depending on W.

Having argued that (8.15) holds we can use the scaling property of E_α^{DM} and rewrite (8.15) as the following limit which is uniform in η:

$$Z^{-3}(\ln\eta)^{-2}E_\alpha^{\mathrm{Q}}(N,Z,B)\to(\ln\eta)^{-2}E_\alpha^{\mathrm{DM}}(\lambda,1,2\pi\eta). \tag{8.16}$$

Both energies E_α^{Q} and E_α^{DM} are defined as infima of functions that are linear in α and are therefore themselves concave in α. It then follows from (8.16) that

$$Z^{-3}(\ln\eta)^{-2}\frac{\partial}{\partial\alpha}E_\alpha^{\mathrm{Q}}(N,Z,B)\to(\ln\eta)^{-2}\frac{\partial}{\partial\alpha}E_\alpha^{\mathrm{DM}}(\lambda,1,2\pi\eta), \tag{8.17}$$

as $Z \to \infty$ unformly in η.

We shall use (8.17) for $\alpha = 0$. From the concavity of $E_\alpha^{\rm Q}$ and $E_\alpha^{\rm DM}$ as functions of α we easily see that

$$\begin{aligned} Z^{-3}(\ln\eta)^{-2}\frac{\partial}{\partial\alpha}E_\alpha^{\rm Q}(N,Z,B)\big|_{\alpha=0} &= Z^{-3}(\ln\eta)^{-2}\int W_{Z,\eta}(x)\rho^{\rm Q}(x)dx \\ &= Z^{-4}\eta^{-1}[\ln(\eta)]^{-1}\int \rho^{\rm Q}(Z^{-1}x_\eta)W(x)dx. \end{aligned}$$

and

$$(\ln\eta)^{-2}\frac{\partial}{\partial\alpha}E_\alpha^{\rm DM}(\lambda,1,2\pi\eta)\big|_{\alpha=0} = \eta^{-1}[\ln(\eta)]^{-1}\int \rho^{\rm DM}(x_\eta;\lambda,1,2\pi\eta)W(x)dx.$$

Thus (8.14) follows from (8.17) which is a consequence of (8.15). ■

Notice that the scaling in (8.13) is identical to the scaling (3.11) introduced to study the hyper-strong limit. In particular, if W is independent of $x_\perp$, i.e., $W(x) = W(x_3)$, on the support of $\rho^{\rm DM}$ we have from Theorem 3.5 and Theorem 4.6 that the right side of (8.14) converges to $\int_{\mathbf{R}} \rho^{\rm HS}(x_3)W(x_3)dx_3$ as $\eta \to \infty$. This proves the following result.

8.2. THEOREM. *Let $\rho^{\rm HS}(x) = \rho^{\rm HS}(x;\lambda)$ be the minimizer for the hyper-strong functional given in Theorem 3.1 and let $N = \lambda Z$. Define the one-dimensional quantum density by*

$$\overline{\rho}^{\rm Q}(x_3) = \int_{|x_\perp|\le\sqrt{2N/B}} \rho^{\rm Q}(x_\perp,x_3)dx_\perp \quad .$$

(If $N \le 2Z$ we can, as a consequence of Corollary 3.6, let the integral extend over all of $\mathbf{R}^2$.) Then

$$[Z^2\ln\eta)]^{-1}\overline{\rho}^{\rm Q}([Z\ln(\eta)]^{-1}x_3) \rightharpoonup \overline{\rho}^{\rm HS}(x_3,\lambda),$$

weakly in $L^1_{\rm loc}(\mathbf{R})$.

IX. IONIZATION AND BINDING OF ATOMS

For reasons that no one really understands at present, enhanced binding of atoms is associated with enhanced ionization. By this we mean the following. In ordinary atoms (with $B = 0$) the maximal number of electrons, $N_c^{\rm Q}$, that can be bound to a nucleus of charge Z satisfies $N_c^{\rm Q}/Z \to 1$ as $Z \to \infty$, as proved in [42]. Thus, the maximal ionization, $N_c^{\rm Q} - Z$, tends to zero on the scale of Z. At the same time, such an atom is well described to leading order by TF theory, which has the property, originally noted by Teller and proved in [30], that atoms never bind. More precisely, in TF theory the energy of a molecule containing two or more infinitely massive nuclei always has an energy that is not less than the sum of the constituent atomic energies. Thus for a real molecule, the binding energy must be of lower order than the atomic energies. We also note that TF theory gives spherically symmetric atoms.

With a magnetic field the situation is unaltered in regions 1, 2 and 3 (see Sect. I). In regions 4 and 5 things begin to change for the first time:

- (i) Atoms become non-spherical
- (ii) The maximal ionization is not zero on the scale of Z
- (iii) Atoms bind together to form molecules with a binding energy $\sum E_{\rm atom} - E_{\rm mol}$ of the same order as the atomic energy $\sum E_{\rm atom}$ itself.

As far as regions 4 and 5 go, we have proved assertion (i) in Theorem 4.5 for the density $\rho^{\rm DM}$, and in Theorem 8.1 we proved that $\rho^{\rm Q}$ is asymptotically the same as $\rho^{\rm DM}$.

Assertions (ii) and (iii) will not be proved here for all of region 4 but they are surely correct because they are resoundingly true in region 5, as we shall demonstrate now. We leave it as an *open problem* to verify (ii) and (iii) for the DM theory for all positive values of the parameter η. For large values of η, assertion (ii) was proved in the DM theory in Corollary 3.6 (recall Theorem 4.6) as a consequence of the study of the hyper-strong theory. We shall now use the hyper-strong theory to conclude assertions (ii) and (iii) for the quantum theory itself, as formulated in Theorems 1.5 and 1.6 in the Introduction.

Proof of Theorem 1.5. (Ionization of atoms): If the theorem is false there is a number $\lambda < 2$ such that the following is true. There are two infinite sequences Z_i and B_i with $Z_i \to \infty$ and with $B_i/Z_i^3 \to \infty$ such that the ratio $E^{\rm Q}(N_i, Z_i, B_i)/E^{\rm Q}([\lambda Z_i], Z_i, B_i) = 1$ for all integers $N_i > [\lambda Z_i]$. (Here $[\lambda Z]$ is the largest integer in λZ.) Set $N_i = [2Z_i]$. By Theorems 1.3, 3.5 and 4.6 the ratio converges, as $i \to \infty$, to $E^{\rm HS}(2)/E^{\rm HS}(\lambda) > 1$ by (3.7). This is a contradiction. ∎

Before leaving the topic of ionization let us comment, as promised in Sect. I, on the $2Z + 1$ theorem [45]. That theorem is applicable to the case in which $H_{\mathbf{A}}$ is replaced by $(\mathbf{p} + \mathbf{A})^2$, and states that the energy of an atom with N electron is not smaller than the energy of an atom with $N - 1$ electrons if $N \geq 2Z + 1$. This result can be translated into a statement about our Hamiltonian (1.1) in which the terms $\boldsymbol{\sigma} \cdot \mathbf{B}$ is included in $H_{\mathbf{A}}$. It says that if $N \geq 2Z + 1$ then $E^{\rm Q}(N, Z, B) \geq E^{\rm Q}(N - 1, Z, B) - B$. We cannot then conclude anything about $N_c^{\rm Q}$.

In order to define the **binding energy** that appears in Theorem 1.6 and in our discussion in this section and in Sect. I, we proceed as follows. First we choose K nuclei with charges $Z_1, Z_2, \ldots, Z_K$ and locate them at $R_1, R_2, \ldots, R_K$ in $\mathbf{R}^3$. (Theorem 1.6 concerns the special case $K = 2$, but here we shall consider the general case). The Hamiltonian H_N in (1.1) is modified in two ways

(i) $-Z|x|^{-1}$ is replaced by $-\sum_{j=1}^{K} Z_j|x-R_j|^{-1}$.

(ii) The nuclear Coulomb repulsion energy $\sum_{1\le i<j\le K} Z_iZ_j|R_i-R_j|^{-1}$ is added to H_N.

The energy is defined by (1.2) as before, but this quantity is then minimized (more precisely, infimized) with respect to $R_1,\dots,R_K$. The final result is denoted by $E^{\mathrm{Q}}(N,Z_1,\dots,Z_K,B)$. The binding energy is defined to be

$$E_{\mathrm{b}}^{\mathrm{Q}}(N,Z_1,\dots,Z_K,B)=\min\{E^{\mathrm{Q}}(N^{\{a\}},Z^{\{a\}},B)+E^{\mathrm{Q}}(N^{\{b\}},Z^{\{b\}},B)\}-E^{\mathrm{Q}}(N,Z_1,\dots,Z_K,B), \tag{9.1}$$

where the minimum is over all decompositions of $\{1,2,\dots,K\}$ into two subsets $\{a\}$ and $\{b\}$ and where $N^{\{a\}}+N^{\{b\}}=N$. A simpler and equally useful notion of binding energy is to restrict the three N's appearing in (9.1) to be neutral, i.e., $N=\sum_{j=1}^{K} Z$, $N^{\{a\}}=\sum_{j\in\{a\}} Z$, $N^{\{b\}}=\sum_{j\in\{b\}} Z$. (Incidentally, it is a fact about TF type theories [30] that if N is neutral then the minimizing values of $N^{\{a\}}$ and $N^{\{b\}}$ are automatically neutral as well. This need not occur in the quantum theory or in the SS, DM or HS theories.)

It is only for simplicity of exposition that Theorem 1.6 was restricted to neutral, diatomic molecules. The true state of affairs, from which Theorem 1.6 follows immediately, is that $E^{\mathrm{Q}}(N,Z_1,\dots,Z_K,B)$ can be calculated easily in the $B/Z^3\to\infty$ limit from knowledge of $E^{\mathrm{HS}}(\lambda)$ — as the following theorem shows.

9.1. THEOREM (Bound atoms are isocentric for large B). *Fix $\lambda>0$ and K. Consider a sequence of molecules with K nuclei, electron number N and magnetic field B in which the parameters tend to infinity in the following way (with $Z:=\sum_{j=1}^{K} Z_j$) : $Z_i\to\infty$, $B/Z^3\to\infty$ and $N/Z=\lambda$. Then*

$$\lim_{Z\to\infty}\{E^{\mathrm{Q}}(N,Z_1,\dots,Z_K,B)/E^{\mathrm{Q}}(N,Z,B)\}=1.$$

Here, as usual, $E^{\mathrm{Q}}(N,Z,B)$ is the energy of an atom with nuclear charge Z.

Proof: We will derive upper and lower bounds of the necessary accuracy.

The lower bound is trivial. For any choice of $R_1,\dots,R_K$ and electronic wave function Ψ, with spin included, we can define the electron density ρ_Ψ as in (1.3) and then define the potential $\Phi=|x|^{-1}*\rho_\Psi$. Let $x_0\in\mathbf{R}^3$ be such that $\Phi(x_0)=\sup_x\Phi(x)$. Clearly, the attractive electron-nuclear energy (see (i) above) is minimized if we now set $R_1=R_2=\ldots=R_K=x_0$. At the same time, for a lower bound we can omit the positive nuclear repulsion (see (ii) above). The result is then $(\Psi,H_N^{(K)}\Psi)\ge(\Psi,H_N\Psi)$, where $H_N^{(K)}$ is our Hamiltonian for K nuclei, and H_N is the one nucleus Hamiltonian (1.1) with a nucleus of charge Z located at x_0. By translation covariance, we can move x_0 to $0 \in \mathbf{R}^3$ without changing the energy. Thus, *for any* Z_i's

$$E^{\mathrm{Q}}(N, Z_1, \ldots, Z_K, B) \geq E^{\mathrm{Q}}(N, Z, B).$$

The upper bound is a bit more complicated. We use Lieb's variational principle [50] (cf. Sect. V) and take as variational density matrix the one given in (5.4) for an atom with electron number N and nuclear charge $Z = \sum_{j=1}^{K} Z_j$ (located at the origin, of course). Since we consider large B/Z^3 the density matrix in (5.4) is of the form given in (4.29) with density $\rho^{\mathrm{SS}}(x)$. Next, we place our K nuclei on the $x_\perp = 0$ axis, close to the origin and with a spacing $D = Z^{-1}(\ln\eta)^{-\varepsilon}$ with $\eta = B/(2\pi Z^3)$. Any fixed $1 < \varepsilon < 2$ will do. The nuclear coordinates are thus $(0,0,\pm D)$, $(0,0,\pm 2D)$, etc. The nuclear repulsion can be bounded by $\sum Z_i Z_j |R_i - R_j|^{-1} \leq \sum Z_i Z_j D^{-1} \leq \frac{1}{2} Z^2 D^{-1} \leq Z^3 (\ln\eta)^{\varepsilon}$. By Theorem 1.4, therefore, the repulsive energy in our state is of lower order — by a factor $(\ln\eta)^{\varepsilon - 2}$.

The remaining step is to show that the negative electron-nuclei energy (see (i) above) is, to leading order, the same as that for one nucleus of charge Z placed at the origin $(0,0,0)$. We use Proposition 3.3. If R is a point on the axis $x_\perp = 0$ we get, using the scalings (3.11) and (3.14), that $\phi(R) := \int Z|x-R|^{-1}\rho^{\mathrm{SS}}(x)dx = Z^3(\ln\eta)^2 \int V_\eta(x)\rho_\eta^{\mathrm{SS}}(x + Z\ln\eta R)dx$. Thus from Proposition 3.3 with $\eta > 3$

$$Z^{-3}(\ln\eta)^{-2}\left|\int Z|x-R|^{-1}\rho^{\mathrm{SS}}(x) - Z^3(\ln\eta)^2\overline{\rho}_\eta^{\mathrm{SS}}(Z\ln\eta|R|)\right| \leq c_\lambda\left(\frac{1+\ln|\ln\eta|}{\ln\eta}\right),$$

Here we are using that $T[\rho_\eta^{\mathrm{SS}}] \leq c'_\lambda$, where c_λ and c'_λ depend only on λ, and that the support of ρ_η^{SS} is in the set $\{x = (x_\perp, x_3) : |x_\perp| \leq \sqrt{\lambda/\pi}\}$. Since $\int (d\sqrt{\overline{\rho}_\eta^{\mathrm{SS}}}/dx_3)^2 dx_3 \leq T[\rho_\eta^{\mathrm{SS}}] \leq c'_\lambda$ we also have a bound on the Lipschitz constant of $\overline{\rho}_\eta^{\mathrm{SS}}$, i.e.,

$$|\overline{\rho}_\eta^{\mathrm{SS}}(Z\ln\eta|R|) - \overline{\rho}_\eta^{\mathrm{SS}}(0)| < c''_\lambda Z\ln\eta|R|.$$

We choose $|R|$ to be less than KD, whence we obtain

$$Z^{-3}(\ln\eta)^{-2}|\phi(R) - Z^3(\ln\eta)^2\overline{\rho}_\eta^{\mathrm{SS}}(0)| < c''_\lambda\left(\frac{1-\ln|\ln\eta|}{|\ln\eta|} + (\ln\eta)^{1-\varepsilon}\right).$$

This permits us to compare $\phi(R_j)$ with $\phi(0)$ and we see that all are equal to leading order. Therefore, $\sum_j (Z_j/Z)\phi(R_j)$ equals $\phi(0)$ to leading order. ■

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