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# Asymptotics of Heavy Atoms in High Magnetic Fields: II. Semiclassical Regions

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**Abstract:** The ground state energy of an atom of nuclear charge $Ze$ in a magnetic field $B$ is exactly evaluated to leading order as $Z \to \infty$ in the following three regions: $B \ll Z^{4/3}$, $B \sim Z^{4/3}$ and $Z^{4/3} \ll B \ll Z^3$. In each case this is accomplished by a modified Thomas–Fermi (TF) type theory. We also analyze these TF theories in detail, one of their consequences being the nonintuitive fact that atoms are spherical (to leading order) despite the leading order change in energy due to the $B$ field. This paper complements and completes our earlier analysis [1], which was primarily devoted to the regions $B \sim Z^3$ and $B \gg Z^3$ in which a semiclassical TF analysis is numerically and conceptually wrong. There are two main mathematical results in this paper, needed for the proof of the exactitude of the TF theories. One is a generalization of the Lieb–Thirring inequality for sums of eigenvalues to include magnetic fields. The second is a semiclassical asymptotic formula for sums of eigenvalues that is *uniform* in the field $B$.

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## I. Introduction

In this paper we complete the study of the ground state energy and the ground state density of large atoms (and molecules) in large, spatially homogeneous magnetic fields that was begun in [1]. Such an atom, with $N$ electrons of charge $-e$ and mass $m_e$ and nuclear charge $Ze$ is described by the nonrelativistic Schrödinger Hamiltonian operator

$$H_N = \sum_{i=1}^{N} \{(\mathbf{p}_i + \mathbf{A}(x_i))^2 + \boldsymbol{\sigma}_i \cdot \mathbf{B} - Z|x_i|^{-1}\} + \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1} . \quad (1.1)$$

We have used units in which $e = 2m_e = \hbar = 1$ and $c = c\hbar e^{-2} = \alpha^{-1} \approx 137$. The magnetic field is $\mathbf{B} = (0, 0, B)$, where $B$ is the magnitude of the field in units of $4B^* := 4m_e^2 e^3 c\hbar^{-3} = 9.6 \times 10^9$ Gauss. We shall make the gauge choice $\mathbf{A}(x) = \frac{1}{2}\mathbf{B} \times x$, and $\operatorname{curl} \mathbf{A} = \mathbf{B}$. The "vector" formed by the three $2 \times 2$ Pauli matrices is denoted by $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, and we see that only $\sigma_3$ enters (1.1), i.e., the spin dependence is simple. The electron charge is $-e$, hence the $+\mathbf{A}(x)$ appearing in (1.1). Since the electrons are fermions the operator $H_N$ acts on the antisymmetric space $\bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$. ($L^p(\mathbf{R}^3)$ denotes, as usual, the space of complex-valued, $p^{\text{th}}$ power absolutely integrable functions while $L^p(\mathbf{R}^3; \mathbf{C}^2)$ denotes $\mathbf{C}^2$-valued, $p^{\text{th}}$ power absolutely integrable function, which we often write in the form $\psi(x, s)$ with $x \in \mathbf{R}^3$ and $s \in \{-\frac{1}{2}, \frac{1}{2}\}$.)

The physical motivation for this study comes primarily from the study of iron atoms ($Z = 26$) on the surface of a neutron star, where $B$ can be as large as $10^{13}$ Gauss, which is about $10^4$ times the natural unit $B^* = 2.4 \times 10^9$ Gauss. See [2] for a recent review.

In order to understand this complex problem in a definitive way we undertake to study the *ground state energy* ($:= \inf \operatorname{spec}(H_N)$) and *electron density* (cf. (2.4) and (5.18)) in the limit $Z \to \infty$ and $B \to \infty$. The $B \to \infty$ limit is obviously justified in the neutron star case, while the $Z \to \infty$ limit reasonably reflects the $Z = 26$ case since ordinary Thomas–Fermi (TF) theory (which is the $Z \to \infty$ limit of atoms without a magnetic field) is known to be accurate to 3–4% when $Z = 26$.[1]

We have been able to give an *exact* answer to the question posed above and our results were summarized and announced in [4] (see also [5]). One of our main conclusions is that *there are five distinct regions* (with respect to both the physics and the mathematics) according to the manner in which $B$ is related to $Z$ as both tend to infinity. These regions are the following:

*Region 1*: $BZ^{-4/3} \to 0$ *as* $Z \to \infty$: The effect of the magnetic field is negligible to leading order. Standard TF theory with $B = 0$ can be applied. See Theorem 5.2(i).

*Region 2*: $BZ^{-4/3} =$ *constant*: A modified, $B$-dependent TF theory is asymptotically exact (Theorem 5.1). The atomic radius behaves as $Z^{-1/3}$ as in standard TF theory (Theorem 5.3).

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[1] This statement of accuracy is technically incorrect because the positive Scott correction, which is about 20% of the total energy must be added to the negative Thomas–Fermi energy [3] to obtain this accuracy; the Scott correction comes entirely from the innermost electrons and, while it affects the total energy and even the density of these innermost electrons, it does not affect the density of most of the electrons

*Region 3*: $BZ^{-4/3} \to \infty$, but $BZ^{-3} \to 0$: 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 (Theorem 5.2(ii)). The atom shrinks with increasing $B$; the radius is proportional to $Z^{1/5}B^{-2/5} = Z^{-1/3}(B/Z^{4/3})^{-2/5}$ (Theorem 5.3).

Since regions 1, 2 and 3 can be exactly described by TF type theories the electronic density of an atom is *spherical* to leading order, and stable atoms are approximately neutral. (This remark will be clarified at the end of this section and in Sect. IV.) *Although B affects the energy and density to leading order, it does not spoil the sphericity*!! The analysis in these regions is semiclassical; the role of an effective Planck's constant is played by $Z^{-1/3}$ in Regions 1 and 2, and by $(B/Z^3)^{1/5}$ in Region 3.

*Region 4*: $BZ^{-3}$ = *constant*: The atom is no longer spherical, but has the form of a 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 $BZ^{-3}$ it reduces to a functional of the density *alone*.

*Region 5*: $BZ^{-3} \to \infty$: 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 $[\ln(B/Z^3)]^{-1}$. Consequently, in the limit $B/Z^3 \to \infty$ *the Coulomb potential reduces effectively 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 molecular binding, as we discuss below.

The present paper is the second and final one in the detailed presentation of our study. Our first paper [1] contains a detailed history of the physical and mathematical aspects of the problem, and we refer the reader there for further information. Suffice it to say here that the physical interest dates mostly from the early 1970's, with the pioneering work of Kadomtsev [6], Ruderman [7] and Mueller, Rau and Spruch [8]. Subsequently, there were many mathematical analyses of the problem in the physics literature, covering many aspects. Noteworthy among them, for our present purpose, is the work of Tomishima, Matsuno and Yonei [9, 10] in which the correct magnetic Thomas–Fermi theory taking all Landau levels into account first appeared, and the recent paper [11] where this and related theories are further studied.

In [1] Regions 4 and 5 were thoroughly analyzed, these being the regions in which semiclassical or Thomas–Fermi methods *fail* to give the right answer. We did, however, find the non-semiclassical theories that give the exact asymptotics in those two regions. Regions 1, 2 and 3 constitute the scope of the present paper, and here a suitable TF theory is correct in each of the three regions. Region 3 is an overlap between the two papers. It appears here because it is susceptible to a TF type analysis; it appeared in [1] because regions 3, 4, 5 have the common feature that "almost all" electrons are in the lowest Landau band (and hence are totally spin polarized), as proved in Sect. VI of [1]. However, [1] did not complete the analysis of Region 3, because we left the proof that there is an exact TF theory for Region 3 to the present paper.

Region 2 was analyzed in detail in [12] but, owing to a not insignificant technicality, the extension to Region 3 was not possible using the ideas in [12] alone. It is possible to handle Region 3 using the result in [1], in which the Region 3 problem was successfully reduced to a density matrix problem. However, the remaining step – the reduction to the TF problem – would require a semiclassical analysis that is not altogether trivial.

To us, the most straightforward course is to present a strategy that treats the three TF regions 1, 2, 3 in a unified way. There are two key mathematical elements in our strategy. One is the extension of the Lieb–Thirring (LT) inequality [13, 14] for the sum of the negative eigenvalues of a one-body Hamiltonian with a fixed potential $V(x)$ to the case of a non-zero but homogeneous magnetic field[2]. That is, we consider $H = H_{\mathbf{A}} + V(x)$ with $H_{\mathbf{A}}$ being the Pauli operator

$$H_{\mathbf{A}} = [\boldsymbol{\sigma}\cdot(\mathbf{p} + \mathbf{A}(x))]^2 = (\mathbf{p} + \mathbf{A}(x))^2 + \boldsymbol{\sigma}\cdot\mathbf{B}\,, \tag{1.2}$$

and we try to estimate the sum of the negative eigenvalues of $H$ in terms of $L^p$ norms of $|V(x)|_- = \max\{0, -V(x)\}$. This inequality is the content of Sect. II. For the reasons given there this extended inequality is intrinsically more complicated than the usual LT inequality – despite the fact that $\boldsymbol{\sigma}\cdot\mathbf{B}$ can be taken to be a constant.

The second mathematical ingredient is the semiclassical limit (i.e., Planck's constant $h \to 0$) of the one-body problem for a particle in a fixed potential and a homogeneous magnetic field. To be more precise, we consider the one-body Hamiltonian

$$H(h, b) = [\boldsymbol{\sigma}\cdot(h\mathbf{p} + b\mathbf{a}(x))]^2 + V(x)\,, \tag{1.3}$$

where $\mathbf{a}(x) = \frac{1}{2}(-x_2, x_1, 0)$ corresponds to a spatially constant magnetic field of unit strength in the 3-direction. Thus $b\mathbf{a}$ is the vector potential for the magnetic field $\mathbf{b} = (0, 0, b)$.

Our goal here is to evaluate, *uniformly in b*, the sum of the negative eigenvalues asymptotically as $h \to 0$.

The usual approach to the semiclassical limit fixes $b$, in which case the magnetic field has no effect – to leading order – on the sum of the negative eigenvalues [15]. Such an approach is insufficient for us because we need the case in which $b \to \infty$ as $h \to 0$; therefore, uniform estimates are important for us. Our asymptotic formula will contain a non-trivial dependence on $b$ to leading order. This semiclassical formula which is of independent interest is proved in Sect. III.

Sections II and III are the ones of most intrinsic *mathematical* interest. They are applied in Sects. IV and V to formulate Thomas–Fermi theories (one for each of the three regions) that *exactly* reproduce the limit of quantum mechanics as $Z, B \to \infty$. Section IV elucidates the mathematical properties of these TF theories, while Sect. V shows they are the correct limits of quantum mechanics.

The semiclassical results of Sect. III are necessary, but not sufficient for the applications in Sect. V. The reason is that the TF potential has no pure, simple scaling with respect to $Z$ (as it does when $B = 0$), or with respect to $B$. Some additional work is needed. There is, however, a simple scaling if the parameter $B/Z^{4/3}$ is held fixed (cf. Eq. (4.24)). A slightly different route to the final results of Sect. V is possible, namely, to avail ourselves of the very special nature of the

[2] It was essentially this step that was missing in [12]

Coulomb potential and to use some potential theoretic arguments to simplify the discussion. Indeed, this approach was used in [12]. Having proved the semiclassical result of Sect. III in full generality, however, we chose to apply it directly (at the expense of a little extra work) rather than to redo the estimates of Sect. III for the special Coulomb potential.

The fact that there are genuinely two parameters in the problem, with different scalings, leads unavoidably to the somewhat cumbersome notation the reader will find in Sects. IV and V.

In addition to the semiclassical results of Sect. III two other tools play a key role in the limit theorems of Sect. V. One is the variational principle given in [16] which yields a sufficiently accurate upper bound for the ground state energy in terms of the one-body density alone. The second tool is the lower bound on the exchange energy given by the Lieb–Oxford inequality [17] and which, in turn, is controlled by the LT inequality of Sect. II.

Finally, let us remark briefly about ionization and binding in Regions 1, 2 and 3. Since these are exactly described to leading order by suitable TF theories, it follows immediately that three things are automatically true about atoms (again, to leading order): (a) Atoms are spherical because the TF equation is rotationally invariant (only $B$, and not its direction, enters) and because the solution to the TF equation is unique (Theorems 4.5 and 4.7); (b) Negative ions do not exist (Theorem 4.9); (c) Atoms do not bind (Theorem 4.10). Each of these is violated in Regions 4 and 5 [1]. There is, however, an interesting fact about Regions 2 and 3 that shows them to be the precursor of Region 4. In Regions 2 and 3 the density of an atom has compact support (Theorem 4.10), which implies (thanks to the spherical symmetry and Newton's Theorem) that the TF density of a neutral molecule is precisely the sum of the densities of the individual atoms (Corollary 4.11), provided the spacing between any two nuclei is not less than the sum of the radii of the individual atoms. In short, screening is perfect in this case and the energy does not decrease as the atoms are pulled farther apart. In Region 1 the energy is a strictly decreasing function of the atomic separation, i.e., the pressure is positive [18, 19]. This is a strong version of Teller's no-binding Theorem. In Regions 2 and 3 the pressure is positive only for sufficiently small spacing, and this anticipates the actual non-zero binding to be found in Region 4.

## II. Generalized Lieb–Thirring Inequality with a Constant Magnetic Field

In this section we discuss the Schrödinger operator for a single particle in a spatially constant magnetic field $\mathbf{B}\in\mathbf{R}^3$ and in a general potential $V$, satisfying $|V|_-\in L^{5/2}(\mathbf{R}^3)\cap L^{3/2}(\mathbf{R}^3)$, where $|V(x)|_- = -V(x)$ if $V(x)\leqq 0$ and is zero otherwise.

We shall estimate the sum of the negative eigenvalues of

$$H = H_{\mathbf{A}} + V(x)\,. \tag{2.1}$$

We remark that the operators $H_{\mathbf{A}}$ and $H$ are essentially selfadjoint on $C_0^\infty(\mathbf{R}^3)$ (see, e.g., [20]). The spectrum of $H_{\mathbf{A}}$ is described by the Landau bands

$$\mathscr{E}_{p\nu} = 2\nu B + p^2\,. \tag{2.2}$$

Here $\nu = 0, 1, 2, \ldots$ and $p \in \mathbf{R}$ is the momentum along the field $\mathbf{B}$. We have chosen coordinates such that $\mathbf{B}$ lies in the 3-direction. In the lowest Landau band (defined by $\nu = 0$) the value of $\boldsymbol{\sigma} \cdot \mathbf{B}$ is $-B$, so the spin points opposite to the field. The higher levels $\nu = 1, \ldots$ are twice as degenerate as the lowest level and contain both directions of the spin.

In estimating the sum of the negative eigenvalues of $H$ we shall treat the contribution coming from the lowest Landau band separately. The reader might think the problem is trivial owing to the fact that the term $\boldsymbol{\sigma} \cdot \mathbf{B}$ is either $+B$ or $-B$. While this observation is correct, it misses the point. If we ignore the $\boldsymbol{\sigma} \cdot \mathbf{B}$ term entirely, then, from the diamagnetic inequality [21], the known Lieb–Thirring bound [13, 14] for $\mathbf{p}^2 + V(x)$ would apply without change for the sum of the negative eigenvalues of $H' = (\mathbf{p} + \mathbf{A}(x))^2 + V(x)$. In our case, however, we are allowed to subtract the term $B$ from $H'$. This means that we are really estimating the negative spectrum of $H'$ together with the part of the positive spectrum of $H'$ lying between 0 and $+B$. The essential spectrum of $H'$ starts, in fact, at $+B$. From this point of view it will be seen that we are now asking a much more subtle question than merely the negative spectrum of $p^2 + V(x)$. A further complication comes from the somewhat surprising observation in [22] that $H$ may have infinitely many negative eigenvalues even when $V$ is smooth and has compact support. (For stronger versions of this result see [23, 24].) A consequence of our Theorem 2.1 below is that these infinitely many eigenvalues are summable.

Our generalized Lieb–Thirring inequality is the following.[3]

**2.1 Theorem (Generalized Lieb–Thirring Inequality).** *Let $|V|_- \in L^{5/2}(\mathbf{R}^3) \cap L^{3/2}(\mathbf{R}^3)$ and let $e_j(B, V) \leqq 0$, $j = 1, \ldots$ denote the negative eigenvalues for the operator $H$ in (2.1). Then*

$$\sum_j |e_j(B, V)| \leqq L_1 B \int |V(x)|_-^{3/2}\, dx + L_2 \int |V(x)|_-^{5/2}\, dx\,, \tag{2.3}$$

*with $L_1 = 4/3\pi$ and $L_2 = 8\sqrt{6}/5\pi$. More generally, for each $0 < \delta < 1$ we can choose $L_1 = (2/3\pi)(1-\delta)^{-1}$ and $L_2 = (2\sqrt{6}/5\pi)\,\delta^{-2}$.*

As in [13] the estimate (2.3) can be turned into a lower bound for the energy of an antisymmetric (fermionic) wave function $\psi \in \bigwedge_{i=1}^N L^2(\mathbf{R}^3; \mathbf{C}^2)$ in terms of the density

$$\rho_\psi(x) := N \sum_{s_i = \pm 1/2} \int |\psi(x, x_1, \ldots, x_N; s_1, \ldots, s_N)|^2 dx_2 \quad dx_N\,, \tag{2.4}$$

where $s_i = \pm 1/2$ is the spin component of particle $i$ along the field $\mathbf{B}$. Indeed, define $w(t)$ as the solution to

$$\frac{3}{2} L_1 B w(t)^{1/2} + \frac{5}{2} L_2 w(t)^{3/2} = t\,, \tag{2.5}$$

and let

$$F_B(t) = t w(t) - L_1 B w(t)^{3/2} - L_2 w(t)^{5/2} \geqq 0\,. \tag{2.6}$$

[3] Laszlo Erdős has recently found a generalization of this result for a restricted class of inhomogeneous fields

Then $F_B(t)$ is the Legendre transform of the function $w \mapsto L_1 B w^{3/2} + L_2 w^{5/2}$, i.e.,

$$F_B(t) = \sup_{w \geqq 0} [tw - L_1 B w^{3/2} - L_2 w^{5/2}] .$$

Notice that $F_B(t) \approx \frac{4}{27} L_1^{-2} B^{-2} t^3$ for $t$ small and $F_B(t) \approx \frac{3}{5}(\frac{2}{5} L_2^{-1})^{2/3} t^{5/3}$ for $t$ large. Theorem 2.1 has the following corollary:

**2.2 Corollary.** *If $\psi$ is a normalized fermionic function in $\bigwedge_{i=1}^N L^2(\mathbf{R}^3; \mathbf{C}^2)$, then*

$$\left\langle \psi \left| \sum_{i=1}^N [\boldsymbol{\sigma}_i \cdot (\mathbf{p}_i + \mathbf{A}(x_i))]^2 \right| \psi \right\rangle \geqq \int F_B(\rho_\psi(x)) dx .$$

*Proof of Corollary.* Choose $W(x) = w(\rho_\psi(x)) \geqq 0$, with $w$ given by (2.5). Assume first for simplicity that $W \in L^{3/2} \cap L^{5/2}$. Then from the variational principle and inequality (2.3) we get

$$\left\langle \psi \left| \sum_{i=1}^N [\boldsymbol{\sigma}_i \cdot (\mathbf{p}_i + \mathbf{A}(x_i))]^2 - W(x_i) \right| \psi \right\rangle \geqq \sum_j e_j(B, W)$$

$$\geqq - L_1 B \int W(x)^{3/2} dx - L_2 \int W(x)^{5/2} dx . \tag{2.7}$$

We then have

$$\left\langle \psi \left| \sum_{i=1}^N [\boldsymbol{\sigma}_i \cdot (\mathbf{p}_i + \mathbf{A}(x_i))]^2 \right| \psi \right\rangle \geqq \int \{\rho_\psi(x) W(x) - L_1 B W(x)^{3/2} - L_2 W(x)^{5/2}\} dx$$

$$= \int F_B(\rho_\psi(x)) dx . \tag{2.8}$$

If $W \notin L^{3/2} \cap L^{5/2}$ we define instead for $M \geqq 0$, $W_M = w(\rho_\psi \chi_M)$, where $\chi_M$ is the characteristic function of the set $\{x \,|\, |x| \leqq M,\ \rho_\psi(x) \leqq M\}$. Then clearly $W_M = \chi_M W_M$. Use $W_M$ in (2.7). On the right side of (2.8) we would now get $\int F_B(\rho_\psi \chi_M)$ and we can here let $M \to \infty$ by monotone convergence since $F_B \geqq 0$. ∎

We now discuss some preliminaries to the proof of Theorem 2.1. As in [13, 14] we use the (modified) Birman–Schwinger principle. For $E > 0$ define the (modified) Birman–Schwinger kernel

$$K_E = \left| V + \frac{1}{2} E \right|_-^{1/2} \left( H_\mathbf{A} + \frac{1}{2} E \right)^{-1} \left| V + \frac{1}{2} E \right|_-^{1/2} . \tag{2.9}$$

The Birman–Schwinger principle says that the number $N_E$ of eigenvalues of $H_\mathbf{A} + V$ less than $-E$ is no larger than the number of eigenvalues of $K_E$ greater than 1.

We shall split $K_E$ into a part coming from the lowest Landau band and a part coming from the higher bands. Let $\Pi_0$ denote the projection in $L^2(\mathbf{R}^3; \mathbf{C}^2)$ onto the lowest band. The integral kernel for $\Pi_0$ is the $2 \times 2$ matrix function (distribution)

$$\Pi_0(x, y) = \frac{B}{2\pi} \exp\{i(x_\perp \times y_\perp) \cdot \mathbf{B}/2 - (x_\perp - y_\perp)^2 B/4\} \delta(x_3 - y_3) \mathscr{P}^\downarrow , \tag{2.10}$$

where $\mathscr{P}^{\downarrow}$ is the projection in $\mathbf{C}^2$ onto the subspace where $\mathbf{B}\cdot\boldsymbol{\sigma} = -B$, $x_\perp$ denotes the component of $x$ perpendicular to the field and $x_3$ the component parallel to the field.

We write $K_E = K_E^0 + K_E^>$, where

$$K_E^0 = \left|V + \frac{1}{2}E\right|_-^{1/2} \Pi_0 \left(H_{\mathbf{A}} + \frac{1}{2}E\right)^{-1} \Pi_0 \left|V + \frac{1}{2}E\right|_-^{1/2}$$
$$= \left|V + \frac{1}{2}E\right|_-^{1/2} \Pi_0 \left(p_3^2 + \frac{1}{2}E\right)^{-1} \Pi_0 \left|V + \frac{1}{2}E\right|_-^{1/2} \tag{2.11}$$

since $\Pi_0 H_{\mathbf{A}} \Pi_0 = \Pi_0 p_3^2 \Pi_0$. (Here, $p_3$ is the operator $-i\partial/\partial x_3$.) Likewise,

$$K_E^> = \left|V + \frac{1}{2}E\right|_-^{1/2} (I - \Pi_0) \left(H_{\mathbf{A}} + \frac{1}{2}E\right)^{-1} (I - \Pi_0) \left|V + \frac{1}{2}E\right|_-^{1/2} \tag{2.12}$$

Recall that $H_{\mathbf{A}}$ commutes with $\Pi_0$. We shall need the following elementary estimate.

**2.3 Lemma.** *If $X$ and $Y$ are positive semi-definite trace class operators, then the number, $N$, of eigenvalues greater than or equal to 1 of $X + Y$ satisfies*

$$N \leqq (1-\delta)^{-1}\operatorname{Tr} X + \delta^{-2}\operatorname{Tr} Y^2 . \tag{2.13}$$

*for each* $0 < \delta < 1$.

*Proof.* Let $\phi_1, \ldots, \phi_N$ be the orthonormal eigenfunctions for $X + Y$ with eigenvalues greater than or equal to 1. For each $i = 1, \ldots, N$ we have either

$$\langle \phi_i | X | \phi_i \rangle \geqq 1 - \delta \quad \text{or} \quad \langle \phi_i | Y | \phi_i \rangle \geqq \delta . \tag{2.14}$$

Since $\langle \phi_i | Y | \phi_i \rangle^2 \leqq \langle \phi_i | \phi_i \rangle \langle \phi_i | Y^2 | \phi_i \rangle = \langle \phi_i | Y^2 | \phi_i \rangle$, we conclude that $(1-\delta)^{-1}\operatorname{Tr} X + \delta^{-2}\operatorname{Tr} Y^2 \geqq \sum_{i=1}^N (1-\delta)^{-1} \langle \phi_i | X | \phi_i \rangle + \delta^{-2} \langle \phi_i | Y^2 | \phi_i \rangle \geqq N$. ■

We calculate $\operatorname{Tr}(K_E^0)$ using the explicit form (2.10) for $\Pi_0$,

$$\operatorname{Tr}(K_E^0) = \operatorname{Tr}\left[\left|V + \frac{1}{2}E\right|_- \Pi_0 \left(p_3^2 + \frac{1}{2}E\right)^{-1}\right]$$
$$= \int \int \left|V(x) + \frac{1}{2}E\right|_- \left\{\operatorname{Tr}_{\mathbf{C}^2}(\Pi_0(x,y)) \left(p_3^2 + \frac{1}{2}E\right)^{-1} (y_3, x_3)\delta(y_\perp - x_\perp)dy\right\} dx$$
$$= \frac{B}{2\pi}(2E)^{-1/2} \int \left|V(x) + \frac{1}{2}E\right|_- dx , \tag{2.15}$$

where we have also used that on the diagonal the one-dimensional resolvent kernel is

$$\left(p_3^2 + \frac{1}{2}E\right)^{-1}(x_3, x_3) = (2\pi)^{-1} \int_{-\infty}^{\infty} \left(p^2 + \frac{1}{2}E\right)^{-1} dp = (2E)^{-1/2} . \tag{2.16}$$

To estimate $\mathrm{Tr}(K_E^>)^2$ we shall use the diamagnetic inequality. Notice first that both $\mathbf{B}\cdot\boldsymbol{\sigma}$ and $(\mathbf{p}+\mathbf{A})^2$ commute with $\Pi_0$. We claim that

$$\mathbf{B}\cdot\boldsymbol{\sigma} \geqq -\frac{1}{3}(\mathbf{p}+\mathbf{A})^2 \tag{2.17}$$

on the orthogonal complement of the lowest Landau band. Indeed, from (2.2) we have in band $\nu$ that $(\mathbf{p}+\mathbf{A})^2+\mathbf{B}\cdot\boldsymbol{\sigma} \geqq 2\nu B \geqq -2\nu\mathbf{B}\cdot\boldsymbol{\sigma}$. Thus, when $\nu \geqq 1$, (which corresponds to the orthogonal complement of the lowest Landau band) we have (2.17). Therefore

$$\begin{aligned}(I-\Pi_0)H_{\mathbf{A}}(I-\Pi_0) &= (I-\Pi_0)[(\mathbf{p}+\mathbf{A})^2+\mathbf{B}\cdot\boldsymbol{\sigma}](I-\Pi_0)\\ &\geqq \frac{2}{3}(I-\Pi_0)(\mathbf{p}+\mathbf{A})^2(I-\Pi_0)\,.\end{aligned}$$

Because of the operator inequality $0<X<Y \Rightarrow X^{-1}>Y^{-1}$, we have that

$$(I-\Pi_0)\left[H_{\mathbf{A}}+\frac{1}{2}E\right]^{-1}(I-\Pi_0) \leqq (1-\Pi_0)\left[\frac{2}{3}(\mathbf{p}+\mathbf{A})^2+\frac{1}{2}E\right]^{-1}(1-\Pi_0)\,. \tag{2.18}$$

From the (pointwise) diamagnetic inequality [21] for the resolvent kernel

$$\left|\left[\frac{2}{3}(\mathbf{p}+\mathbf{A})^2+\frac{1}{2}E\right]^{-1}(x,y)\right| \leqq \left[\frac{2}{3}\mathbf{p}^2+\frac{1}{2}E\right]^{-1}(x-y)\,, \tag{2.19}$$

we obtain

$$\begin{aligned}\mathrm{Tr}[(K_E^>)^2] &\leqq \mathrm{Tr}\left[\frac{2}{3}(\mathbf{p}+\mathbf{A})^2+\frac{1}{2}E\right]^{-2}\\ &\leqq 2\int\int\left|V(x)+\frac{1}{2}E\right|_-\left\{\left[\frac{2}{3}\mathbf{p}^2+\frac{1}{2}E\right]^{-1}(x-y)\right\}^2\left|V(y)+\frac{1}{2}E\right|_-dx\,dy\\ &\leqq 2\int\left|V(x)+\frac{1}{2}E\right|_-^2dx\int\left\{\left[\frac{2}{3}\mathbf{p}^2+\frac{1}{2}E\right]^{-1}(y)\right\}^2dy\end{aligned} \tag{2.20}$$

The factor of 2 in (2.20) comes from the trace over $\mathbf{C}^2$. The last integral in (2.20) equals

$$(2\pi)^{-3}\int\left[\frac{2}{3}\mathbf{p}^2+\frac{E}{2}\right]^{-2}d^3\mathbf{p} = 3^{3/2}(16\pi)^{-1}E^{-1/2}\,. \tag{2.21}$$

*Proof of Theorem 2.1.* Since $N_E$ is the number of eigenvalues of $H_{\mathbf{A}}+V(x)$ below $-E$ we get (from Lemma 2.3)

$$\sum_j|e_j(B,V)| = \int_0^\infty N_E\,dE \leqq \int_0^\infty(1-\delta)^{-1}\mathrm{Tr}(K_E^0)+\delta^{-2}\mathrm{Tr}[(K_E^>)^2]\,dE\,. \tag{2.22}$$

From (2.15) the first term is

$$\frac{1}{1-\delta}\int_0^\infty \operatorname{Tr}(K_E^0)dE = \frac{B}{2\pi(1-\delta)}\int\int_0^\infty (2E)^{-1/2}\left|V(x)+\frac{1}{2}E\right|_- dE\,dx$$
$$= \frac{B}{2\pi(1-\delta)}\int\int_0^\infty (2E)^{-1/2}|V(x)|_-^{1/2}\left|V(x)+\frac{1}{2}E|V(x)|_-\right|_- dE\,dx$$
$$= \frac{B}{2\pi(1-\delta)}\int |V(x)|_-^{3/2}dx\int_0^2 (2E)^{-1/2}\left(1-\frac{1}{2}E\right)dE$$
$$= \frac{2B}{3\pi(1-\delta)}\int |V(x)|_-^{3/2}dx. \tag{2.23}$$

The second term in (2.22) can be estimated, using Eqs. (2.20) and (2.21), as follows.

$$\int_0^\infty \delta^{-2}\operatorname{Tr}[(K_E^{>})^2]dE \leqq 3^{3/2}(8\pi\delta^2)^{-1}\int\int_0^\infty E^{-1/2}\left|V(x)+\frac{1}{2}E\right|_-^2 dE\,dx$$
$$= 3^{3/2}(8\pi\delta^2)^{-1}\int |V(x)|_-^{5/2}dx\int_0^2 E^{-1/2}\left(1-\frac{1}{2}E\right)^2 dE$$
$$= \frac{2\sqrt{6}}{5\pi\delta^2}\int |V(x)|_-^{5/2}dx\,. \quad \blacksquare \tag{2.24}$$

As an application of Theorem 2.1 we shall derive a lower bound to the ground state energy of an atom in a constant magnetic field $\mathbf{B} = (0, 0, B)$. The nuclear charge is $Z$ (in our units) and the number of electrons, $N$, is arbitrary. The Hamiltonian on $\bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$ that we consider here has no electron-electron repulsion:

$$\tilde{H} = \sum_{i=1}^N [\boldsymbol{\sigma}_i\cdot(\mathbf{p}_i + \mathbf{A}(x_i))]^2 - Z|x_i|^{-1}. \tag{2.25}$$

Since $\tilde{H}$ is less than the true Hamiltonian (1.1) (which contains repulsion), the following theorem gives a true lower bound to the ground state energy.

**2.4 Theorem (Lower Bound for Atomic Energies).** *The ground state energy $\tilde{E}(N, B, Z)$ for* (2.25) *satisfies the following two bounds, in which $\lambda = N/Z$ and $\beta = B/Z^{4/3}$:*

$$\tilde{E} \geqq -\frac{5}{3}\left(\frac{\pi}{2}\right)^{2/5} Z^{7/3}\lambda^{3/5}\beta^{2/5}\left(1+\frac{1}{5}6^{3/2}2^{3/5}\pi^{2/5}(\lambda^{2/3}\beta)^{-3/5}\right), \tag{2.26}$$

$$\tilde{E} \geqq -3(\pi\sqrt{6})^{2/3}Z^{7/3}\lambda^{1/3}\left(1+\frac{1}{9}6^{-5/6}\pi^{-2/3}\lambda^{2/3}\beta\right). \tag{2.27}$$

*Proof.* The ground state energy is the sum of the lowest $N$ eigenvalues (including spin) of the operator $H_A - Z|x|^{-1}$ on $L^2(\mathbf{R}^3; \mathbf{C}^2)$. Choose some radius $R > 0$ and note that $V(x) \geqq V_<(x) - Z/R$ with $V_<(x) = V(x) + Z/R$ for $|x| \leqq R$ and $V_<(x) = 0$ otherwise. Then $\tilde{E} \geqq -NZ/R +$ the sum of the negative eigenvalues of $H_{\mathbf{A}} + V_<$. Thus, from Theorem 2.1,

$$\tilde{E} \geqq -NZ/R - \frac{\pi}{3}BR^{3/2}Z^{3/2} - 2\pi\sqrt{6}R^{1/2}Z^{5/2}\,. \tag{2.28}$$

The optimum choice for $R$ is found by minimizing the right side of (2.28). This is too complicated to do. The estimate (2.26) follows by minimizing the first two terms only, thereby obtaining $R = (2N/\pi B)^{2/5} Z^{-1/5}$, whereas (2.27) follows by minimizing the first and last terms, thereby obtaining $R = (N/\pi\sqrt{6})^{2/3} Z^{-1}$. ■

*Remark.* Clearly (2.26) is useful for large $B$ while (2.27) is useful for small $B$. If $N = Z$ (neutral atom) the dividing line is $B \approx Z^{4/3}$ and (2.27) yields the usual $Z^{7/3}$ energy of a neutral atom with no magnetic field. In fact, $E \approx -Z^2 N^{1/3}$ in (2.27) is always correct for $B = 0$, even if $N \neq Z$, as TF theory shows. The right side of (2.26) will turn out to be of the correct order of magnitude when $B$ is large, but not super-large. For $N = Z$ this is $E \approx -Z^{9/5} B^{2/5}$ in the regime $Z^{4/3} \leqq B \leqq Z^3$. If $B \gg Z^3$, (2.27) is too negative; in that super-large $B$ regime the atom is no longer spherical, and

$$E \approx -Z^3 [\ln(Z^3/B)]^2 . \tag{2.29}$$

The regime $B \gg Z^3$ was analyzed in [1]. In fact, the larger regime $B \gg Z^{4/3}$ was analyzed in [1] because, as proved there, that regime is characterized by all the electrons almost totally confined to the lowest Landau band. For the convenience of the reader we shall repeat here (in Theorem 2.5 and Lemma 2.6) the rationale behind (2.29). The lowest Landau band confinement (proved in [1], Theorem 1.2) will be assumed here and we shall derive a lower bound of the form (2.29) under this assumption. We are thus looking for a lower bound to the sum of the first $N$ negative eigenvalues of the operator

$$\Pi_0 (H_A - Z|x|^{-1}) \Pi_0 = \Pi_0 (p_3^2 - Z|x|^{-1}) \Pi_0 , \tag{2.30}$$

where $\Pi_0$ is the projection onto the lowest Landau band given in (2.10).

**2.5 Theorem.** *Let $e_j^{(0)}(B, Z), j = 1, 2, \ldots$ denote the negative eigenvalues for the restricted operator* (2.30) *on $L^2(\mathbf{R}^3; \mathbf{C}^2)$. Then*

$$\sum_{j=1}^{N} e_j^{(0)}(B, Z) \geqq -2NZ^2 [\ln(2^{3/2} Z^{-1} N^{-1/2} B^{1/2} + 1)]^2 - \frac{9}{4} NZ^2 . \tag{2.31}$$

*In the case $N \approx Z$ and $B \gg Z^3$* (2.31) *reduces to the form* (2.29). *Notice that the error term $NZ^2$ differs only by a logarithm from the leading term.*[4]

As preparation for the proof of this theorem we need the following lemma (essentially identical to Lemma 2.1 in [1]).

**2.6 Lemma (Energy of One-Dimensional Coulomb Problem).** *For $Z > 0$ and $a > 0$, let $h_{Z,a}$ be the operator on $L^2(\mathbf{R})$ given by*

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

*Then the first and second eigenvalues, $\mu_1$ and $\mu_2$, satisfy*

$$\mu_1 \geqq -Z^2 \{1 + [\sinh^{-1}(1/Za)]^2\} ,$$

$$\mu_2 \geqq -Z^2/4 .$$

[4] In [1], (4 11), a slightly better estimate is given

*Proof.* By scaling, we see that $h_{Z,a} = Z^2$ 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),

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

with $I = \int \psi^2$. The fourth line was obtained from the third by noting that $\psi(1)^2 \leqq 2\int_1^\infty |\psi(x)[d\psi(x)/dx]| dx$. The bound on $\mu_1$ is obtained by minimizing the last expression with respect to $T$.

To estimate $\mu_2$ we first replace $-Z(|x|^2 + a^2)^{-1/2}$ with the lower bound $-Z|x|^{-1}$. Thus, if $\psi_2$ denotes the second eigenfunction,

$$\mu_2 \geqq \langle \psi_2 | p^2 - Z|x|^{-1} | \psi_2 \rangle \,. \tag{2.32}$$

Since the potential $x \mapsto Z(|x|^2 + a^2)^{-1/2}$ is symmetric about $x = 0$, the second normalized eigenfunction $\psi_2$ must have a node at $x = 0$. Minimizing the right side of the inequality (2.32) over normalized functions having a node at the origin is equivalent to minimizing the energy of the hydrogen atom with respect to radial functions. Thus we obtain $\mu_2 \geqq -Z^2/4$. ■

*Proof of Theorem 2.5.* Denote the eigenfunction corresponding to $e_j^{(0)}$ by $m_j^{(0)}$, $j = 1, 2, \ldots$. Since all $m_j^{(0)}$ are in the lowest Landau band the spin is always opposite to the field **B** and we might consider the $m_j^{(0)}$ as belonging to $L^2(\mathbf{R}^3)$ rather than $L^2(\mathbf{R}^3; \mathbf{C}^2)$. Consider the projection on $L^2(\mathbf{R}^3)$ with integral kernel

$$\gamma(x; y) = \sum_{j=1}^{n} m_j^{(0)}(x) \overline{m_j^{(0)}(y)} \,.$$

Since $\gamma$ projects onto the lowest Landau band we have $\gamma = \Pi_0 \gamma \Pi_0$. (Note that here $\Pi_0$ is a projection in $L^2(\mathbf{R}^3)$, i.e., given by (2.10) without $\mathscr{P}^{\downarrow}$.) From this we shall now conclude that for the reduced operator $\gamma_{x_\perp}$ on $L^2(\mathbf{R})$ given by the kernel

$$\gamma_{x_\perp}(x_3; y_3) = \gamma(x_\perp, x_3; x_\perp, y_3) , \tag{2.33}$$

we have the operator inequality

$$0 \leqq \gamma_{x_\perp} \leqq \frac{B}{\pi} I_{L^2(\mathbf{R})} . \tag{2.34}$$

Here $I_{L^2(\mathbf{R})}$ is the identity in $L^2(\mathbf{R})$.

Indeed, given $f \in L^2(\mathbf{R})$ with $\|f\| = 1$ we can use (2.10) and the facts that $0 \leqq \gamma \leqq I_{L^2(\mathbf{R}^3)}$ and $\Pi_0^2 = \Pi_0$ to obtain $\Pi_0 \gamma \Pi_0 \leqq \Pi_0$, and hence

$$\begin{aligned} \langle f | \gamma_{x_\perp} | f \rangle &= \int \overline{f(x_3)} (\Pi_0 \gamma \Pi_0)(x_3, x_\perp; y_3, x_\perp) f(y_3) dx_3 dy_3 \\ &\leqq \int \overline{f(x_3)} \Pi_0(x_3, x_\perp; y_3, x_\perp) f(y_3) dx_3 dy_3 \\ &= \int |f(x_3)|^2 \Pi_0(x, x)\, dx_3 = B/2\pi . \end{aligned}$$

For the sum of the negative eigenvalues of the operator (2.30) we find

$$\begin{aligned} \sum_{j=1}^{N} e_j^{(0)}(B, Z) &= \mathrm{Tr}[\gamma(p_3^2 - Z|x|^{-1})] \\ &= \int \mathrm{Tr}_{L^2(\mathbf{R})}[\gamma_{x_\perp}(p_3^2 - Z(x_3^2 + |x_\perp|^2)^{-1/2})] dx_\perp . \end{aligned} \tag{2.35}$$

As a consequence of (2.34) we can get a lower bound for the right side of (2.35) by replacing $\gamma_{x_\perp}$ with the projection onto eigenfunctions for $p_3^2 - Z(x_3^2 + |x_\perp|^2)^{-1/2}$ (as an operator on $L^2(\mathbf{R})$ depending on the parameter $|x_\perp|$) multiplied by $B/2\pi$. Thus

$$\sum_{j=1}^{N} e_j^{(0)}(B, Z) \geqq \frac{B}{2\pi} \int_{|x_\perp|^2 \leqq 2N/B} \mu_1(x_\perp) dx_\perp - N \sup_{x_\perp} |\mu_2(x_\perp)| , \tag{2.36}$$

where $\mu_1(x_\perp)$ and $\mu_2(x_\perp)$ are, respectively, the first and second eigenvalues of $p_3^2 - Z(x_3^2 + |x_\perp|^2)^{-1/2}$ on $L^2(\mathbf{R})$. The domain of integration for the first integral is due to the restriction $\int \mathrm{Tr}(\gamma_{x_\perp})\, dx_\perp = N$ which, in the case when $\gamma_{x_\perp}$ is either zero or greater than $B/2\pi$ multiplied by a one-dimensional projection, implies that $\gamma_{x_\perp}$ is zero for $|x_\perp|^2 > 2N/B$. Here we are of course using the fact that $\mu_1(x_\perp)$ is a monotone increasing function of $|x_\perp|$ so that the optimal support for $x_\perp \mapsto \gamma_{x_\perp}$ is a disc centered at the origin.

We shall now derive a bound whose leading term is determined by the first eigenvalue $\mu_1(x_\perp)$ . To do this we use the estimates of $\mu_1(x_\perp)$ and $\mu_2(x_\perp)$ in Lemma 2.6 (with $a = |x_\perp|$). Inserting these bounds into (2.36) and using $\sinh^{-1}(x) = \ln(x + \sqrt{1 + x^2})$ yields

$$\sum_{j=1}^{N} e_j(B, Z) \geqq -\frac{B}{2\pi} Z^2 \int_{|x_\perp|^2 \leqq 2N/B} \left\{ \left( \ln\left( \frac{1 + \sqrt{(Z|x_\perp|)^2 + 1}}{Z|x_\perp|} \right) \right)^2 + 1 \right\} dx_\perp - \frac{N}{4} Z^2 .$$

The estimate (2.31) is then easily seen from

$$\frac{B}{2\pi}Z^2 \int_{|x_\perp|^2 \leqq 2N/B} \left(\ln\left(\frac{1+\sqrt{(Z|x_\perp|)^2+1}}{Z|x_\perp|}\right)\right)^2 dx_\perp$$

$$\leqq \frac{B}{2\pi}\int_{|x_\perp|^2 \leqq 2NZ^2/B} \left(\ln\left(\frac{1+\sqrt{2NZ^2B^{-1}+1}}{|x_\perp|}\right)\right)^2 dx_\perp$$

$$\leqq \frac{B}{\pi}\int_{|x_\perp|^2 \leqq 2NZ^2/B} \left(\ln\left(\frac{1+\sqrt{2NZ^2B^{-1}+1}}{\sqrt{2NZ^2B^{-1}}}\right)\right)^2 + \left(\ln\left(\frac{|x_\perp|}{\sqrt{2NZ^2B^{-1}}}\right)\right)^2 dx_\perp$$

$$= 2NZ^2(\ln(2^{1/2}N^{-1/2}Z^{-1}B^{1/2} + \sqrt{1+2N^{-1}Z^{-2}B}))^2 + NZ^2 ,$$

where we have used that $\int_{|x_\perp|\leqq 1}(\ln|x_\perp|)^2 dx_\perp = \pi/2$. ■

For the $B\to\infty$ limit it is natural to ask how Theorem 2.1 changes if the operator $H_{\mathbf{A}} + V(x)$ is restricted to the lowest Landau band, i.e., if we consider the operator $\Pi_0(H_{\mathbf{A}} + V(x))\,\Pi_0$ instead of $H_{\mathbf{A}} + V(x)$. The following theorem answers this question. The constant in the inequality of this theorem corresponds to the constant $L_1$ of Theorem 2.1 with $\delta = 0$.

**2.7 Theorem.** *If* $|V|_-\in L^{3/2}(\mathbf{R}^3)$ *let* $e_j^{(0)}(B, V), j = 1, 2, \ldots,$ *denote the negative eigenvalues of* $\Pi_0(H_{\mathbf{A}} + V(x))\Pi_0$ *on* $L^2(\mathbf{R}^3; \mathbf{C}^2)$, *where* $\Pi_0$ *is the projection* (2.10) *onto the lowest Landau band. Then*

$$\sum_j |e_j^{(0)}(B, V)| \leqq \frac{2}{3\pi}B\int |V(x)|_-^{3/2}dx . \tag{2.37}$$

*Proof.* The proof of (2.37) uses a slightly modified Birman–Schwinger principle, which we now briefly outline.

We shall estimate the number $N_E^{(0)}$ of eigenvalues of $\Pi_0(H_{\mathbf{A}} + V)\Pi_0$ less than $-E$, i.e., the eigenvalues less than zero of

$$\left(H_{\mathbf{A}} + \frac{1}{2}E\right) + \Pi_0\left(V(x) + \frac{1}{2}E\right)\Pi_0 \tag{2.38}$$

We shall replace $V(x) + \frac{1}{2}E$ by the lower bound $-|V(x) + \frac{1}{2}E|_-$. This change will only increase the number of eigenvalues as can easily be seen from the variational principle. Let $f\in L^2(\mathbf{R}^3; \mathbf{C}^2)$ be an eigenfunction for

$$H_{\mathbf{A}} + \frac{1}{2}E - \Pi_0\left|V + \frac{1}{2}E\right|_- \Pi_0 \tag{2.39}$$

with eigenvalue $-\zeta < 0$. Then $\Pi_0 f = f$ and

$$f = \Pi_0\left(H_{\mathbf{A}} + \frac{1}{2}E + \zeta\right)^{-1}\Pi_0\left|V + \frac{1}{2}E\right|_- f .$$

If we define $g = |V + \frac{1}{2}E|_-^{1/2} f$ we obtain

$$g = \left|V + \frac{1}{2}E\right|_-^{1/2} \Pi_0 \left(H_{\mathrm{A}} + \frac{1}{2}E + \zeta\right)^{-1} \Pi_0 \left|V + \frac{1}{2}E\right|_-^{1/2} g . \tag{2.40}$$

Note that $g \in L^2(\mathbf{R}^3; \mathbf{C}^2)$ since $|V|_- \in L^{3/2}$ and $f \in L^6$ by the standard Sobolev inequality.

The operator on the right side of (2.40) is monotonically decreasing in $\zeta$. All the eigenvalues greater than 1 for the operator with $\zeta = 0$, i.e., for the operator

$$K_E^0 = \left|V + \frac{1}{2}E\right|_-^{1/2} \Pi_0 \left(H_{\mathrm{A}} + \frac{1}{2}E\right)^{-1} \Pi_0 \left|V + \frac{1}{2}E\right|_-^{1/2} , \tag{2.41}$$

will eventually decrease to 1 as $\zeta$ increases. Thus $N_E^{(0)}$ is bounded by the number of eigenvalues greater than 1 for $K_E^0$. But this number we estimate by $\mathrm{Tr}\, K_E^0$, and this we computed in the proof of Theorem 2.1; see Eqs. (2.11) and (2.23). ■

*Remark.* Using the method of Theorem 2.4, but with the inequality (2.37) instead of (2.3), we can get a lower bound for the sum of the negative eigenvalues of $\Pi_0(H_{\mathrm{A}} - Z|x|^{-1})\Pi_0$ different from the bound in Theorem 2.5. Thus, if $e_j^{(0)}(B, Z), j = 1, 2, \ldots$, again denote the negative eigenvalues of $\Pi_0(H_{\mathrm{A}} - Z|x|^{-1})\Pi_0$, we obtain the two bounds

$$\sum_j e_j^{(0)}(B, Z) \geqq -\frac{5}{6}\left(\frac{\pi}{2}\right)^{2/5} Z^{6/5} N^{3/5} B^{2/5} \tag{2.42}$$

and

$$\sum_j e_j^{(0)}(B, Z) \geqq -2NZ^2[\ln(2^{3/2} Z^{-1} N^{-1/2} B^{1/2} + 1)]^2 - \frac{9}{4} NZ^2 . \tag{2.43}$$

Inequality (2.42) is derived from Theorem 2.7 while (2.43) is a restatement of inequality (2.31) in Theorem 2.5.

The first inequality, (2.42), is best when $B \lesssim NZ^2$ while (2.43) is better when $B \gtrsim NZ^2$.

We conclude this section with a generalization of Theorem 2.4 to potentials other than the Coulomb potential. This result is needed for the quantum mechanical limit in Sect. V.

**2.8 Proposition.** *Suppose $v = v_1 + v_2$ with $v_1 \in L^{5/2}(\mathbf{R}^3) \cap L^{3/2}(\mathbf{R}^3)$ and $v_2 \in L^\infty(\mathbf{R}^3)$. Consider the Hamiltonian*

$$\tilde{H}_{N,B,Z} = \sum_{i=1}^N [\boldsymbol{\sigma}_i \cdot (\mathbf{p}_i + \mathbf{A}(x_i))]^2 + Z\ell^{-1} v(\ell^{-1} x) , \tag{2.44}$$

*where $\ell = Z^{-1/3}(1 + \beta)^{-2/5}$, with $\beta = B/Z^{4/3}$. The ground state energy of this Hamiltonian on the space $\bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$ is bounded below by*

$$-Z^2 \ell^{-1} c_\lambda(v) = -Z^{7/3}(1 + \beta)^{2/5} c_\lambda(v) , \tag{2.45}$$

*where $c_\lambda(v)$ depends only on $\lambda = N/Z$ and $v$.*

*Proof.* On the space $\bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$ we have the lower bound

$$\tilde{H}_{N,B,Z} \geqq \sum_{i=1}^N [\boldsymbol{\sigma}_i \cdot (\mathbf{p}_i + \mathbf{A}(x_i))]^2 + Z\ell^{-1} v_1(\ell^{-1} x) - NZ\ell^{-1} \|v_2\|_\infty .$$

If we now use the LT inequality (2.3) we get

$$\tilde{H}_{N,B,Z} \geqq -L_1 B Z^{3/2}\ell^{3/2}\int |v_1(x)|^{3/2}dx - L_2 Z^{5/2}\ell^{1/2}\int |v_1(x)|^{5/2}dx - NZ\ell^{-1}\|v_2\|_\infty .$$

The choice $\ell = Z^{-1/3}(1+\beta)^{-2/5}$ allows one to bound all three terms below by expressions of the form (2.45). ■

As a consequence we immediately get the following result which is also needed in Sect. V.

**2.9 Corollary.** *Let $\tilde{H}_{N,B,Z}$ be defined as in Proposition 2.8. If $\psi \in \bigwedge^N L^2(\mathbf{R}^3;\mathbf{C}^2)$ satisfies $\langle\psi|\tilde{H}_{N,B,Z}|\psi\rangle \leqq 0$ we get a bound on the kinetic energy:*

$$\langle\psi|\sum_{i=1}^{N}[\boldsymbol{\sigma}_i\cdot(\mathbf{p}_i+\mathbf{A}(x_i))]^2|\psi\rangle \leqq Z^2\ell^{-1}c'_\lambda(v) = Z^{7/3}(1+\beta)^{2/5}c'_\lambda(v)\,, \tag{2.46}$$

*where, as above, $c'_\lambda(v)$ depends only on $\lambda$ and $v$.*

*Proof.* This is clear since Proposition 2.8 holds (with a different $c_\lambda(v)$) if we replace $\tilde{H}_{N,B,Z}$ by the operator

$$\tilde{H}'_{N,B,Z} = \tilde{H}_{N,B,Z} - \frac{1}{2}\sum_{i=1}^{N}[\boldsymbol{\sigma}_i\cdot(\mathbf{p}_i+\mathbf{A}(x_i))]^2. \quad ■$$

## III. Semiclassics in a Constant Magnetic Field

Our goal in this section is to prove a semiclassical formula for the sum of the negative eigenvalues of a Hamiltonian of the form (1.1). We introduce a semiclassical parameter $h > 0$ and consider the operator

$$H(h,b) = [\boldsymbol{\sigma}\cdot(h\mathbf{p} + b\mathbf{a}(x))]^2 + V(x)\,, \tag{3.1}$$

where $\mathbf{a}(x) = \frac{1}{2}(-x_2, x_1, 0)$ corresponds to a spatially constant magnetic field of unit strength in the 3-direction. Thus $b\mathbf{a}$ is the vector potential for the magnetic field $\mathbf{b} = (0,0,b)$. The potential $V$ as before satisfies $|V|_- \in L^{5/2}(\mathbf{R}^3) \cap L^{3/2}(\mathbf{R}^3)$. As usual $H(h,b)$ acts on $L^2(\mathbf{R}^3;\mathbf{C}^2)$. We are interested in the asymptotic properties of $H(h,b)$ as $h \to 0$.

If we fix the magnetic field strength $b > 0$ and ask for the leading term in $h^{-1}$ of the sum of the negative eigenvalues, it is well-known, and we shall prove it again below, that it has no dependence on $b$ [15]. It is simply the standard expression $-(2/15)\,\pi^{-2}h^{-3}\int|V(x)|_-^{5/2}dx$.

Our goal, however, is a semiclassical expression analogous to the LT estimate (2.3) which holds for all values of the magnetic field strength $b$. More precisely we shall prove a semiclassical approximation to the sum of the negative eigenvalues of the operator (3.1) which holds *uniformly* in $b$.

It is somewhat surprising that it is at all possible to find a semiclassical approximation valid uniformly in the magnetic field strength. In fact, the corresponding classical phase space is, as we shall see, not the standard phase space with conjugate variables $x$ and $\mathbf{p}$.

The possibility of doing semiclassics in a strong magnetic field was originally realized in [25] and in [12]. Much of the analysis presented here was done in [12] in the special case when $b$ is of order $h^{-1}$. In this case one can avoid the use of the generalized LT inequality. Reference [25] contains a local analysis of the density of states.[5] In our proof below we follow the coherent state approach used in [12].

Before giving the semiclassical formula for the sum of the eigenvalues we shall briefly describe the corresponding classical phase space. The phase space can be thought of as a union of phase spaces, one for each Landau band. The phase space corresponding to the Landau band with index $\nu \geqq 0$ is $\mathbf{R}^4$ with coordinates $(x_1, x_2, x_3, p)$, $p$ being the momentum along the field. The symplectic form on $\mathbf{R}^4$ is

$$\frac{b}{2\pi h} dx_1 \wedge dx_2 + \frac{1}{2\pi} dx_3 \wedge dp \, .$$

The volume form is then $bh^{-1}(2\pi)^{-2} dx_1 \wedge dx_2 \wedge dx_3 \wedge dp$. The semiclassical expression for the sum of the negative eigenvalues of $H(h, b)$ corresponding to Landau band $\nu \geqq 0$ is thus, with $\varepsilon_{p,\nu}(h, b) = h^2(p^2 + 2bh^{-1}\nu)$,

$$\begin{aligned} -\frac{b}{(2\pi)^2 h} \int |\varepsilon_{p,\nu}(h, b) + V(x)|_- \, dp\, dx_1 dx_2 dx_3 \\ = -\frac{h^{-2}b}{3\pi^2} \int | V(x) + 2\nu bh|_-^{3/2} dx \, . \end{aligned} \tag{3.2}$$

If we recall that the higher bands $\nu > 0$ are twice as degenerate as the lowest band $\nu = 0$ (because of the presence of the spin) we arrive at the following semiclassical expression for the sum of the negative eigenvalues of $H(h, b)$ from (3.1):

$$E_{\mathrm{scl}}(h, b, V) = -\frac{1}{3\pi^2} h^{-2} b \int \left( |V(x)|_-^{3/2} + 2 \sum_{\nu=1}^{\infty} |V(x) + 2\nu bh|_-^{3/2} \right) dx \, . \tag{3.3}$$

Notice that if $b$ is fixed and $h \to 0$ the sum in (3.3) can be replaced by an integral and we get the standard semiclassical expression $-(2/15)\pi^{-2} h^{-3} \int |V(x)|_-^{5/2} dx$. In the other extreme limit $h^{-1} \ll b$ the sum in (3.3) is absent and we have only a contribution from the lowest Landau band. This latter case is a semiclassical equivalent of the confinement of electrons to the lowest Landau band which we discussed in [1].

If we compare the semiclassical expression (3.3) with the estimate from the LT inequality (2.3) we see that the two terms in (2.3) correspond, respectively, to the $b \to \infty$ (first term) and $b \to 0$ (last term) asymptotics of (3.3).

We note that the function which appears in the semiclassical expression (3.3) can be written as $h^{-3} P_{hb}(|V|_-)$, where $P_B \colon \mathbf{R}_+ \to \mathbf{R}_+$, given by

$$P_B(w) = \frac{B}{3\pi^2} \left( w^{3/2} + 2 \sum_{\nu=1}^{\infty} |2\nu B - w|_-^{3/2} \right) , \tag{3.4}$$

is the *pressure* of the free Landau gas, i.e., the non-interacting electron gas in a constant magnetic field of magnitude $B$, as a function of the *chemical potential*, $w$, of the gas. The function $P_B$ is convex and its derivative

$$P_B'(w) = \frac{B}{2\pi^2} \left( w^{1/2} + 2 \sum_{\nu=1}^{\infty} |2\nu B - w|_-^{1/2} \right) , \tag{3.5}$$

[5] Motivated by our work, the local analysis in [25] has recently been extended in [26] to give a local version of Theorem 3 1 below with good error bounds

is the particle number density of the Landau gas. As in (3.2) we have the following representations:

$$h^{-3}P_{hb}(w) = \sum_{\nu} \frac{d_\nu(h, b)}{2\pi} \int |\varepsilon_{p,\nu}(h, b) - w|_- dp \,, \tag{3.6}$$

and

$$h^{-3}P'_{hb}(w) = \sum_{\nu} \frac{d_\nu(h, b)}{2\pi} \int_{\varepsilon_{p,\nu}(h,b) < w} dp \,, \tag{3.7}$$

where $d_0(h, b) = b/(2\pi h)$ and $d_\nu(h, b) = b/(\pi h)$ if $\nu > 0$.

We turn now to the proof that (3.3) is indeed the correct semiclassical expression for the sum of the negative eigenvalues.

**3.1 Theorem (Semiclassics in a Magnetic Field).** *Let $e_j(h, b, V), j = 1, 2, \ldots,$ denote the negative eigenvalues of the Hamiltonian* (3.1) *with $|V|_- \in L^{3/2}(\mathbf{R}^3) \cap L^{5/2}(\mathbf{R}^3)$. Then*

$$\lim_{h \to 0} \left( \sum_j e_j(h, b, V) / E_{\rm scl}(h, b, V) \right) = 1 \,, \tag{3.8}$$

*uniformly in the magnetic field strength $b$. Here $E_{\rm scl}$ is given by the semiclassical formula* (3.3).[6]

*Proof. Step 1.* The function $P(w) := h^{-3}P_{hb}(w)$ satisfies the bounds (compare also with the LT inequality (2.3))

$$k_1 h^{-2} b w^{1/2} + k_2 h^{-3} w^{3/2} \leqq P'(w) \leqq K_1 h^{-2} b w^{1/2} + K_2 h^{-3} w^{3/2} \,, \tag{3.9}$$

where $k_1, k_2, K_1$ and $K_2$ are positive constants. From this we have

$$c_1 h^{-2} b w^{3/2} + c_2 h^{-3} w^{5/2} \leqq P(w) \leqq C_1 h^{-2} b w^{3/2} + C_2 h^{-3} w^{5/2} \,, \tag{3.10}$$

where $c_1 = 2k_1/3$, $c_2 = 2k_1/5$, $C_1 = 2K_1/3$ and $C_2 = 2K_2/5$. Thus $E_{\rm scl}(h, b, V) = -\int P(|V(x)|_-)\, dx$ satisfies

$$\tilde{c} \leqq \{h^{-3} + h^{-2} b\}^{-1} |E_{\rm scl}(h, b, V)| \leqq \tilde{C} \,, \tag{3.11}$$

where, except for the trivial case $V \geqq 0$ almost everywhere, $\tilde{c} > 0$. We thus have to prove that

$$\lim_{h \to 0} \left( \{h^{-2} b + h^{-3}\}^{-1} \left( E_{\rm scl}(h, b, V) - \sum_j e_j(h, b, V) \right) \right) = 0 \,, \tag{3.12}$$

uniformly in $b$. We shall do this by giving upper and lower bounds to $\sum_j e_j(h, b, V)$. To achieve this goal we apply the method of coherent states.

*Step 2 (Coherent states).* To define our coherent states we introduce the projection $\Pi_\nu$ in $L^2(\mathbf{R}^3; \mathbf{C}^2)$ onto the Landau band with index $\nu \geqq 0$ for $((h\mathbf{p} + b\mathbf{a}) \cdot \boldsymbol{\sigma})^2$. We can write $\Pi_\nu = \Pi_\nu^{(2)} \otimes \mathbf{1}$, where $\Pi_\nu^{(2)}$ is a projection in $L^2(\mathbf{R}^2; \mathbf{C}^2)$ obtained by suppressing the direction $x_3$ along the field. The integral kernel for $\Pi_0$ was given in

[6] The statement implies, in particular, that if $V$ is negative on a set of positive measure then the Hamiltonian $H(h, b)$ has negative eigenvalues for $h$ small enough

(2.10) with $B = b/h$. In general the integral kernels are

$$\Pi_\nu^{(2)}(x_\perp, y_\perp) = \frac{b}{2\pi h}\exp\{i(x_\perp \times y_\perp)\cdot \mathbf{b}/2h - |x_\perp - y_\perp|^2 b/4h\}$$

$$\times\left(L_\nu\left(|x_\perp - y_\perp|^2\frac{b}{2h}\right)\mathscr{P}^\uparrow + L_{\nu-1}\left(|x_\perp - y_\perp|^2\frac{b}{2h}\right)\mathscr{P}^\downarrow\right). \tag{3.13}$$

Here $L_\nu$ are Laguerre polynomials normalized by $L_\nu(0) = 1$ and, to be consistent with (2.10), $L_{-1} \equiv 0$. As before $\mathscr{P}^\uparrow$ and $\mathscr{P}^\downarrow$ denote the projections in $\mathbf{C}^2$ onto the subspaces where $\mathbf{B}\cdot\boldsymbol{\sigma} = B$ and $\mathbf{B}\cdot\boldsymbol{\sigma} = -B$ respectively. Since the Landau level eigenfunctions form a complete set in $L^2(\mathbf{R}^2; \mathbf{C}^2)$ we have the identity $\sum_\nu \Pi_\nu^{(2)} = \mathbf{1}_{L^2(\mathbf{R}^2;\mathbf{C}^2)}$.

We shall not need the explicit form (3.13) but only the fact that

$$\Pi_\nu^{(2)}(x_\perp, x_\perp) = d_\nu(h, b) = \frac{b}{\pi h}\begin{cases} 1/2 & \text{if } \nu = 0 \\ 1 & \text{if } \nu > 0 \end{cases}. \tag{3.14}$$

This simply says that in each Landau level the two-dimensional density of states perpendicular to the magnetic field is $b/2\pi h$, not counting spin degeneracy.

The coherent states we introduce following [12] are given by the map

$$\Pi\colon \mathbf{N}_0 \times \mathbf{R}^4 \ni (\nu, u, p) \mapsto \Pi(\nu, u, p)$$

from the nonnegative integers times the classical phase space of two-dimensional motion to operators on $L^2(\mathbf{R}^3; \mathbf{C}^2)$, where the operator $\Pi(\nu, u, p)$ has the integral kernel

$$\Pi(\nu, u, p)(x, y) = g_r(x - u)\Pi_\nu^{(2)}(x_\perp, y_\perp)e^{ip(x_3 - y_3)}g_r(y - u)\,. \tag{3.15}$$

Here $g_r(x) = r^{-3/2}g(x/r)$, where $0 \leqq g \in C_0^\infty(\mathbf{R}^3)$ with $\int g^2 = 1$ and $\operatorname{supp} g \subseteq \{|x| \leqq 1\}$. We shall choose $r > 0$ later. Note that $\Pi(\nu, u, p)$ is not a rank-one operator and therefore $\Pi$ is not a coherent state map in the usual sense. It is reminiscent of the coherent *operators* introduced in [27]. The operator $\Pi(\nu, u, p)$ satisfies the coherent operator identities

$$\sum_{\nu=0}^{\infty}(2\pi)^{-1}\iint \Pi(\nu, u, p)\,du\,dp = 1_{L^2(\mathbf{R}^3;\mathbf{C}^2)}\,, \tag{3.16}$$

$$\operatorname{Tr}_{L^2(\mathbf{R}^3;\mathbf{C}^2)}[\Pi(\nu, u, p)] = d_\nu(h, b)\,, \tag{3.17}$$

with $d_\nu(h, b)$ given in (3.14).

If we use the following easily derived version of the IMS localization formula, valid for all $f$ and $g$,

$$\langle f|g_r[(h\mathbf{p} + b\mathbf{a})\cdot\boldsymbol{\sigma}]^2 g_r|f\rangle = \langle f|g_r^2[(h\mathbf{p} + b\mathbf{a})\cdot\boldsymbol{\sigma}]^2|f\rangle + h^2\langle f|(\nabla g_r)^2|f\rangle\,, \tag{3.18}$$

we get from (3.15) and (3.17) that

$$\operatorname{Tr}[((h\mathbf{p} + b\mathbf{a})\cdot\boldsymbol{\sigma})^2\Pi(\nu, u, p)] = d_\nu(h, b)\varepsilon_{p,\nu}(h, b) + d_\nu(h, b)h^2\int(\nabla g_r)^2\,. \tag{3.19}$$

Here we have also used

$$((h\mathbf{p} + b\mathbf{a})\cdot\boldsymbol{\sigma})^2\Pi_\nu^{(2)}(x_\perp, y_\perp)e^{ip(x_3 - y_3)} = \varepsilon_{p,\nu}(h, b)\,\Pi_\nu^{(2)}(x_\perp, y_\perp)e^{ip(x_3 - y_3)}\,. \tag{3.20}$$

Likewise, from (3.18) and (3.20) we obtain

$$\begin{aligned}\langle f|((h\mathbf{p}+b\mathbf{a})\cdot\boldsymbol{\sigma})^2|f\rangle &= \int\langle f|g_r(\cdot-u)^2((h\mathbf{p}+b\mathbf{a})\cdot\boldsymbol{\sigma})^2|f\rangle du\\ &=\int\langle f|g_r(\cdot-u)((h\mathbf{p}+b\mathbf{a})\cdot\boldsymbol{\sigma})^2 g_r(\cdot-u)|f\rangle du - h^2\int(\nabla g_r)^2\\ &=\sum_{v=0}^{\infty}(2\pi)^{-1}\int\int\varepsilon_{p,v}(h,b)\langle f|\Pi(v,u,p)|f\rangle du\,dp - h^2\int(\nabla g_r)^2\,.\end{aligned} \tag{3.21}$$

Finally we have, for a potential $V(x)$, the identities

$$\mathrm{Tr}[V\Pi(v,u,p)] = d_v(h,b)\,V*g_r^2(u) \tag{3.22}$$

and

$$\langle f|V*g_r^2|f\rangle = \sum_v(2\pi)^{-1}\int\int V(u)\langle f|\Pi(v,u,p)|f\rangle du\,dp\,. \tag{3.23}$$

*Step 3* (*Upper bound on* $\sum_j e_j$). We shall use the coherent operators from Step 2 to construct a trial density matrix $\gamma$.

Given $\varepsilon>0$, choose $R>0$ such that

$$\int_{|x|\geqq R}|V(x)|_-^{3/2}dx<\varepsilon \quad\text{and}\quad \int_{|x|\geqq R}|V(x)|_-^{5/2}dx<\varepsilon\,. \tag{3.24}$$

Define the function $M(v,u,p)$ on the phase space to be the characteristic function of the set

$$\{(v,u,p)|\varepsilon_{p,v}(h,b)\leqq|V(u)|_-\ \text{and}\ |u|\leqq R\}\,, \tag{3.25}$$

and define the operator $\gamma$ on $L^2(\mathbf{R}^3;\mathbf{C}^2)$ by

$$\gamma=\sum_{v=0}^{\infty}(2\pi)^{-1}\int\int M(v,u,p)\Pi(v,u,p)du\,dp\,. \tag{3.26}$$

From (3.16), $\gamma$ satisfies the density matrix condition $0\leqq\gamma\leqq\mathbf{1}$. Thus from the variational principle we get

$$\begin{aligned}\sum_j e_j(h,b,V)\leqq \mathrm{Tr}[H(h,b)\gamma] = \sum_v(2\pi)^{-1}\int\int M(v,u,p)d_v(h,b)\{\varepsilon_{p,v}(h,b)\\ + h^2[\textstyle\int(\nabla g_r)^2] - |V|_-*g_r^2(u)\}du\,dp\,,\end{aligned}$$

where we have used (3.19) and (3.22). From the definition (3.25) of $M$ we get, by comparison with (3.2), that

$$\begin{aligned}\sum_j e_j(h,b,V)\leqq &-\int_{|u|\leqq R}P(|V(u)|_-)du+\int_{|u|\leqq R}P'(|V(u)|_-)\\ &\times[|V(u)|_- - |V|_-*g_r^2(u)]du\\ &+h^2\int(\nabla g_r)^2\int_{|u|\leqq R}P'(|V(u)|_-)du\,,\end{aligned} \tag{3.27}$$

where $P$ is the semiclassical function defined in Step 1, and we have used that if $|u|\leqq R$ then

$$\sum_v(2\pi)^{-1}d_v(h,b)\int M(v,u,p)dp = P'(|V(u)|_-)\,, \tag{3.28}$$

by (3.7).

To conclude that the upper bound in (3.27) agrees with the semiclassical formula to leading order we note first that by (3.10) and the choice of $R$

$$-\int_{|u|\leqq R} P(|V(u)|_-)du \leqq -\int P(|V(u)|_-)du + C_1 h^{-2} b\varepsilon + C_2 h^{-3}\varepsilon\,. \tag{3.29}$$

We next show that the last term in (3.27) is small. To this end we use the estimate (3.9) from Step 1 and Hölder's inequality to conclude that

$$\begin{aligned}\int_{|u|\leqq R} P'(|V(u)|_-)du &\leqq C\int_{|u|\leqq R}(bh^{-2}|V(u)|_-^{1/2} + h^{-3}|V(u)|_-^{3/2})du\\ &\leqq C'bh^{-2}R^2\left(\int_{|u|\leqq R}|V(u)|_-^{3/2}du\right)^{1/3} + Ch^{-3}\int_{|u|\leqq R}|V(u)|_-^{3/2}du\,.\end{aligned} \tag{3.30}$$

By recalling that this is being multiplied by $h^2\int(\nabla g_r)^2 = h^2 r^{-2}\int(\nabla g)^2$, we see that if we choose $r = h^{1-\alpha}$ for some $0 < \alpha < 1$ then the last term in (3.27) is bounded by

$$(\text{const.})\{h^{-3} + R^2 bh^{-2}\}h^{2\alpha}\,, \tag{3.31}$$

which, according to (3.11), is of lower order than the main term.

We turn to the second term in (3.27). Using the bound (3.9) from Step 1 we conclude that

$$\begin{aligned}&\int_{|u|\leqq R} P'(|V(u)|_-)[|V(u)|_- - |V|_- * g_r^2(u)]du\\ &\leqq C_R h^{-2} b\||V|_-\|_{3/2}^{1/2}\||V|_- * g_r^2 - |V|_-\|_{3/2}\\ &\quad + C_R h^{-3}\||V|_-\|_{5/2}^{3/2}\||V|_- * g_r^2 - |V|_-\|_{5/2}\,.\end{aligned} \tag{3.32}$$

Since $r = h^{1-\alpha}\to 0$ as $h\to 0$ and $|V|_- * g_r^2 \to |V|_-$ in $L^{3/2}(\mathbf{R}^3)$ and in $L^{5/2}(\mathbf{R}^3)$ we have from (3.29), (3.31) and (3.32) that

$$\limsup_{h\to 0}\frac{\sum_j e_j(h, b, V)}{-\int P(|V(u)|_-)du} \leqq 1$$

uniformly in $b$.

*Step 4* (*Lower bound on* $\sum_j e_j$). It is clear that in proving the lower bound we can replace the potential $V$ by $-|V|_-$. As in Step 3 we want to restrict to a bounded region $\{|x| \leqq R\}$ with $R$ determined by $\varepsilon$ as in (3.24). Choose $0 \leqq \theta_1, \theta_2 \in C^\infty(\mathbf{R}^3)$ with $\theta_1^2 + \theta_2^2 = 1$, $\theta_1(x) = 1$ if $|x| \leqq R$ and $\theta_2(x) = 1$ if $|x| \geqq 2R$.

Since $\sum_j e_j(h, b, V) = \inf\sum_j\langle f_j|H(h, b)|f_j\rangle$, where the infimum is over all orthonormal families $f_1, \ldots, f_N$, $N \geqq 1$, it suffices to prove a lower bound on $\sum_j\langle f_j|H(h, b)|f_j\rangle$ independent of $f_1, \ldots, f_N$, $N \geqq 1$. From the formula (3.18) we have

$$\begin{aligned}\langle f_j|H(h, b)|f_j\rangle &= \langle f_j|\theta_1(((h\mathbf{p} + b\mathbf{a})\cdot\boldsymbol{\sigma})^2 - |V|_-)\theta_1|f_j\rangle\\ &\quad + \langle f_j|\theta_2(((h\mathbf{p} + b\mathbf{a})\cdot\boldsymbol{\sigma})^2 - |V|_-)\theta_2|f_j\rangle\\ &\quad - h^2\langle f_j|(\nabla\theta_1)^2 + (\nabla\theta_2)^2|f_j\rangle\,.\end{aligned}$$

For $\delta > 0$ (to be chosen below) we write the sum over $j$ as

$$\sum_{j=1}^{N} \langle f_j | H(h,b) | f_j \rangle = \sum_{j=1}^{N} \langle f_j | \theta_1((1-\delta)((h\mathbf{p} + b\mathbf{a}) \cdot \boldsymbol{\sigma})^2 - |V|_- * g_r^2)\theta_1 | f_j \rangle$$

$$+ \sum_{j=1}^{N} \langle f_j | \theta_1(\delta((h\mathbf{p} + b\mathbf{a}) \cdot \boldsymbol{\sigma})^2 - |V|_-$$

$$+ |V|_- * g_r^2 - h^2(\nabla\theta_1)^2 - h^2(\nabla\theta_2)^2)\theta_1 | f_j \rangle$$

$$+ \sum_{j=1}^{N} \langle f_j | \theta_2(((h\mathbf{p} + b\mathbf{a}) \cdot \boldsymbol{\sigma})^2 - |V|_-$$

$$- h^2(\nabla\theta_1)^2 - h^2(\nabla\theta_2)^2)\theta_2 | f_j \rangle \,. \tag{3.33}$$

The main contribution to the sum of the negative eigenvalues comes from the first sum in (3.33). The two last sums we control using the LT inequality (2.3). Indeed, using (2.3) it is very easy to see that the last sum in (3.33) for $h$ small enough is bounded below by

$$-C\varepsilon(h^{-2}b + h^{-3}) \,. \tag{3.34}$$

The second term is just as easy to estimate. In fact, since $r = h^{1-\alpha}$, and $\alpha < 1$ we can choose $h$ small enough so that

$$\int \big| |V|_- - |V|_- * g_r^2 + h^2(\nabla\theta_1)^2 + h^2(\nabla\theta_2)^2 \big|^q < \varepsilon$$

for $q = 3/2$ and $q = 5/2$. The second sum in (3.33) is thus bounded below by

$$-C\varepsilon(h^{-2}b\delta^{-1/2} + h^{-3}\delta^{-3/2}) \,. \tag{3.35}$$

We are left with estimating the first sum in (3.33). From the identities (3.16), (3.21) and (3.23) we obtain that the first sum in (3.33) is equal to

$$\sum_{\nu} (2\pi)^{-1} \int\int [(1-\delta)(\varepsilon_{p,\nu}(h,b) - h^2 r^{-2} I_g) - |V(u)|_-] \sum_{j=1}^{N} \langle f_j | \theta_1 \Pi(\nu, u, p)\theta_1 | f_j \rangle du\, dp \,, \tag{3.36}$$

where we are writing $I_g = \int (\nabla g)^2$. The function $\sum_{j=1}^{N} \langle f_j | \theta_1 \Pi(\nu, u, p)\theta_1 | f_j \rangle$ satisfies the following two relations:

$$0 \leqq \sum_{j=1}^{N} \langle f_j | \theta_1 \Pi(\nu, u, p)\,\theta_1 | f_j \rangle \leqq d_\nu(h,b)$$

and

$$\sum_{j=1}^{N} \langle f_j | \theta_1 \Pi(\nu, u, p)\,\theta_1 | f_j \rangle = 0 \quad \text{if } |u| \geqq 2R + r \,.$$

It is thus clear that we get a lower bound to (3.36) if we replace $\sum_j \langle f_j | \theta_1 \Pi \theta_1 | f_j \rangle$ by the function $\widetilde{M}(\nu, u, p)$ defined to be $d_\nu(h,b)$ multiplied by the characteristic function of the set

$$\{(\nu, u, p) \,|\, (1-\delta)(\varepsilon_{p,\nu}(h,b) - h^2 r^{-2} I_g) - |V(u)|_- \leqq 0 \text{ and } |u| \leqq 2R + r\} \,. \tag{3.37}$$

By inserting this into (3.36) we find the lower bound to be

$$-\sum_{\nu}(2\pi)^{-1}d_\nu(h,b)\int \int_{|u|\leq 2R+r} |(1-\delta)(\varepsilon_{p,\nu}(h,b)-h^2r^2I_g)-|V(u)|_-|_-\,du\,dp$$

$$\geqq -(1-\delta)\int_{|u|\leq 2R+r} P((1-\delta)^{-1}|V(u)|_- + h^{2\alpha}I_g)du\,,$$

where we have used (3.6) and $r = h^{1-\alpha}$. Let $W(u) = (1-\delta)^{-1}|V(u)|_- + h^{2\alpha}I_g$. Since $P$ is an increasing, convex function and $W(u) \geqq |V(u)|_-$ we get for $\delta < 1/2$ that

$$\begin{aligned} 0 &\leqq P(W(u)) - P(|V(u)|_-) \leqq P'(W(u))(W(u) - |V(u)|_-) \\ &\leqq (K_1h^{-2}bW(u)^{1/2} + K_2h^{-3}W(u)^{3/2})[2\delta|V(u)|_- + h^{2\alpha}I_g]\,, \end{aligned} \tag{3.38}$$

where we have again used the estimate (3.9). Integrating (3.38) over the set where $|u| \leqq 2R + r$ and using Hölder's inequality we obtain the bound

$$\begin{aligned} &\int_{|u|\leq 2R+r} P(W(u)) - P(|V(u)|_-)du \\ &\leqq (\text{const.})\Bigg[h^{-2}b\left(\int_{|u|\leq 2R+r} W(u)^{3/2}du\right)^{1/3}(\delta\||V|_-\|_{3/2} + h^{2\alpha}I_g(2R+r)^2) \\ &\quad + h^{-3}\left(\int_{|u|\leq 2R+r} W(u)^{5/2}du\right)^{3/5}(\delta\||V|_-\|_{5/2} + h^{2\alpha}I_g(2R+r)^{6/5})\Bigg]\,. \end{aligned} \tag{3.39}$$

Combining (3.34), (3.35) and (3.39) we easily see that for $h$ small enough, depending on $R$ (and hence $\varepsilon$), $\delta$, $g$ and $V$, we have the lower bound

$$\begin{aligned} \sum_{j=1}^{N} e_j(h,b,V) \geqq & -\int P(|V(u)|_-)du - C\varepsilon((1+\delta^{-1/2})h^{-2}b + (1+\delta^{-3/2})h^{-3}) \\ & - C\delta(h^{-2}b + h^{-3})\,, \end{aligned}$$

where the constant $C$ depends only on $V$ and $g$. We can now choose first $\delta$ and then $\varepsilon$ to make the errors above as small as we please. We have thus shown that

$$\liminf_{h\to 0} \frac{\sum_j e_j(h,b,V)}{-\int P(|V(u)|_-)du} \geqq 1$$

uniformly in $b$. ■

*Remark.* In the application of Theorem 3.1 in Sect. V we shall need a slight generalization of this result. In fact, the potential $V$ there will depend on $h$ and $b$. As an inspection of the proof of Theorem 3.1 shows, the uniform limit in (3.8) is still valid if the dependence of $V$ on $h$ and $b$ satisfies the following conditions:

(i) The quantities $hb(1+hb)^{-1}\int|V|_-^{3/2}$ and $(1+hb)^{-1}\int|V|_-^{5/2}$ are bounded uniformly in $h$ and $b$.
(ii) For every $\varepsilon > 0$ there is an $R$ independent of $h$ and $b$ such that

$$hb(1+hb)^{-1}\int_{|x|\geq R}|V(x)|_-^{3/2}dx \leqq \varepsilon \quad \text{and} \quad (1+hb)^{-1}\int_{|x|\geq R}|V(x)|_-^{5/2}dx \leqq \varepsilon\,.$$

(iii) If $j_r(x) = r^{-3}j(x/r)$, where $0 \leqq j \in C_0^\infty(\mathbf{R}^3)$ with $\int j = 1$, then

$$hb(1+hb)^{-1}\int(|V|_- * j_r - |V|_-)^{3/2} \to 0 \quad \text{as} \quad r \to 0\,,$$

and

$$(1+hb)^{-1}\int(|V|_- * j_r - |V|_-)^{5/2} \to 0 \quad \text{as} \quad r \to 0\,,$$

uniformly in $h$ and $b$.

## IV. Thomas–Fermi Theory with a Magnetic Field

In this section we study the properties of the Thomas–Fermi theory for electrons moving in a magnetic field $\mathbf{B}$ and an exterior potential $V$. The most important case for atomic physics is that of spatially *uniform* $\mathbf{B}$, and $V$ of the form $V(x) = -\sum_{k=1}^{K} Z_k |x - X_k|^{-1}$ with $Z_k > 0$ and $X_k \in \mathbf{R}^3$ fixed. It is not substantially more difficult to develop the theory for more general potentials and nonuniform magnetic fields, and we shall do so below. One bonus of such a general treatment is that local properties of the electronic density and the magnetic moment can then be studied by considering local variations of the potential and the magnetic field.

We shall assume that the magnetic field is locally bounded, $\mathbf{B}(\cdot) \in L^\infty_{\text{loc}}(\mathbf{R}^3; \mathbf{R}^3)$. The exterior potentials we consider have the form $V = V_1 + V_2$ with $V_1 \in L_c^{5/2}$ ($L^{5/2}$ functions of compact support) and $V_2 \in L^\infty$ with $\sup_{|x| \geqq R} |V(x)| \to 0$ as $R \to \infty$. The energy functional is

$$\mathscr{E}[\rho; \mathbf{B}, V] = \int_{\mathbf{R}^3} \tau_{B(x)}(\rho(x))\, dx + \int_{\mathbf{R}^3} V(x)\rho(x)\, dx + D(\rho, \rho)\,, \tag{4.1}$$

where $D(f, g) = \frac{1}{2}\int\int f(x) g(y) |x - y|^{-1} dx\, dy$, $B(x) = |\mathbf{B}(x)|$, and $\tau_B$ is the energy density of a gas of noninteracting electrons in a uniform magnetic field of strength $B$. The density $\rho$ belongs to a class of nonnegative functions to be specified below.

We shall refer to the functional (4.1) as the *Magnetic Thomas–Fermi* (MTF) *functional.* When need arises to distinguish it from other functionals we shall write $\mathscr{E}^{\text{MTF}}$ instead of simply $\mathscr{E}$. Notice that $\mathscr{E}$ depends only on the intensity $B(\cdot)$ of the magnetic field, and is independent of its direction. Nevertheless, we shall retain the boldface $\mathbf{B}$ in the notation (4.1) for $\mathscr{E}$ while discussing inhomogeneous fields, but shift to the simpler $B$ in the latter part of this section when we specialize to homogeneous fields.

The functional (4.1) (with homogeneous $\mathbf{B}$ and $V(x) = -Z|x|^{-1}$) was introduced in [9] for spinless particles and extended to include the electron spin in [10]. It was also studied, together with some related theories, in [11] and has been applied to astrophysical problems, e.g., in [28–31]. The forerunner of (4.1) is the Thomas–Fermi theory for strong magnetic fields [6], that takes only the lowest Landau band into account. This theory, which will be called the STF theory below, is discussed in a number of references, e.g., in [8] and [32–36]. For other aspects and variants of magnetic Thomas–Fermi theory see [37–41].

The present section is devoted to the mathematical properties of Thomas–Fermi theory based on the functional (4.1). The discussion proceeds along similar lines to those in [19] and [42] for the case $B = 0$. We start by collecting some facts about the kinetic energy density $\tau_B(\rho)$ that replaces the simpler expression for the $B = 0$ case, i.e., $\frac{3}{5}(3\pi^2)^{2/3}\rho^{5/3}$.

**Properties of the Kinetic Energy.** The kinetic energy density $\tau_B$ is, by definition, the Legendre transform of the pressure $P_B$ given by (3.4), i.e.,

$$\tau_B(t) = \sup_{w \geqq 0} [tw - P_B(w)] \tag{4.2}$$

with

$$P_B(w) = \frac{B}{3\pi^2}\left( w^{3/2} + 2\sum_{\nu=1}^{\infty} |2\nu B - w|_-^{3/2} \right).$$

From the properties of $P_B$ it follows immediately that $t \mapsto \tau_B(t)$ is nonnegative, strictly convex and once continuously differentiable in $t$ with $\tau_B(0) = \tau_B'(0) = 0$. More explicitly, if $w(t) > 0$ is the unique solution to

$$P_B'(w(t)) = t\ , \tag{4.3}$$

for $t > 0$, then

$$\tau_B(t) = tw(t) - P_B(w(t))\ . \tag{4.4}$$

Conversely, $P_B$ is the Legendre transform of $\tau_B$, so

$$\tau_B'(t) = w(t)\ , \tag{4.5}$$

i.e., $\tau_B'$ is the inverse of $P_B'$. The pressure $P_B$ satisfies the scaling relation

$$P_{\alpha B}(w) = \alpha^{5/2} P_B(\alpha^{-1} w) \tag{4.6}$$

for $\alpha > 0$, which implies a similar relation for $\tau_B$,

$$\tau_{\alpha B}(t) = \alpha^{5/2} \tau_B(\alpha^{-3/2} t)\ . \tag{4.7}$$

Since $\tau_B(t)$ is continuous in $t$ it follows from (4.7) that it is also continuous in $B$. Equations (4.3)–(4.4) define $\tau_B$ only for $B \neq 0$, but in the limit $B \to 0$ the function $\tau_B$ is the kinetic energy density in zero magnetic field, i.e.,

$$\tau_0(t) := \frac{3}{5}\kappa_0 t^{5/3} \tag{4.8}$$

with $\kappa_0 = (3\pi^2)^{2/3}$. Note that $\tau_0(t)$ is the Legendre transform of the pressure $P_0(w) := \lim_{B \to 0} P_B(w) = (2/15\pi^2)\, w^{5/2}$. The energy functional of standard TF theory, $\mathscr{E}^{\mathrm{TF}}$, may thus be considered a special case of (4.1) with $\mathbf{B} \equiv 0$.

To investigate $\tau_B$ further we note first that

$$P_B'(w) = \frac{B}{2\pi^2} w^{1/2} \tag{4.9}$$

if $w \leqq 2B$. For large $w$ or small $B$, on the other hand, $P_B'$ is close to $P_0'(w) = \lim_{B \to 0} P_B'(w) = (1/3\pi^2) w^{3/2}$. The difference is conveniently estimated using the Poisson summation formula

$$\frac{1}{2}F(0) + \sum_{n=1}^{\infty} F(n) = \int_0^{\infty} F(x)dx + 2\mathrm{Re} \sum_{n=1}^{\infty} \int_0^{\infty} F(x) e^{i2\pi n x} dx\ , \tag{4.10}$$

which holds for all continuous, real valued, absolutely integrable functions $F$. Applying (4.10) to $F(x) = \left|x - \frac{w}{2B}\right|_-^{1/2}$ we obtain[7]

$$P'_B(w) = \frac{1}{3\pi^2}w^{3/2} + B^{3/2}\frac{1}{2^{1/2}\pi^3}\sum_{n=1}^{\infty}\frac{1}{n^{3/2}}$$

$$\times\left[\sin\left(\frac{n\pi w}{B}\right)C\left(\left(\frac{2nw}{B}\right)^{1/2}\right) - \cos\left(\frac{n\pi w}{B}\right)S\left(\left(\frac{2nw}{B}\right)^{1/2}\right)\right], \quad (4.11)$$

where $C$ and $S$ are the Fresnel integrals

$$C(x) = \int_0^x \cos(\pi t^2/2)\,dt \quad \text{and} \quad S(x) = \int_0^x \sin(\pi t^2/2)dt\,.$$

In deriving (4.11) from (4.10) we used the identity

$$\int_0^a x^{1/2}e^{-i2\pi nx}dx = \frac{1}{i4\pi n^{3/2}}\int_0^{2(na)^{1/2}} e^{-i\pi t^2/2}dt - \frac{1}{i2\pi n}a^{1/2}e^{-i2\pi na}\,, \quad (4.12)$$

which may be obtained by partial integration.

From (4.11) and the limit relation $\lim_{x\to\infty}S(x) = \lim_{x\to\infty}C(x) = \frac{1}{2}$ we find that

$$|P'_B(w) - P'_0(w)| \leqq 0.03\,B^{3/2}\,, \quad (4.13)$$

with $0.03 \approx 2^{-3/2}\pi^{-3}\zeta(\frac{3}{2}) = \lim_{v\to\infty}|P'_1(2v) - P'_0(2v)|$. The oscillating terms under the sum in (4.11) are responsible for the de Haas–van Alphen effect in the electron gas.

Equations (4.9) and (4.13) lead easily to some estimates on $\tau_B$ that we list in the following lemma. (Recall that $\tau'_B$ is the inverse of $P'_B$.) Pictures of $\tau'_B$ and $\tau_B$ can be found in [11], Fig. 4.

**4.1 Lemma (Estimates on $\tau_B$).**

(i) *For all $B$ and $t \geqq 0$,*

$$\tau'_B(t) \leqq \kappa_1 t^{2/3} \quad \textit{and hence} \quad \tau_B(t) \leqq \frac{3}{5}\kappa_1 t^{5/3} \quad (4.14)$$

*with $\kappa_1 = (4\pi^2)^{2/3}$.*

(ii) *For $t \leqq \frac{1}{\sqrt{2}\pi^2}B^{3/2}$,*

$$\tau_B(t) = \kappa_2\frac{t^3}{B^2} \quad (4.15)$$

*with $\kappa_2 = 4\pi^4/3$.*

(iii) *For $t \geqq \frac{1}{\sqrt{2}\pi^2}B^{3/2}$ one has*

$$0.83\kappa_0 t^{2/3} \leqq \tau'_B(t) \quad \textit{and hence} \quad \kappa_3 t^{5/3} \leqq \tau_B(t) \quad (4.16)$$

*with $\kappa_3 = 0.83\frac{3}{5}\kappa_0$.*

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[7] We thank Einar Gudmundsson for pointing out to us that $P'_B$ can be written in this way. See also [43, 44 and 45]

(iv) *For all $B$ and $t \geqq 0$,*

$$|\tau_B'(t) - \tau_0'(t)| \leqq (0.07\pi^{4/3})B^{3/2}t^{-1/3}$$

*and hence*

$$|\tau_B(t) - \tau_0(t)| \leqq (0.11\pi^{4/3})B^{3/2}t^{2/3}\ . \tag{4.17}$$

(v) *For all $B$ and $t \geqq 0$,*

$$t\tau_B'(t) \leqq 3\tau_B(t) \quad \textit{and} \quad \left|\tau_B(t) - \frac{3}{5}t\tau_B'(t)\right| \leqq (0.14\pi^{4/3})B^{3/2}t^{2/3}\ . \tag{4.18}$$

*Proof.* (i) The function $\tau_B'$ is the inverse of $P_B'$, so (4.14) is equivalent to $P_B'(w) \geqq (w/\kappa_1)^{3/2}$. For $w \leqq 2B$ this inequality follows from (4.9); for $w \geqq 2B$ we use (4.13).

(ii) Since $t \leqq \frac{1}{\sqrt{2}\pi^2}B^{3/2} =: t_*(B)$ is equivalent to $w \leqq 2B$, this follows immediately from (4.9).

(iii) This follows from (4.13), using that $w \geqq 2B$ for $t \geqq t_*(B)$ .

(iv) For $t \leqq t_*(B)$ the assertion follows from (4.15), so let us assume that $t \geqq t_*(B)$. From (4.13) we obtain $|t - \frac{1}{3\pi^2}\tau_B'(t)^{3/2}| \leqq 0.03B^{3/2}$, which implies $(3\pi^2 t)^{2/3}(1 - 0.03B^{3/2}/t)^{2/3} \leqq \tau_B'(t) \leqq (3\pi^2 t)^{2/3}(1 + 0.03B^{3/2}/t)^{2/3}$, and (4.17) follows because $|(1 + x)^{2/3} - 1| \leqq |x|$ for $|x| \leqq 1$.

(v) For $t \leqq t_*(B)$ we have $t\tau_B'(t) = 3\tau_B(t)$ by (4.15). For $t \geqq t_*(B)$ , the inequality $t\tau_B'(t) \leqq 3\tau_B(t)$ follows from (4.14) and (4.16). The second inequality in (4.18) follows from (4.17), because $|\tau_B(t) - \frac{3}{5}t\tau_B'(t)| \leqq |\tau_B(t) - \tau_0(t)| + \frac{3}{5}t|\tau_0'(t) - \tau_B'(t)|$. ■

Using (4.14)–(4.16) we can establish some inequalities that will be used repeatedly in the sequel. If $\Omega \subset \mathbf{R}^3$ is any bounded, measurable set we introduce the decomposition $\Omega = \Omega_1 \cup \Omega_2$ with

$$\Omega_1 = \{x \in \Omega \mid \rho(x) > 2^{-1/2}\pi^{-2}B(x)^{3/2}\}$$

and

$$\Omega_2 = \{x \in \Omega \mid \rho(x) \leqq 2^{-1/2}\pi^{-2}B(x)^{3/2}\}\ .$$

From (4.16) we obtain for any nonnegative, measurable function $\rho$

$$\int_\Omega \rho(x)^{5/3}dx \leqq \frac{1}{\kappa_3}\int_{\Omega_1} \tau_{B(x)}(\rho(x))dx + \kappa_4\|B\|_{\Omega_2}^{5/2}\mathrm{Vol}(\Omega_2) \tag{4.19}$$

with $\|B\|_{\Omega_2} = \sup\{|\mathbf{B}(x)|\,|\,x \in \Omega_2\}$ and $\kappa_4 = 2^{-5/6}\pi^{-10/3}$. Using the Hölder inequality $\|\rho\|_{5/3} \leqq \|\rho\|_3^{3/5}\|\rho\|_1^{2/5}$ and (4.15) we obtain another estimate:

$$\int_\Omega \rho(x)^{5/3}dx$$
$$\leqq \frac{1}{\kappa_3}\int_{\Omega_1} \tau_{B(x)}(\rho(x))dx + \frac{1}{\kappa_2}\|B\|_{\Omega_2}^{2/3}\left(\int_{\Omega_2}\rho(x)dx\right)^{2/3}\left(\int_{\Omega_2}\tau_{B(x)}(\rho(x))dx\right)^{1/3}\ . \tag{4.20}$$

The inequality (4.19) has the advantage of being independent of $\int\rho$, whereas (4.20) has the virtue of not involving the volume of $\Omega$.

**Properties of the MTF Functional.** We begin our study of the functional (4.1) by considering its domain of definition. This domain consists of the following class of measurable functions:

$$\mathscr{C}_{\mathbf{B}} := \{\rho \mid \rho \geqq 0, \int\rho(x)dx < \infty, \int\tau_{B(x)}(\rho(x))dx < \infty, D(\rho,\rho) < \infty\}\ . \tag{4.21}$$

**4.2 Proposition (Domain of $\mathscr{E}$).** (i) *If $\rho, \rho' \in \mathscr{C}_{\mathbf{B}}$ and $s, s' \geqq 0$, then $s\rho + s'\rho' \in \mathscr{C}_{\mathbf{B}}$. Thus $\mathscr{C}_{\mathbf{B}}$ is a convex cone.*
(ii) *If $\mathbf{B}(\cdot), \mathbf{B}'(\cdot) \in L^{\infty}_{\mathrm{loc}}(\mathbf{R}^3; \mathbf{R}^3)$, and either $|\mathbf{B}'(x)| = \alpha|\mathbf{B}(x)|$ with $\alpha > 0$, or $\mathbf{B}'(x) = \mathbf{B}(x) + \mathbf{B}_1(x)$ with $\mathbf{B}_1$ of compact support, then $\mathscr{C}_{\mathbf{B}'} = \mathscr{C}_{\mathbf{B}}$.*
(iii) *For all $\mathbf{B} \in L^{\infty}_{\mathrm{loc}}$,*

$$L^{5/3}(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) \cap \{\rho|\rho \geqq 0\} \subset \mathscr{C}_{\mathbf{B}} \subset L^{5/3}_{\mathrm{loc}}(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) \cap \{\rho \,|\, \rho \geqq 0\} .$$

*If $\mathbf{B}$ is uniformly bounded, then $\mathscr{C}_{\mathbf{B}} = L^{5/3}_{\mathrm{loc}}(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) \cap \{\rho \,|\, \rho \geqq 0\}$.*

*Proof*: (i) The conditions $\rho \geqq 0, \int\rho < \infty$ and $D(\rho, \rho) < \infty$ obviously define a convex cone. If $\rho, \rho' \in \mathscr{C}_{\mathbf{B}}$ and $s + s' \leqq 1$ with $s, s' \geqq 0$, then $\int\tau_B(s\rho + s'\rho)$ is finite by convexity and *monotonicity of $t \mapsto \tau_B(t)$*. Furthermore, by (4.18) we have

$$\frac{d}{ds}\tau_B(st) = t\tau_B'(st) \leqq 3s^{-1}\tau_B(st) ,$$

and thus

$$\tau_B(st) \leqq s^3\tau_B(t)$$

for $s \geqq 1$. Hence $\mathscr{C}_{\mathbf{B}}$ is a convex cone.

(ii) The case $|\mathbf{B}'| = \alpha|\mathbf{B}|$ is dealt with by means of the scaling relation (4.7), the case $\mathbf{B}' = \mathbf{B} + \mathbf{B}_1$ by noting that $\tau_{B(x)}(\rho(x))$ and $\tau_{B'(x)}(\rho(x))$ differ only for $x$ in the support of $\mathbf{B}_1$.

(iii) By (4.14), $\tau_B(t) \leqq (\text{const.})t^{5/3}$ uniformly in $\mathbf{B}$, and Young's inequality implies that

$$D(\rho, \rho) \leqq (\text{const.})\,(\|\rho\|_1\|\rho\|_{5/3} + \|\rho\|_1^2) .$$

Hence

$$L^{5/3}(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) \cap \{\rho|\rho \geqq 0\} \subset \mathscr{C}_{\mathbf{B}} .$$

By (4.20), $\int_\Omega\rho^{5/3}$ is bounded for all $\rho \in \mathscr{C}_{\mathbf{B}}$ and all $\Omega$ such that $\|B\|_\Omega < \infty$. Hence $\mathscr{C}_{\mathbf{B}} \subset L^{5/3}_{\mathrm{loc}}(\mathbf{R}^3)$ for all $\mathbf{B} \in L^{\infty}_{\mathrm{loc}}(\mathbf{R}^3)$, and $\mathscr{C}_{\mathbf{B}} \subset L^{5/3}(\mathbf{R}^3)$ if $\mathbf{B}$ is uniformly bounded. ∎

Since $\int V_1\rho$ is defined for all $\rho \in L^{5/3}_{\mathrm{loc}}(\mathbf{R}^3)$ and $V_1 \in L^{5/2}_c(\mathbf{R}^3)$, and since $\int V_2\rho$ is defined for $\rho \in L^1(\mathbf{R}^3)$ and $V_2 \in L^\infty(\mathbf{R}^3)$, it follows from Proposition 4.1(iii) that $\mathscr{E}[\rho; \mathbf{B}, V]$ is defined for all $\rho \in \mathscr{C}_{\mathbf{B}}$.

**4.3 Proposition (Convexity and Boundedness of $\mathscr{E}$).** *The functional $\rho \mapsto \mathscr{E}[\rho; \mathbf{B}, V]$ is strictly convex on $\mathscr{C}_{\mathbf{B}}$. It is bounded below on*

$$\mathscr{C}_{\mathbf{B},N} := \{\rho \in \mathscr{C}_{\mathbf{B}} \,|\int\rho \leqq N\}$$

*for all $N < \infty$. If $V(x) = O(|x|^{-1})$ at infinity, then $\mathscr{E}$ is bounded below uniformly on $\mathscr{C}_{\mathbf{B}}$ for each fixed $\mathbf{B}$ and $V$.*

*Proof.* The first term in (4.1) is strictly convex because $t \mapsto \tau_B(t)$ is strictly convex, the second term is linear, and the quadratic form $\rho \mapsto D(\rho, \rho)$ is strictly convex. Hence $\mathscr{E}$ is strictly convex in $\rho$.

To establish a lower bound for $\mathscr{E}$ on $\mathscr{C}_{\mathbf{B},N}$ we may ignore the positive term $D(\rho, \rho)$. Write $V = V_1 + V_2$ with $V_1 \in L^{5/2}(\mathbf{R}^3)$ of compact support $\Omega$, and with $V_2 \in L^\infty(\mathbf{R}^3)$. We have

$$\int V_2(x)\rho(x)dx \geqq -N\|V_2\|_\infty$$

and

$$\int V_1(x)\,\rho(x)\,dx \geqq -\|V_1\|_{5/2}\left(\int_\Omega \rho^{5/3}dx\right)^{3/5} .$$

By the estimate (4.19), the right side of the last inequality is bounded below by

$$-\ (\text{const.})\left[\int_\Omega \tau_{B(x)}(\rho(x))dx + \|B\|_\Omega^{5/2}\cdot \mathrm{Vol}(\Omega)\right]^{3/5} \|V_1\|_{5/2} ,$$

which is controlled by the kinetic energy $\int \tau_{B(x)}(\rho(x))dx$. Hence $\mathscr{E}$ is bounded below on $\mathscr{C}_{\mathbf{B},N}$.

If $|V(x)| \leqq Z/|x|$ for large $|x|$ we may use the inequality

$$-\int_{|x|\geqq R}\frac{Z\rho(x)}{|x|} + \frac{1}{2}\int_{|x|\geqq R}\int_{|y|\geqq R}\frac{\rho(x)\rho(y)}{|x-y|}dx\,dy \geqq -\frac{Z^2}{2R}$$

(cf. [42], Theorem II.3) to replace the estimate on $\int V_2\rho$ by an $N$-independent estimate on $\int V_2\rho + D(\rho,\rho)$. Hence, in this case, $\mathscr{E}$ is bounded below on $\mathscr{C}_{\mathbf{B}}$, uniformly in $N$. ■

The *Thomas–Fermi energy* corresponding to $\mathscr{E}$ is defined as

$$E(N,\mathbf{B},V) := \inf\{\mathscr{E}[\rho;\mathbf{B},V]\,|\,\rho\in\mathscr{C}_{\mathbf{B},N}\} . \tag{4.22}$$

**4.4 Proposition.** *$E(N, B, V)$ is nonincreasing and convex as a function of $N$ for fixed* **B** *and $V$. Moreover,*

$$E(N,\mathbf{B},V) = \inf\{\mathscr{E}[\rho;\mathbf{B},V]\,|\,\rho\in\mathscr{C}_{\mathbf{B}}, \textstyle\int\rho = N\} .$$

*Proof.* Since **B** and $V$ are fixed we omit them from the notation. Since $\mathscr{C}_N \subset \mathscr{C}_{N'}$ for $N < N'$, $E$ is obviously nonincreasing. Let $\varepsilon > 0$ be given and choose $\rho_\varepsilon\in\mathscr{C}_N$, $\rho'_\varepsilon\in\mathscr{C}_{N'}$ with $|\mathscr{E}[\rho_\varepsilon] - E(N)| < \varepsilon$ and $|\mathscr{E}[\rho'_\varepsilon] - E(N')| < \varepsilon$. Then, for $0 \leqq t \leqq 1$, we have $t\rho_\varepsilon + (1-t)\,\rho'_\varepsilon\in\mathscr{C}_{tN+(1-t)N'}$, and

$$\begin{aligned} E(tN+(1-t)N') &\leqq \mathscr{E}[t\rho_\varepsilon + (1-t)\rho'_\varepsilon] \leqq t\mathscr{E}[\rho_\varepsilon] + (1-t)\mathscr{E}[\rho'_\varepsilon] \\ &\leqq tE(N) + (1-t)E(N') + 2\varepsilon . \end{aligned}$$

Hence $N\mapsto E(N)$ is convex. The last statement of our proposition is a consequence of the assumption that $V(x)\to 0$ as $x\to\infty$ and the $B$-independent upper bound $\tau_{\mathbf{B}}(t) \leqq (\text{const.})t^{5/3}$ for the kinetic energy. Because of this, one can always add charges far away from the origin in such a way that the energy change is arbitrarily small. ■

We shall later discuss the dependence of $E$ on **B**, but for the moment we note that $E$ has a simple scaling behavior. Suppose one scales the charge density,

$$\rho(x) \to \rho_a(x) := a^2\rho(a^{1/3}x) ,$$

with $a > 0$, so that $N\to aN$. If at the same time

$$\mathbf{B}(x)\to \mathbf{B}_a(x) := a^{4/3}\mathbf{B}(a^{1/3}x) ,$$

$$V(x)\to V_a(x) := a^{1/3}V(a^{1/3}x) ,$$

then

$$\mathscr{E}[\rho;\mathbf{B},V]\to \mathscr{E}[\rho_a;\mathbf{B}_a,V_a] = a^{7/3}\mathscr{E}[\rho;\mathbf{B},V] . \tag{4.23}$$

In particular we have the following **scaling relation for the energy**:

$$E(aN, \mathbf{B}_a, V_a) = a^{7/3} E(N, \mathbf{B}, V) . \tag{4.24}$$

**4.5 Theorem (Existence and Uniqueness of a Minimizer).** *There is a unique* $\rho = \rho_{N,\mathbf{B},V} \in \mathscr{C}_{\mathbf{B},N}$ *with* $\mathscr{E}[\rho_{N,\mathbf{B},V}; \mathbf{B}, V] = E(N, \mathbf{B}, V)$.

*Proof.* The uniqueness is a consequence of strict convexity, so we have only to prove existence. Let $\rho^{(n)}$ be a sequence in $\mathscr{C}_{\mathbf{B},N}$ with $\mathscr{E}[\rho^{(n)}; \mathbf{B}, V] \to E(N, \mathbf{B}, V)$. We have

(a) $\int \tau_B(\rho^{(n)})$ is bounded in $n$, since $\mathscr{E}[\rho; \mathbf{B}, V] - \frac{1}{2}\int \tau_B(\rho)$ is bounded below on $\mathscr{C}_{\mathbf{B},N}$ by Proposition 4.3. By (4.19) this implies that $\int_\Omega \rho^{(n)5/3}$ is bounded for all compact $\Omega \subset \mathbf{R}^3$.

(b) $D(\rho^{(n)}, \rho^{(n)})$ is bounded in $n$, since $\mathscr{E}[\rho; \mathbf{B}, V] - \frac{1}{2}D(\rho, \rho)$ is bounded below on $\mathscr{C}_{\mathbf{B},N}$, again by the argument of Proposition 4.3.

Let $\Omega_\nu \subset \Omega_{\nu+1}$ be an increasing sequence of compact sets exhausting $\mathbf{R}^3$. By (a), $\rho^{(n)}$ is a bounded sequence in the reflexive Banach space $L^{5/3}(\Omega_\nu)$ for each $\nu$. Using the Banach–Alaoglu theorem for each of these spaces and a Cantor diagonalization procedure we conclude that there is a function, $\rho^{(\infty)} \in L^{5/3}_{\text{loc}}(\mathbf{R}^3)$, and a subsequence, again denoted by $\rho^{(n)}$, that converges weakly to $\rho^{(\infty)}$ in $L^{5/3}(\Omega_\nu)$ for all $\nu$. In order to prove the theorem it is sufficient to show that $\rho^{(\infty)} \in \mathscr{C}_{\mathbf{B},N}$, and

$$\liminf_n \mathscr{E}[\rho^{(n)}; \mathbf{B}, V] \geqq \mathscr{E}[\rho^{(\infty)}; \mathbf{B}, V] ,$$

because then $\rho^{(\infty)}$ has the required properties of a minimizer. We note first that clearly $\rho^{(\infty)} \geqq 0$. From (4.14) one easily deduces that the convex functional

$$f \mapsto \int_\Omega \tau_B(|f|)$$

is strongly continuous on $L^{5/3}(\Omega)$ for all compact $\Omega$ and hence weakly lower semicontinuous on this space by Mazur's theorem. It follows that

$$\int_\Omega \tau_B(\rho^{(\infty)}) \leqq \liminf_n \int_\Omega \tau_B(\rho^{(n)}) \leqq \liminf_n \int_{\mathbf{R}^3} \tau_B(\rho^{(n)}) ,$$

and hence

$$\int_{\mathbf{R}^3} \tau_B(\rho^{(\infty)}) \leqq \liminf_n \int_{\mathbf{R}^3} \tau_B(\rho^{(n)}) .$$

Let $\chi_\Omega$ denote the characteristic function of a compact set $\Omega$. Since $D(f,f) \leqq (\text{const.})(\|f\|_1 \|f\|_{5/3} + \|f\|_1^2)$, one sees that $f \mapsto D(f\chi_\Omega, f\chi_\Omega)$ is continuous on $L^{5/3}(\Omega)$. By an argument analogous to that above, using that $\rho^{(\infty)} \geqq 0$, we obtain

$$D(\rho^{(\infty)}, \rho^{(\infty)}) \leqq \liminf_n D(\rho^{(n)}, \rho^{(n)}) .$$

For a given $\varepsilon > 0$ we can write $V = V_1 + V_2$ with $V_1 \in L^{5/2}$ having support in the set $\{x \,|\, |x| \leqq R\}$ and with $\sup_{|x| \geqq R} |V_2(x)| < \varepsilon/N$. By the weak convergence of $\rho^{(n)}$ in $L^{5/3}_{\text{loc}}(\mathbf{R}^3)$, the sequence $\int V_1 \rho^{(n)}$ converges to $\int V_1 \rho^{(\infty)}$. Moreover, $|\int V_2 \rho| < \varepsilon N^{-1} \int_{|x| \geqq R} \rho < \varepsilon$. Hence $\lim_{n\to\infty} \int V \rho^{(n)} = \int V \rho^{(\infty)}$.

To complete the proof it remains to show that $\int \rho^{(\infty)} \leqq N$. Suppose on the contrary that $\int \rho^{(\infty)} > N$. Then $\int_\Omega \rho^{(\infty)} > N$ for some compact set $\Omega$, and since the characteristic function of $\Omega$ belongs to $L^{5/2}(\Omega)$, this would contradict the weak convergence of $\rho^{(n)}$ in $L^{5/3}(\Omega)$. ∎

Next we discuss the question when the minimizing $\rho \in \mathscr{C}_{\mathbf{B},N}$ satisfies $\int \rho = N$ and solves the variational equation for the functional $\mathscr{E}$. Define

$$N_c(\mathbf{B}, V) := \sup\{N \mid E(N, \mathbf{B}, V) < E(N', \mathbf{B}, V) \text{ for all } N' < N\} . \qquad (4.25)$$

**4.6 Proposition (Critical Particle Number).** *The function $N \mapsto E(N, \mathbf{B}, V)$ is strictly convex for $N < N_c$. If $N \leqq N_c$, then the minimizer $\rho_{N,\mathbf{B},V} \in \mathscr{C}_{\mathbf{B},N}$ satisfies $\int \rho_{N,\mathbf{B},V} = N$. If $N > N_c$, then $\rho_{N,\mathbf{B},V} = \rho_{N_c,\mathbf{B},V}$.*

*Proof.* As in Proposition 4.3 we omit $\mathbf{B}$ and $V$ from the notation. Strict convexity of $E$ for $N < N_c$ follows from the existence of a minimizer for all $N$ and the strict convexity of $\mathscr{E}$, since $\rho_{N'} \neq \rho_N$ for $N' < N \leqq N_c$. Suppose $\int \rho_N = N' < N \leqq N_c$. Then $\mathscr{E}[\rho_N] \geqq E(N') > E(N)$, which contradicts the definition of $\rho_N$. Suppose $N > N_c$ and $\rho_N \neq \rho_{N_c}$. Then $E\left(\dfrac{N + N_c}{2}\right) \leqq \mathscr{E}\left[\dfrac{\rho_N + \rho_{N_c}}{2}\right] < \frac{1}{2}E(N) + \frac{1}{2}E(N_c) \leqq E(N_c)$ by strict convexity of $\mathscr{E}$, which contradicts the definition of $N_c$. ∎

**4.7 Theorem (Thomas–Fermi Equation).** *If $N \leqq N_c$, then the minimizing density $\rho \in \mathscr{C}_{\mathbf{B}}$ with $\int \rho = N$ satisfies the Thomas–Fermi equation*

$$\tau'_{B(x)}(\rho(x)) = |V(x) + \rho * |x|^{-1} + \mu|_- \qquad (4.26)$$

*for some (unique) $\mu = \mu(N, \mathbf{B}, V) \geqq 0$. Conversely, if $\rho$ and $\mu$ satisfy* (4.26) *with $\rho \in \mathscr{C}_{\mathbf{B}}$, then $\rho$ minimizes $\mathscr{E}$ on $\mathscr{C}_{\mathbf{B},N}$ with $N = \int \rho$, and $\mu = \mu(N, \mathbf{B}, V)$. If $N = N_c$, then $\mu = 0$.*

**4.8 Theorem (Chemical Potential).** *$E(N, \mathbf{B}, V)$ is continuously differentiable as a function of $N$ with $\partial E/\partial N = -\mu$ if $N \leqq N_c$, and $\partial E/\partial N = 0$ if $N \geqq N_c$.*

These theorems can be proved in the same way as Theorems 4.6 and 4.7 in [19], cf. also [42], Theorem II.10.

The Thomas–Fermi equation (4.26) can be written in another form. By (4.3)–(4.5) the inverse of $\tau'_B$ is $P'_B$, so (4.26) is equivalent to

$$\rho(x) = P'_{B(x)}(|V_{\text{eff}}(x)|_-) , \qquad (4.27)$$

where the *effective potential*, $V_{\text{eff}}$, corresponding to $\rho \in \mathscr{C}_{\mathbf{B}}$ and $\mu \geqq 0$, is defined by

$$V_{\text{eff}}(x) = V(x) + \rho * |x|^{-1} + \mu . \qquad (4.28)$$

By the definition (4.4) of $\tau_{\mathbf{B}}$, the solution of (4.27) satisfies

$$P_{B(x)}(|V_{\text{eff}}(x)|_-) = \rho(x)|V_{\text{eff}}(x)|_- - \tau_{B(x)}(\rho(x)) .$$

Since by (4.26), $V_{\text{eff}}(x) \geqq 0$ implies $\rho(x) = 0$, this may equivalently be written as

$$-P_{B(x)}(|V_{\text{eff}}(x)|_-) = \tau_{B(x)}(\rho(x)) + V_{\text{eff}}(x)\rho(x) . \qquad (4.29)$$

Upon integration over $x$, this formula (for homogeneous $B$) provides the link between the Thomas–Fermi energy functional and the semiclassical expression (3.3) for the negative spectrum of $H_{\mathbf{A}} + V_{\text{eff}}$.

So far we have only assumed that $V \in L_c^{5/2} + L^\infty$ with $V(x) \to 0$ at $\infty$. For the next result we consider potentials of a more specific form.

**4.9 Theorem (Maximum Charge).** (i) *Suppose* $V(x)$ *has the form*

$$V(x) = -\int \frac{dM(y)}{|x-y|} + V_0(x), \tag{4.30}$$

*where* $dM$ *is a nonnegative measure of compact support, and* $V_0 \in L_c^{5/2} + L^\infty$ *satisfies* $|V_0(x)| \leqq C/|x|$ *for* $|x| \geqq R$ *with some* $C, R < \infty$. *Then* $N_c \geqq Z - C$, *where* $Z = \int dM$. *In particular, if* $|x| V_0(x) \to 0$ *for* $|x| \to \infty$, *then* $N_c \geqq Z$.

(ii) *Suppose* $V(x)$ *has the form in* (4.30) *with* $V_0 \geqq 0$, $V_0 \in L_c^{5/2} + L^\infty$ *tending to* 0 *at* $\infty$ *and in which* $dM$ *is a nonnegative measure of compact support having the following properties: The set* $D = \{x \mid \int |x-y|^{-1} dM(y) = \infty\}$ *is a closed set of Lebesgue measure zero, and the potential* $x \mapsto \int |x-y|^{-1} dM(y)$ *is continuous on* $\mathbf{R}^3 \backslash D$. *Then* $N_c \leqq Z$.

*Proof.* (i) Suppose $N_c < Z - C$, so that the absolute minimizer $\rho$ of $\mathscr{E}$ satisfies $\int \rho < Z - C - \varepsilon$ with some $\varepsilon > 0$. Put

$$\psi(x) = \int \frac{dM(y) - \rho(y) dy}{|x-y|},$$

and if $f$ is a function on $\mathbf{R}^3$ let $[f](r)$ denote the mean value of $f$ over the surface of a sphere of radius $r$ around the origin. For $r$ sufficiently large we have

$$[\psi - V_0](r) \geqq \frac{Z - \int \rho - C}{r} \geqq \frac{\varepsilon}{r}.$$

Being an absolute minimizer $\rho$ satisfies the TF equation (4.26) with $\mu = 0$,

$$\tau_B'(\rho) = |-\psi + V_0|_- .$$

Since $\tau_B'(\rho) \leqq \kappa_1 \rho^{2/3}$ by (4.14), it follows that

$$[\rho](r) \geqq \frac{\varepsilon}{\kappa_1^{3/2}} \cdot \frac{1}{r^{3/2}},$$

which contradicts the integrability of $\rho$ on $\mathbf{R}^3$.

(ii) Let $\rho$ be a solution to the TF equation

$$\tau_B'(\rho) = |-\psi + V_0 + \mu|_-$$

with $\psi$ as above and $\mu \geqq 0$. We claim that $\psi(x) \geqq 0$ for all $x$. Indeed, the set $A = \{x \mid \psi(x) < 0\}$ is open and does not intersect the set $D$ by our assumptions on $dM$. Moreover, because $V_0 \geqq 0$ and $\mu \geqq 0$ it follows from the TF equation that $\rho = 0$ on $A$. Hence $-\Delta\psi/4\pi = -\rho + dM = dM \geqq 0$ on $A$, so $\psi$ is superharmonic on $A$. It therefore takes its infimum on the boundary of $A$, where $\psi = 0$. Since $\psi < 0$ on $A$ this shows that $A$ is empty and $\psi(x) \geqq 0$ everywhere. Since $\lim_{r \to \infty} r[\psi](r) = \int dM - \int \rho$ it follows that $\int \rho \leqq Z$. ∎

Theorem 4.9 implies in particular that the maximum number of electrons that can be bound by a potential of the form

$$V(x) = -\sum_{k=1}^{K} \frac{Z_k}{|x - X_k|}, \tag{4.31}$$

with $Z_k > 0$, $X_k \in \mathbf{R}^3$, is $N_c = Z := \sum_k Z_k$. In other words, *negative ions do not exist in* MTF *theory.*

A result of a similar nature is the following *no-binding theorem* which asserts that molecules are unstable with respect to splitting into isolated atoms if the nuclear repulsion is taken into account. The proof is the same as in Theorem 3.23 in [19].

**4.10 Theorem (No Binding).** *Let $V$ be of the form* (4.31) *with $K \geqq 2$ and, for $1 \leqq n < K$, write $V = V^{(1)} + V^{(2)}$ with $V^{(1)}(x) = -\sum_{k=1}^{n} Z_k|x - X_k|^{-1}$. Let*

$$\tilde{E}(N, \mathbf{B}, V) := E(N, \mathbf{B}, V) + \sum_{1 \leqq i < j \leqq K} Z_i Z_j |X_i - X_j|^{-1}$$

*be the total energy including the nuclear repulsion, and in the same way define the energy of the separate parts*

$$\tilde{E}(N_1, \mathbf{B}, V^{(1)}) := E(N_1, \mathbf{B}, V^{(1)}) + \sum_{1 \leqq k < l \leqq n} Z_k Z_l |X_k - X_l|^{-1}$$

*and*

$$\tilde{E}(N_2, \mathbf{B}, V^{(2)}) := E(N_2, \mathbf{B}, V^{(2)}) + \sum_{n+1 \leqq p < q \leqq K} Z_p Z_q |X_p - X_q|^{-1}.$$

*Then for all $N$*

$$\tilde{E}(N, \mathbf{B}, V) \geqq \min_{N_1 + N_2 = N} \{\tilde{E}(N_1, \mathbf{B}, V^{(1)}) + \tilde{E}(N_2, \mathbf{B}, V^{(2)})\} .$$

Although magnetic Thomas–Fermi theory, like any other theory of Thomas–Fermi type, does not exhibit molecular binding, it shows preliminary signs of an enhanced binding due to the magnetic field that becomes dramatic in the region of super-strong fields. By this we mean the following. In standard TF theory (without a magnetic field) not only is it impossible to lower the energy of a molecule by bringing the nuclei closer together, but the energy is even a *strictly decreasing function of the nuclear separation* [18]. In the presence of a magnetic field, on the other hand, atoms have a finite radius in Thomas–Fermi theory as we shall prove below. This observation was first made in [9] for the Strong TF theory of Region 3 (defined in (4.36) and (4.45)) with a constant magnetic field, but it is also true in regions 2, 3, 4, 5 (in Regions 4 and 5, "finite radius" refers to directions perpendicular to **B**). As a consequence, magnetic Thomas–Fermi theory admits "zero pressure" states, in which the atoms are far enough apart so that their supports are nonoverlapping. If we pass to the region of hyper-strong fields, $B \gg Z^3$, we have a large "negative pressure". In other words, molecules are strongly bound; the binding energy of a diatomic molecule (for $Z \to \infty$) is six times as large as the ground state energy of each individual atom [1].

We now state a general theorem about the radius of molecules in magnetic Thomas–Fermi theory. If $\rho$ is the minimizer for $\mathscr{E}$ with $\int \rho \leqq N$ we define

$$R_{\max} = R_{\max}(N, \mathbf{B}, V) := \inf\{R \,|\, \rho(x) = 0 \text{ a.e. for } |x| \geqq R\} .$$

**4.11 Theorem (Finite Radius).** *Assume that the potential $V$ is of the form* (4.30) *with $V_0 \in L^{5/2}(\mathbf{R}^3)$ of compact support and, furthermore, that the magnetic field strength satisfies $B(x) \geqq B_0$ for some constant $B_0 > 0$. Let $0 \leqq R_0 < \infty$ be the smallest radius for which $dM$ and $V_0$ are supported in the ball $\{x \,|\, |x| \leqq R_0\}$ and for which $V(x) \geqq -2B_0$ for $|x| = R_0$. Then*

$$R_{\max} \leqq \max\{5R_0, 3.8\pi^{2/5} R_0^{1/5} B_0^{-1/5}\} .$$

*In particular, for the atomic potential* $V(x) = -Z/|x|$ *we obtain*

$$R_{\max} \leqq \max\left\{\frac{5}{2}ZB_0^{-1}, 3.3\pi^{2/5}Z^{1/5}B_0^{-2/5}\right\}. \tag{4.32}$$

*Proof.* Because of the support properties of $V_0$ and $dM$ the effective potential satisfies $-(4\pi)^{-1}\Delta V_{\text{eff}}(x) = \rho(x)$ when $|x| \geqq R_0$. Thus $V_{\text{eff}}$ is superharmonic on the set $\{x \| x| \geqq R_0\}$. Since $V_{\text{eff}}(x) \geqq V(x) \geqq -2B_0$ on the boundary of this set and $V(x)$ tends to 0 as $|x| \to \infty$ we conclude, using the superharmonicity, that $V_{\text{eff}}(x) \geqq -2B_0R_0/|x|$ for all $|x| \geqq R_0$. Since $B(x) \geqq B_0$ we get from (4.9) that $P'_{B(x)}(|V_{\text{eff}}|_-) = (2\pi^2)^{-1}B(x)|V_{\text{eff}}(x)|_-^{1/2}$ for such $x$. We can therefore write the TF equation (4.26) for $|x| \geqq R_0$ as

$$-\Delta V_{\text{eff}}(x) = 4\pi\rho(x) = 2\pi^{-1}B(x)|V_{\text{eff}}(x)|_-^{1/2}. \tag{4.33}$$

We now pick an $R > R_0$ and compare $-V_{\text{eff}}$ with the function

$$f_R(x) = \frac{B_0^2}{36\pi^2}\begin{cases}(R-|x|)^4, & \text{if } |x| \leqq R\\ 0 & \text{otherwise}\end{cases}.$$

We compute $\Delta(R-|x|)^4 = 12(R-|x|)^2 - 8|x|^{-1}(R-|x|)^3 \leqq 12(R-|x|)^2$ if $|x| \leqq R$. Thus we have for all $|x| > 0$ that $\Delta f_R(x) \leqq 2\pi^{-1}B_0 f_R(x)^{1/2}$. Notice that $\Delta f_R$ is continuous at $|x| = R$. If for some $0 < \delta < 1$ we choose $R = \max\{\delta^{-1}R_0, 72\pi^2B_0^{-1}R_0\delta^{-1}(1-\delta)^{-4}\}$, we shall prove that for $|x| \geqq \delta R$, $V_{\text{eff}}(x) \geqq -f_R(x)$. Since $f_R(x) = 0$ for $|x| \geqq R$ the statement of the theorem then follows from (4.33) by choosing $\delta = 1/5$. Let $\Omega$ be the set $\{|x| \geqq \delta R | V_{\text{eff}}(x) < -f_R(x)\}$. We have to to show that $\Omega$ is empty. First we prove that $\Omega$ is an open set with $V_{\text{eff}}(x) = -f_R(x)$ on its boundary $\partial\Omega$. Since $|V_{\text{eff}}(x)|_- \to 0$ as $|x| \to \infty$ we only have to show that $V_{\text{eff}}(x) \geqq -f_R(x)$ for $|x| = \delta R$. By the choice of $R$, $\delta R \geqq R_0$, and hence for $|x| = \delta R$ we have

$$V_{\text{eff}}(x) \geqq -2B_0R_0/(\delta R) \geqq -(36\pi^2)^{-1}B_0^2(1-\delta)^4R^4 = -f_R(x),$$

where we have again used the choice of $R$. On the open set $\Omega$ we have $\Delta(V_{\text{eff}} + f_R(x)) \leqq 2\pi^{-1}B(x)(-|V_{\text{eff}}(x)|_-^{1/2} + f_R(x)^{1/2}) \leqq 0$. Hence $V_{\text{eff}}(x) + f_R(x)$ is a negative superharmonic function on $\Omega$ and since it is zero on the boundary we conclude that $\Omega$ must be empty. The atomic estimate (4.32) follows from the observation that $R_0 = Z/(2B_0)$ if $V(x) = -Z|x|^{-1}$. ■

As mentioned above, the existence of neutral zero pressure molecular states is a simple consequence of this theorem.

**4.12 Corollary (Existence of Zero Pressure Molecular States).** *Assume that* **B** *satisfies the same conditions as in Theorem* 4.11. *Then the neutral* MTF *molecular energy,*

$$\tilde{E}(N, B, V) = E(N, \mathbf{B}, V) + \sum_{1\leqq k<l\leqq K} Z_kZ_l|X_k - X_l|^{-1},$$

*with $V$ as in* (4.31) *and $N = \sum_k Z_k$, is independent of the positions $X_k$, $k = 1, \ldots, K$ of the nuclei as long as the smallest nuclear separation $\min_{k\neq l}|X_k - X_l|$ is greater than twice the largest atomic radius $2\max_k R_{\max}(Z_k, \mathbf{B}, -Z_k|\cdot|^{-1})$.*

*Proof.* Let $\rho_k$, $k = 1, \ldots, K$ be the (atomic) minimizer for $\mathscr{E}[\cdot, \mathbf{B}, V_k]$ with $\int \rho_k = Z_k$, where $V_k = -Z_k|x - X_k|^{-1}$. By Theorem 4.11 the densities $\rho_k$, $k = 1, \ldots, K$ have disjoint supports if the nuclear separation is as stated. Moreover, by uniqueness, $\rho_k$ is spherically symmetric about $X_k$. By Newton's Theorem we compute

$$\mathscr{E}\left[\sum_k \rho_k; \mathbf{B}, V\right] + \sum_{k<l} Z_k Z_l |X_k - X_l|^{-1} = \sum_k E(Z_k, \mathbf{B}, V_k) .$$

We can now either appeal to the no-binding Theorem 4.10 to conclude that $\rho = \sum_k \rho_k$ is the minimizer for $\mathscr{E}[\cdot; \mathbf{B}, V]$ with $\int \rho = \sum_k Z_k$, or we could arrive at the same conclusion by again applying Newton's Theorem to show that $\rho$ is indeed the solution to the corresponding TF equation with $\mu = 0$. ■

We now discuss the behavior of the energy $E$ as a functional of the magnetic field $\mathbf{B}(\cdot)$. We first consider continuity and differentiability of $\tau_B(\rho)$ with respect to $B$.

**4.13 Lemma.** (i) *For fixed $t$, $B \mapsto \tau_B(t)$ is differentiable in $B$ with*

$$\frac{d}{dB}\tau_B(t) = \frac{5}{2B}\left[\tau_B(t) - \frac{3}{5}t\tau_B'(t)\right] \tag{4.34}$$

*for $B \neq 0$, and $d\tau_B(t)/dB|_{B=0} = 0$.*
(ii) *For all $B$, $B_0$, $t \geqq 0$,*

$$|\tau_B(t) - \tau_{B_0}(t)| \leqq (\text{const.})|B^{3/2} - B_0^{3/2}|\, t^{2/3} . \tag{4.35}$$

*Proof.* (i) Differentiability at $B \neq 0$ and the formula (4.34) follow from the scaling relation (4.7) and differentiability of $t \mapsto \tau_1(t)$. If $B = 0$ the statement follows from Eq. (4.17).

(ii) If $B = 0$ or $B_0 = 0$, Eq. (4.35) is just Eq. (4.17). If $B, B_0 > 0$, we write

$$\tau_B(t) - \tau_{B_0}(t) = \int_{B_0}^{B} \frac{d}{dB'}\tau_{B'}(t)dB'$$

and use (4.34) and (4.18). ■

**4.14 Proposition (Continuity in B).** *If $|\mathbf{B}(\cdot)| \to |\mathbf{B}_0(\cdot)|$ in $L^\infty_{\text{loc}}(\mathbf{R}^3)$, then $E(N, \mathbf{B}, V) \to E(N, \mathbf{B}_0, V)$ and $\mu(N, \mathbf{B}, V) \to \mu(N, \mathbf{B}_0, V)$. Moreover, the minimizing density $\rho_{N,\mathbf{B},V}$ converges to $\rho_{N,\mathbf{B}_0,V}$ weakly in $L^{5/3}_{\text{loc}}$.*

*Proof.* Since $N$ and $V$ are fixed, they will be omitted in the notation. Let $\chi_R$ denote the characteristic function of $\{x \,|\, |x| \leqq R\}$. Since $V$ tends to zero at infinity we can, for each $\varepsilon > 0$, find a radius $R$ such that $\bar\rho_{\mathbf{B}} := \rho_{\mathbf{B}}\chi_R$ and $\bar\rho_{\mathbf{B}_0} := \rho_{\mathbf{B}_0}\chi_R$ satisfy

$$E(\mathbf{B}) \leqq \mathscr{E}[\bar\rho_{\mathbf{B}}; \mathbf{B}] \leqq E(\mathbf{B}) + \varepsilon$$

and

$$E(\mathbf{B}_0) \leqq \mathscr{E}[\bar\rho_{\mathbf{B}_0}; \mathbf{B}_0] \leqq E(\mathbf{B}_0) + \varepsilon .$$

Now we have

$$\begin{aligned} E(\mathbf{B}_0) &\leqq \mathscr{E}[\bar\rho_{\mathbf{B}}; \mathbf{B}_0] = \mathscr{E}[\bar\rho_{\mathbf{B}}; \mathbf{B}] + \int_{|x| \leqq R} (\tau_{B_0}(\rho_B) - \tau_B(\rho_B)) \\ &\leqq E(\mathbf{B}) + \varepsilon + (\text{const.}) \sup_{|x| \leqq R} |B(x)^{3/2} - B_0(x)^{3/2}| N^{2/3} R , \end{aligned}$$

where we have used the previous lemma. Interchanging $\mathbf{B}$ and $\mathbf{B}_0$ we obtain an estimate in the other direction. The convergence of the energies is thus proved. Since $E$ is convex and differentiable in $N$, the chemical potentials $\mu(N, \mathbf{B}, V) = -\partial E(N, \mathbf{B}, V)/\partial N$ also converge if $B(x) \to B_0(x)$ in $L^\infty_{\text{loc}}(\mathbf{R}^3)$.

Convergence of the densities follows in a standard way by considering perturbations of the potential of the form $\alpha U$ with $U \in L_c^{5/2}$ and $\alpha \in \mathbf{R}$. Let $E(\mathbf{B}, \alpha)$ denote the energy with $V$ replaced by $V + \alpha U$. By the Feynman–Hellmann argument (see Theorem II.16 in [42]), $E(\mathbf{B}, \alpha)$ is differentiable in $\alpha$ with $\partial E(\mathbf{B}, \alpha)/\partial\alpha|_{\alpha=1} = \int \rho_{\mathbf{B}} U$. Moreover, $E(\mathbf{B}, \alpha)$ is concave in $\alpha$ (since it is an infimum over linear functions of $\alpha$), so convergence of $E(\mathbf{B}, \alpha)$ entails convergence of the derivatives $\partial E(\mathbf{B}, \alpha)/\partial \alpha$. ■

**The Strong Field Limit of MTF.** We shall now discuss the behavior of $E(N, \mathbf{B}, V)$ for large $\mathbf{B}$. We do this by comparing the energy with the result of another TF theory, which we refer to as the *Strong Thomas–Fermi* (STF) *theory*, whose energy functional, $\mathscr{E}^{\text{STF}}[\rho; \mathbf{B}, V]$, is defined as in (4.1), but with $\tau_B$ replaced by

$$\tau_B^{\text{STF}}(t) := \kappa_2 \frac{t^3}{B^2} \tag{4.36}$$

with $\kappa_2 = 4\pi^4/3$. The energy density $\tau_B^{\text{STF}}$ is obtained by taking only the lowest Landau level of the free electron gas into account. We shall prove that in the strong field limit, when $\mathbf{B}$ is replaced by $\alpha\mathbf{B}$ with $\alpha \to \infty$, the energy defined with $\mathscr{E}$ approaches the energy defined with $\mathscr{E}^{\text{STF}}$ after a suitable scaling.

The domain of definition of the functional $\mathscr{E}^{\text{STF}}$ is

$$\mathscr{C}_{\mathbf{B}}^{\text{STF}} = \left\{ \rho \,\middle|\, \rho \geqq 0, \int \rho(x)\, dx < \infty, D(\rho, \rho) < \infty, \int \frac{\rho(x)^3}{B(x)^2} dx < \infty \right\}. \tag{4.37}$$

We note that $\rho(x) = 0$ a.e. where $\mathbf{B}(x) = 0$ if $\rho \in \mathscr{C}_{\mathbf{B}}^{\text{STF}}$. The proof of the next proposition is straightforward.

**4.15 Proposition (Domain of $\mathscr{E}^{\text{STF}}$).** *The domain $\mathscr{C}_{\mathbf{B}}^{\text{STF}}$ is contained in $\mathscr{C}_{\mathbf{B}} \cap L^3_{\text{loc}}(\mathbf{R}^3)$. If $\mathbf{B}$ is uniformly bounded away from 0 then*

$$\mathscr{C}_{\mathbf{B}}^{\text{STF}} \supset L^3(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) \cap \{\rho \,|\, \rho \geqq 0\}\,.$$

*If $\mathbf{B}$ is uniformly bounded, then*

$$\mathscr{C}_{\mathbf{B}}^{\text{STF}} \subset L^3(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) \cap \{\rho \,|\, \rho \geqq 0\}\,.$$

*Consequently, if $\mathbf{B}$ is both bounded away from zero and uniformly bounded, then*

$$\mathscr{C}_{\mathbf{B}}^{\text{STF}} = L^3(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) \cap \{\rho \,|\, \rho \geqq 0\}\,.$$

Because of the stronger increase of $\tau_B^{\text{STF}}(t)$ with $t$, the class of acceptable exterior potentials is larger than for $\tau_B$. For $\tau_B^{\text{STF}}$ we can allow $V = V_1 + V_2$ with $V_1 \in L_c^{3/2}$, $V_2 \in L^\infty$ and $V \to 0$ as $|x| \to \infty$. When comparing $\mathscr{E}^{\text{STF}}$ with $\mathscr{E}$ we shall, however, assume that $V$ is in the smaller class appropriate to $\mathscr{E}$.

The results of Proposition 4.1 through Corollary 4.12 for $\mathscr{C}_{\mathbf{B}}$ and $\mathscr{E}$ all hold *mutatis mutandis* for $\mathscr{C}_{\mathbf{B}}^{\text{STF}}$ and $\mathscr{E}^{\text{STF}}$ with one minor exception: To ensure that

$$E^{\text{STF}}(N, \mathbf{B}, V) := \inf\{\mathscr{E}^{\text{STF}}[\rho; \mathbf{B}, V] \,|\, \int \rho \leqq N\}$$

is equal to

$$\inf\{\mathscr{E}^{\text{STF}}[\rho; \mathbf{B}, V] \,|\, \int \rho = N\}$$

one must assume that $\mathbf{B}$ is uniformly bounded away from 0, since otherwise we cannot be sure that the kinetic energy does not blow up when we remove excess charge to spatial $\infty$. The proofs for $\mathscr{E}^{\mathrm{STF}}$ are even simpler than for $\mathscr{E}$, since the energy density $\tau_B^{\mathrm{STF}}$ has a simpler form than $\tau_B$.

The functional $\mathscr{E}^{\mathrm{STF}}$ has the same scaling behavior as $\mathscr{E}$ with respect to the transformations $\rho(x) \to a^2\rho(a^{1/3}x)$, $\mathbf{B}(x) \to a^{4/3}\mathbf{B}(a^{1/3}x)$, $V(x) \to a^{4/3}V(a^{1/3}x)$, but in addition $\mathscr{E}^{\mathrm{STF}}$ can be scaled independently in $\mathbf{B}$ with $\int\rho$ fixed: For $\alpha > 0$ define

$$\mathbf{B}_\alpha(x) := \alpha\mathbf{B}(\alpha^{2/5}x) ,$$

$$V_\alpha(x) := \alpha^{2/5}V(\alpha^{2/5}x) ,$$

$$\rho_\alpha(x) := \alpha^{6/5}\rho(\alpha^{2/5}x) .$$

(This should not be confused with the transformation $\mathbf{B}(x) \to \mathbf{B}_a(x) = a^{4/3}\mathbf{B}(a^{1/3}x)$ etc. discussed earlier.) Then one has

$$\mathscr{E}^{\mathrm{STF}}[\rho_\alpha; \mathbf{B}_\alpha, V_\alpha] = \alpha^{2/5}\mathscr{E}^{\mathrm{STF}}[\rho; \mathbf{B}, V] , \tag{4.38}$$

and consequently

$$E^{\mathrm{STF}}(N, \mathbf{B}_\alpha, V_\alpha) = \alpha^{2/5}E^{\mathrm{STF}}(N, \mathbf{B}, V) . \tag{4.39}$$

**4.16 Proposition (Strong Field Limit).** *For each fixed* $\mathbf{B}$, $V$ *and* $N$, *the scaled energy* $\alpha^{-2/5}E(N, \mathbf{B}_\alpha, V_\alpha)$ *is a monotonically increasing function of* $\alpha$ *that converges to* $E^{\mathrm{STF}}(N, \mathbf{B}, V)$ *as* $\alpha \to \infty$ (i.e., $E(N, \mathbf{B}_\alpha, V_\alpha)/E^{\mathrm{STF}}(N, \mathbf{B}_\alpha, V_\alpha) \to 1$ *as* $\alpha \to \infty$). *Moreover,* $\rho_\alpha$ *converges weakly in* $L^{5/3}_{\mathrm{loc}}(\mathbf{R}^3)$ *to the minimizer* $\rho_\infty = \rho^{\mathrm{STF}}$ *of* $\mathscr{E}^{\mathrm{STF}}$ *with* $\int\rho^{\mathrm{STF}} \leqq N$.

*Proof.* If $\rho \in \mathscr{C}_\mathbf{B}$, then $\rho_\alpha \in \mathscr{C}_{\mathbf{B}_\alpha}$ by Proposition 4.1(ii). The only $\alpha$-dependent term in $\alpha^{-2/5}\mathscr{E}[\rho_\alpha, \mathbf{B}_\alpha, V_\alpha]$ is $\alpha^{9/10}\int\tau_{B(x)}(\alpha^{-3/10}\rho(x))dx$. For convenience, define $t = \alpha^{3/10}$ and consider

$$\frac{d}{dt}t^3\int\tau_B(t^{-1}\rho(x))dx = t^2\int[3\tau_B(t^{-1}\rho(x)) - \tau'_B(t^{-1}\rho(x))]dx .$$

By (4.18), this is positive, which proves monotonicity of $\alpha^{-2/5}\mathscr{E}[\rho_\alpha; \mathbf{B}_\alpha, V_\alpha]$ in $\alpha$ for fixed $\rho$. This, in turn, implies monotonicity of $\alpha^{-2/5}E(N, \mathbf{B}_\alpha, V_\alpha)$.

Define, with $t = \alpha^{3/10}$ as before,

$$\mathscr{E}_t[\rho; \mathbf{B}, V] := t^3\int\tau_{B(x)}(t^{-1}\rho(x))dx + \int V(x)\rho(x)dx + D(\rho, \rho) .$$

Then $\alpha^{-2/5}\mathscr{E}[\rho_\alpha; \mathbf{B}_\alpha, V_\alpha] = \mathscr{E}_t[\rho; \mathbf{B}, V]$. Let $\rho^{(t)}$ be the unique minimizer of $\mathscr{E}_t$ with $\int\rho^{(t)} \leqq N$, i.e., $\rho^{(t)}(x) = t^{-4}\rho(t^{-4/3}x)$, where $\rho$ is the minimizer of $\mathscr{E}$ with $\mathbf{B}_\alpha$ and $V_\alpha$. For each $\varepsilon > 0$, one can find $R < \infty$ (independent of $t$) such that

$$\mathscr{E}_t[\rho^{(t)}\chi_R] \leqq \mathscr{E}_t[\rho^{(t)}] + \varepsilon .$$

Define

$$\tilde{\rho}^{(t)}(x) = \begin{cases} 0 & \text{if } \rho^{(t)}(x) > \kappa t B(x)^{3/2} \\ \rho^{(t)}(x)\chi_R(x) & \text{if } \rho^{(t)}(x) \leqq \kappa t B(x)^{3/2} \end{cases}$$

with $\kappa = 2^{1/2}\pi^{-2}$. Then $\tilde{\rho}^{(t)} \in \mathscr{C}_\mathbf{B}^{\mathrm{STF}}$, and because of (4.15)

$$E^{\mathrm{STF}} \leqq \mathscr{E}^{\mathrm{STF}}[\tilde{\rho}^{(t)}] = \mathscr{E}_t[\tilde{\rho}^{(t)}] \leqq \mathscr{E}_t[\rho^{(t)}] + \varepsilon + \int\limits_{\rho^{(t)} > \kappa t B^{3/2}} |V(x)|\rho^{(t)}(x)\chi_R(x)dx .$$

To estimate the last term we use the TF equation (4.26) which, together with (4.16), implies that $\rho^{(t)}(x) \leqq t^{-2}|V(x)|^{3/2}$ if $\rho^{(t)}(x) > \kappa t B(x)^{3/2}$. Hence the last term is no larger than $t^{-2}\int_{|x|\leqq R}|V(x)|^{5/2}dx$, which goes to zero as $t \to \infty$. The convergence of $\rho_\alpha$ to $\rho^{\mathrm{STF}}$ follows from the convergence of the energies exactly as in Proposition 4.14. ■

**Homogeneous Fields.** In the remaining part of this section we focus attention on homogeneous magnetic fields. We establish some properties of the Thomas–Fermi energy and density that are important for the proof of the limit theorems in the next section.

According to (4.23)–(4.24) the MTF theory allows an exact simultaneous scaling of the potential $V$ and the magnetic field intensity $B$, and by Proposition 4.16 an approximate independent scaling of $B$ for large $B$. To account for both of these scalings we now consider potentials of the form

$$V_{Z,B}(x) = Z\ell^{-1}v(\ell^{-1}x)\,, \tag{4.40}$$

where $v \in L^{5/2} + L^\infty$ with $v(x) \to 0$ as $|x| \to \infty$, $Z > 0$, and the scale factor $\ell = \ell(Z, B) \leqq 1$ is a smooth function of $Z$ and $B$ with the behavior $\ell \sim Z^{-1/3}$ for $B \ll Z^{4/3}$ and $\ell \sim Z^{-1/3}(B/Z^{4/3})^{-2/5}$ for $B \gg Z^{4/3}$. One possible choice for $\ell$ is

$$\ell(Z, B) = Z^{-1/3}(1 + \beta)^{-2/5} \tag{4.41}$$

with $\beta = B/Z^{4/3}$. For convenience we keep this choice, but other possibilities could of course be discussed in the same way. In the atomic case, $v(x) = -|x|^{-1}$, and $V_{Z,B}(x) = -Z|x|^{-1}$ is independent of $B$.

In the following we regard $v$ as fixed. The MTF functional (4.1) depends on $B$ and $Z$ and we write

$$\mathcal{E}^{\mathrm{MTF}}_{B,Z}[\rho] = \int \tau_B(\rho(x))dx + \int V_{Z,B}(x)\rho(x)dx + D(\rho, \rho)\,. \tag{4.42}$$

The corresponding energy depends on $N$, $B$, $Z$:

$$E^{\mathrm{MTF}}(N, B, Z) = \inf\{\mathcal{E}^{\mathrm{MTF}}_{B,Z}[\rho] \mid \rho \in L^1 \cap L^{5/3}, \rho \geqq 0, \int\rho \leqq N\}\,. \tag{4.43}$$

Besides $\mathcal{E}^{\mathrm{MTF}}_{B,Z}$ we also consider the standard TF functional

$$\mathcal{E}^{\mathrm{TF}}_Z[\rho] = \frac{3}{5}\kappa_0\int\rho(x)^{5/3}dx + \int V_{Z,0}(x)\rho(x)dx + D(\rho, \rho) \tag{4.44}$$

with $\kappa_0 = (3\pi^2)^{2/3}$, and the TF functional for strong fields

$$\mathcal{E}^{\mathrm{STF}}_{B,Z}[\rho] = \frac{\kappa_2}{B^2}\int\rho(x)^3dx + \int V_{Z,B}(x)\rho(x)dx + D(\rho, \rho)\,, \tag{4.45}$$

with $\kappa_2 = 4\pi^4/3$. The corresponding energies are denoted by $E^{\mathrm{TF}}(N, Z)$ and $E^{\mathrm{STF}}(N, B, Z)$, respectively. In the same way we distinguish other quantities related to these functionals by the superscripts MTF, TF and STF. The scaling relations are

$$E^{\mathrm{TF}}(N, Z) = Z^{7/3}E^{\mathrm{TF}}(\lambda, 1)\,,$$

$$E^{\mathrm{MTF}}(N, B, Z) = Z^{7/3}E^{\mathrm{MTF}}(\lambda, \beta, 1)\,,$$

$$E^{\mathrm{STF}}(N, B, Z) = Z^{7/3}\beta^{2/5}E^{\mathrm{STF}}(\lambda, 1, 1)\,,$$

with $\lambda = N/Z$, $\beta = B/Z^{4/3}$. In order to extract an additional factor $(1+\beta)^{2/5}$ from $\mathscr{E}^{\mathrm{MTF}}$ we define

$$\hat{\mathscr{E}}_\beta[\rho] := \int \hat{\tau}_\beta(\rho(x))dx + \int v(x)\rho(x)dx + D(\rho,\rho) \tag{4.46}$$

with

$$\hat{\tau}_\beta(t) := (1+\beta)^{-8/5}\tau_\beta((1+\beta)^{6/5}t) = (1+\beta)^{2/5}\tau_{\beta(1+\beta)^{-4/5}}(t)\ , \tag{4.47}$$

where we have used (4.7). Notice that $\lim_{\beta\to 0}\hat{\tau}_\beta(t) = \tau_0(t) = \kappa_0 t^{5/3}$, with $\kappa_0 = 3(2\pi^2)^{2/3}/5$, is the kinetic energy density of standard TF theory at $B = 0$, and $\lim_{\beta\to\infty}\hat{\tau}_\beta(t) = \kappa_2 t^3 = \hat{\tau}_\infty(t)$, with $\kappa_2 = 4\pi^4/3$, is the kinetic energy of the STF theory at $B = 1$.

The energy corresponding to (4.46) is

$$\hat{E}(\lambda,\beta) = \inf\{\hat{\mathscr{E}}_\beta[\rho]\,|\,\rho\in L^1\cap L^{5/3}, \rho \geqq 0, \textstyle\int\rho \leqq \lambda\}\ . \tag{4.48}$$

We have

$$E^{\mathrm{MTF}}(N,B,Z) = Z^2\ell^{-1}\hat{E}(\lambda,\beta) = Z^{7/3}(1+\beta)^{2/5}\hat{E}(\lambda,\beta), \tag{4.49}$$

and the minimizers $\rho^{\mathrm{MTF}}_{N,B,Z}$ of $\mathscr{E}^{\mathrm{MTF}}_{B,Z}$ and $\rho_{\lambda,\beta}$ of $\hat{\mathscr{E}}_\beta$ are related by

$$\rho^{\mathrm{MTF}}_{N,B,Z}(x) = Z\ell^{-3}\rho_{\lambda,\beta}(\ell^{-1}x) = Z^2(1+\beta)^{6/5}\rho_{\lambda,\beta}(Z^{1/3}(1+\beta)^{2/5}x)\ . \tag{4.50}$$

The kinetic energy density $\hat{\tau}_\beta$ is the Legendre transform of the scaled pressure

$$\hat{P}_\beta(w) := (1+\beta)^{-8/5}P_\beta((1+\beta)^{2/5}w) = (1+\beta)^{-3/5}P_{\beta(1+\beta)^{-2/5}}(w) \tag{4.51}$$

(by the scalings (4.6) and (4.7)), i.e., if $\hat{P}'_\beta(w(t)) = t$, then $\hat{\tau}_\beta(t) = tw(t) - \hat{P}_\beta(w(t))$. The TF equation for $\rho_{\lambda,\beta}$ can be written in either of the equivalent forms

$$\hat{\tau}'_\beta(\rho_{\lambda,\beta}) = |v_{\mathrm{eff}}|_-\ , \tag{4.52}$$

or

$$\rho_{\lambda,\beta} = \hat{P}'_\beta(|v_{\mathrm{eff}}|_-)\ , \tag{4.53}$$

where the scaled effective potential is

$$v_{\mathrm{eff}}(x) = v(x) + \rho_{\lambda,\beta} * |x|^{-1} + \mu(\lambda,\beta)\ , \tag{4.54}$$

with $\mu(\lambda,\beta) = -\partial\hat{E}(\lambda,\beta)/\partial\lambda$. For later reference we note also the scaled form of (4.29):

$$-\hat{P}_\beta(|v_{\mathrm{eff}}|_-) = \hat{\tau}_\beta(\rho_{\lambda,\beta}(x)) + v_{\mathrm{eff}}(x)\,\rho_{\lambda,\beta}(x)\ . \tag{4.55}$$

For fixed $\beta$, $\mu(\lambda,\beta)$ is a nonnegative, decreasing function of $\lambda$, and $\mu$ takes the value 0 if and only if the critical particle number $\lambda_c(\beta) = \sup\{\lambda|\mu(\lambda,\beta) > 0\} = N_c(B, V_{Z,B})/N$ is finite. Then $\mu(\lambda_c(\beta),\beta) = 0$. Moreover, for all $\lambda \geqq 0$,

$$\int\rho_{\lambda,\beta}(x)dx = \min\{\lambda, \lambda_c(\beta)\}\ .$$

For Coulomb potentials $\lambda_c(\beta)$ is finite and independent of $\beta$ by Theorem 4.9.

We now study the properties of $\hat{E}(\lambda,\beta)$ and $\mu(\lambda,\beta)$ as functions of $\beta$ for fixed $\lambda$.

**4.17 Proposition (Uniform Bounds on the Energy).** *For fixed $\lambda$, $\hat{E}(\lambda,\beta)$ and $\mu(\lambda,\beta)$ are continuous functions of $\beta$ with*

$$\lim_{\beta\to 0}\hat{E}(\lambda,\beta) = E^{\mathrm{MTF}}(\lambda,0,1) = E^{\mathrm{TF}}(\lambda,1)\ ,$$

$$\lim_{\beta\to\infty}\hat{E}(\lambda,\beta) = \lim_{\beta\to\infty}\beta^{-2/5}E^{\mathrm{MTF}}(\lambda,\beta,1) = E^{\mathrm{STF}}(\lambda,1,1)$$

*and*

$$\lim_{\beta\to 0}\mu(\lambda,\beta)=\mu^{\mathrm{TF}}(\lambda,1) \quad \text{and} \quad \lim_{\beta\to\infty} = \mu^{\mathrm{STF}}(\lambda,1,1)\,.$$

*In particular, $|\hat{E}(\lambda,\beta)|$ is uniformly bounded in $\beta$. Moreover, the three parts of the energy,*

$$\hat{T}_{\lambda,\beta}:=\int\hat{\tau}_\beta(\rho_{\lambda,\beta}),\quad \hat{A}_{\lambda,\beta}:=\int v\rho_{\lambda,\beta},\quad \hat{R}_{\lambda,\beta}:=D(\rho_{\lambda,\beta},\rho_{\lambda,\beta})$$

*are all bounded in absolute value uniformly in $\beta$ for $\lambda$ fixed.*

*If $v<0$ on a set of positive measure, and $\lambda>0$, then $\hat{E}(\lambda,\beta)$ is bounded away from zero uniformly in $\beta$:*

$$\hat{E}(\lambda,\beta)\leqq -c_\lambda \tag{4.56}$$

*for some $c_\lambda>0$.*

*Proof.* Continuity of $\hat{E}$ and the limit relations follow from Propositions 4.14 and 4.16 (with trivial modifications due to slightly different scaling). The uniform lower bound on $\hat{E}(\lambda,\beta)$ is an immediate consequence. The bounds on $\hat{T}_{\lambda,\beta}$, $\hat{A}_{\lambda,\beta}$ and $\hat{R}_{\lambda,\beta}$ follow by considering first the energy functional with $\hat{\tau}_\beta$ replaced by $\frac{1}{2}\hat{\tau}_\beta$, then with $D(\rho,\rho)$ replaced by $\frac{1}{2}D(\rho,\rho)$ and finally $v$ replaced by $\frac{1}{2}v$.

To obtain an upper bound on $\hat{E}(\lambda,\beta)$ strictly less than zero we note that $\hat{\tau}_\beta(t)\leqq(\text{const.})(1+\beta)^{2/5}t^{5/3}$ for all $\beta$ by (4.14), and $\lim_{\beta\to\infty}\hat{E}(\lambda,\beta)=E^{\mathrm{STF}}(\lambda,1,1)$ is the Thomas–Fermi energy with kinetic term $\tau(\rho)=\kappa_2\rho^3$. Hence it suffices to prove that the Thomas–Fermi energy, with $\tau(\rho)$ either of the form $k\rho^{5/3}$ or $k\rho^3$, $k>0$, is bounded away from zero for every $\lambda>0$. By convexity and monotonicity of the energy in $\lambda$ it is sufficient to show this for one $\lambda$. Suppose on the contrary that the energy is 0 for all $\lambda$. Then $\mu=0$ for all $\lambda$, and the TF equation becomes $\tau'(\rho)=|v+\rho*|x|^{-1}|_-$. It is clear that $\rho=0$ is not a solution if $v<0$ on a set of positive measure. ■

In view of the last proposition it is natural to include the limiting cases $\beta=0$ and $\beta=\infty$ in the definitions (4.43)–(4.45). Thus we define $\hat{E}(\lambda,0):=\lim_{\beta\to 0}\hat{E}(\lambda,\beta)=E^{\mathrm{TF}}(\lambda,1)$ and $\hat{E}(\lambda,\infty):=\lim_{\beta\to\infty}\hat{E}(\lambda,\beta)=E^{\mathrm{STF}}(\lambda,1,1)$. Note that $\hat{E}(\lambda,0)$ corresponds to the kinetic energy density (4.8), i.e. $\hat{\tau}_0(t)=\tau_0(t)=(3\kappa_0/5)t^{5/3}$, and $\hat{E}(\lambda,\infty)$ corresponds to

$$\hat{\tau}_\infty(t):=\lim_{\beta\to\infty}\hat{\tau}_\beta(t)=(4\pi^4/3)t^3\,. \tag{4.57}$$

Next we consider some properties of the minimizers $\rho_{\lambda,\beta}$. As above, $\beta=0$ and $\beta=\infty$ label the minimizers of the functional (4.46) with kinetic energy $\tau_0$ and $\hat{\tau}_\infty$, respectively.

**4.18 Proposition (Uniform Bounds on the Density).** *Let $\lambda=N/Z$ be fixed.*

(i) *$\|\rho_{\lambda,\beta}\|_1$ and $\|\rho_{\lambda,\beta}\|_{5/3}$ are uniformly bounded in $\beta$.*
(ii) *If $0\leqq\beta_0\leqq\infty$ and $\beta\to\beta_0$, then $\rho_{\lambda,\beta}\rightharpoonup\rho_{\lambda,\beta_0}$ weakly in $L^{5/3}_{\mathrm{loc}}(\mathbf{R}^3)$.*
(iii) *If $j_r(x)=r^{-3}j(x/r)$, where $0\leqq j\in C_0^\infty(\mathbf{R})$ satisfies $\int j(x)dx=1$, then*

$$D(\rho_{\lambda,\beta}-\rho_{\lambda,\beta}*j_r,\rho_{\lambda,\beta}-\rho_{\lambda,\beta}*j_r)\to 0$$

*uniformly in $\beta$ as $r\to 0$.*

*Proof.* (i) The uniform $L^1$-bound is trivial because $\int\rho_{\lambda,\beta}\leqq\lambda$ by definition of $\rho_{\lambda,\beta}$. For the $L^{5/3}$ bound we note that by (4.20) and scaling we have for $\rho\in L^1\cap L^{5/3}$

with $\int\rho \leqq \lambda$,

$$\int\rho^{5/3} \leqq (\text{const.})\left[(1+\beta)^{-2/5}\hat{T}_\beta(\rho) + \lambda^{2/3}\left(\frac{\beta}{1+\beta}\right)^{2/3}\hat{T}_\beta(\rho)^{1/3}\right], \qquad (4.58)$$

where $\hat{T}_\beta(\rho) := \int\hat{\tau}_\beta(\rho)$. If $\rho = \rho_{\lambda,\beta}$ it follows from Proposition 4.17 that $\|\rho_{\lambda,\beta}\|_{5/3}$ is uniformly bounded in $\beta$.

(ii) Convergence of the densities follows from the convergence of the energies according to Proposition 4.17 in the same way as in Proposition 4.14.

(iii) Write

$$D(\rho - \rho * j_r, \rho - \rho * j_r) = (\text{const.})\int|\hat{\rho}(p)|^2(1-\hat{j}(rp))^2|p|^{-2}dp\ ,$$

where $\hat{f}(p) = \int e^{ipx}f(x)\,dx$ denotes the Fourier transform. By Hölder's inequality this can be bounded from above by

$$(\text{const.})\left(\int|\hat{\rho}(p)|^{5/2}dp\right)^{4/5}\left(\int(1-\hat{j}(rp))^{10}|p|^{-10}dp\right)^{1/5}.$$

The first factor is bounded by (const.) $\|\rho\|_{5/3}^2$ by the Hausdorff–Young inequality. Now $\hat{j}$ is smooth with $\hat{j}(0) = 1$. Hence $|1-\hat{j}(p)| = (\text{const.})|p|$ for small $|p|$, and

$$\int(1-\hat{j}(rp))^{10}|p|^{-10}dp = r^7\int(1-\hat{j}(p))^{10}|p|^{-10}dp = (\text{const.})r^7\ .$$

Altogether we thus obtain

$$D(\rho_{\lambda,\beta} - \rho_{\lambda,\beta} * j_r, \rho_{\lambda,\beta} - \rho_{\lambda,\beta} * j_r) \leqq \text{const.}\|\rho_{\lambda,\beta}\|_{5/3}^2 r^{7/5}\ ,$$

and $\|\rho_{\lambda,\beta}\|_{5/3}$ is uniformly bounded in $\beta$ by (i). ■

Finally, we consider the effective potential $v_{\text{eff}}$ defined by (4.54). It depends on $\lambda$ and $\beta$ through $\rho_{\lambda,\beta}$ and $\mu(\lambda,\beta)$. In order to apply the semiclassical Theorem 3.1 to prove the limit theorem in the next section, we need uniform estimates on $v_{\text{eff}}$, cf. the Remark following Theorem 3.1.

**4.19 Proposition (Uniform Bounds on the Effective Potential).** *Let $\lambda$ be fixed.*

(i) *The norms $\||v_{\text{eff}}|_-\|_{3/2}$ and $\||v_{\text{eff}}|_-\|_{5/2}$ are bounded uniformly in $\beta$.*

(ii) *For each $\varepsilon > 0$ there is a radius $R$ independent of $\beta$ such that $\int_{|x|\geqq R}|v_{\text{eff}}(x)|_-^p dx \leqq \varepsilon$ for $p = 3/2$ and $p = 5/2$.*

(iii) *If $j_r$ is as in Proposition* 4.18 (iii), then *$|v_{\text{eff}}|_- * j_r \to |v_{\text{eff}}|_-$ in $L^{3/2}$ and $L^{5/2}$, uniformly in $\beta$ as $r \to 0$.*

*Proof.* Since $|v_{\text{eff}}|_- \leqq |v|_-$ and $|v|_- \in L^{5/2}_{\text{loc}} \subset L^{3/2}_{\text{loc}}$ by assumption, statement (ii) implies (i). To prove (ii), we note first that $\hat{P}_\beta(w) \leqq w\hat{P}'_\beta(w)$ by convexity. From the TF equation $\hat{P}'_\beta(|v_{\text{eff}}|_-) = \rho_{\lambda,\beta}$ and the lower bound (3.9) we obtain the estimates

$$|v_{\text{eff}}|_-^{3/2} \leqq (\text{const.})\beta^{-1}(1+\beta)\,\rho_{\lambda,\beta}|v_{\text{eff}}|_- \qquad (4.59)$$

and

$$|v_{\text{eff}}|_-^{5/2} \leqq (\text{const.})(1+\beta)^{3/5}\rho_{\lambda,\beta}|v_{\text{eff}}|_-\ . \qquad (4.60)$$

If $\beta \geqq 1$, it follows from (4.59) that

$$\int_{|x|\geqq R}|v_{\text{eff}}|_-^{3/2} \leqq (\text{const.})\|\rho_{\lambda,\beta}\|_1 \sup_{|x|\geqq R}|v(x)|_-\ ,$$

and

$$\int_{|x|\geqq R}|v_{\text{eff}}|^{5/2} \leqq (\text{const.})\|\rho_{\lambda,\beta}\|_1 \sup_{|x|\geqq R}|v(x)|_-^2\ .$$

Since $\|\rho_{\lambda,\beta}\|_1 \leqq \lambda$ and $v \to 0$ at infinity, we have thus proved (ii) for $\beta \geqq 1$. Statement (ii) for $\beta \leqq 1$ and $p = 5/2$ follows in the same way from (4.60). The case $p = 3/2$, $\beta \leqq 1$ is a little more delicate. First we recall from Proposition 4.17 that for $\lambda$ fixed, $\mu(\lambda, \beta)$ is a continuous function of $\beta$. Hence there is a $\beta_0$ (possibly depending on $\lambda$), such that $\mu(\lambda, \beta_0) = \min_{\beta \in [0,1]} \mu(\lambda, \beta)$. If $\mu(\lambda, \beta_0) > 0$, we are done, for $v \to 0$ at $\infty$ implies that $|v(x) + \mu(\lambda, \beta_0)|_- = 0$ for $x$ outside a ball of finite radius, and $|v_{\text{eff}}|_- \leqq |v + \mu(\lambda, \beta)|_- \leqq |v + \mu(\lambda, \beta_0)|_-$. If $\mu(\lambda, \beta_0) = 0$ we argue as follows. By (4.14) we have $\hat{\tau}'_\beta(t) \leqq ct^{2/3}/$ with some $c < \infty$ for $\beta \leqq 1$. Consider the TF equation

$$c\tilde{\rho}^{2/3} = |v + \tilde{\rho} * |x|^{-1} + \mu|_- \, .$$

From Corollary 3.10 in [19] one easily deduces that it has a unique solution $\tilde{\rho}_\mu \in L_1$ for all $\mu \geqq 0$ with $\int \tilde{\rho}_0 \leqq \int \rho_{\lambda,\beta_0}$, because $\lambda_c(\beta_0) = \int \rho_{\lambda,\beta_0} < \infty$ and $\hat{\tau}'_{\beta_0}(t) \leqq ct^{2/3}$. Corollary 3.10 in [19] implies also that for all $\beta \geqq 0$,

$$\tilde{\rho}_{\mu(\lambda,\beta)} * |x|^{-1} \leqq \rho_{\lambda,\beta} * |x|^{-1} \, ,$$

and hence

$$|v(x) + \rho_{\lambda,\beta} * |x|^{-1} + \mu(\lambda, \beta)|_- \leqq |v(x) + \tilde{\rho}_{\mu(\lambda,\beta)} * |x|^{-1} + \mu(\lambda, \beta)|_- \, . \quad (4.61)$$

On the other hand, by Corollary 3.8 in [19] we have

$$|v(x) + \tilde{\rho}_\mu * |x|^{-1} + \mu|_- \leqq |v(x) + \tilde{\rho}_0 * |x|^{-1}|_-$$

for all $\mu > 0$. Combined with (4.58) and the TF equation for $\tilde{\rho}_0$ this gives the uniform bound

$$|v_{\text{eff}}(x)|_-^{3/2} \leqq |v(x) + \tilde{\rho}_0 * |x|^{-1}|_-^{3/2} \leqq c^{3/2} \tilde{\rho}_0(x) \, ,$$

which concludes the proof of (ii) because $\tilde{\rho}_0 \in L^1$.

We now consider statement (iii). Because of (ii) it suffices to prove that for all $R < \infty$, $\int_{|x| \leqq R} ||v_{\text{eff}}|_- - |v_{\text{eff}}|_- * j_r|^{5/2} \to 0$ uniformly in $\beta$ as $r \to 0$. By Jensen's inequality we have, since $\int j_r = 1$,

$$\int_{|x| \leqq R} ||v_{\text{eff}}|_- - |v_{\text{eff}}|_- * j_r|^{5/2} \leqq \int \left( \int_{|x| \leqq R} ||v_{\text{eff}}(x)|_- - |v_{\text{eff}}(x-y)|_-|^{5/2} dx \right) j_r(y) dy$$

$$\leqq \int \left( \int_{|x| \leqq R} ||v(x)|_- - |v(x-y)|_-|^{5/2} dx \right) j_r(y) dy$$

$$+ \int \|\rho_{\lambda,\beta} * [|\cdot|^{-1} - |\cdot - y|^{-1}]\|_{5/2}^{5/2} j_r(y) \, dy \, .$$

The first term converges to 0 because $v \in L^{5/2}_{\text{loc}}$. For the second term we use Young's inequality:

$$\|\rho_{\lambda,\beta} * [|\cdot|^{-1} - |\cdot - y|^{-1}]\|_{5/2}^{5/2} \leqq \|\rho_{\lambda,\beta}\|_1^{5/2} \cdot \||\cdot|^{-1} - |\cdot - y|^{-1}\|_{5/2}^{5/2}$$

$$\leqq \|\rho_{\lambda,\beta}\|_1^{5/2} \cdot (\text{const.}) |y|^{1/2} \, .$$

Hence the second term is no larger than $(\text{const.})\lambda^{5/2} r^{1/2}$. ■

## V. Magnetic Thomas–Fermi Theory as a Limit of Quantum Mechanics

We now consider the quantum mechanical Hamiltonian for $N$ electrons in a homogeneous magnetic field of strength $B$ and an exterior potential $V_{Z,B}$ as in (4.40), i.e.,

$$V_{Z,B}(x) = Z\ell^{-1}v(\ell^{-1}x) ,$$

with $v \in L^{5/2} + L^{\infty}$, $v(x) \to 0$ for $|x| \to \infty$. With $\mathbf{a}(x) = \frac{1}{2}(-x_2, x_1, 0)$ as in Sect. III we write the Hamiltonian as

$$H_{N,B,Z} = \sum_{i=1}^{N} \{[\boldsymbol{\sigma}_i \cdot (\mathbf{p}_i + B\mathbf{a}(x_i))]^2 + V_{Z,B}(x_i)\} + \sum_{i<j}^{N} |x_i - x_j|^{-1} . \tag{5.1}$$

It operates on wave functions $\psi \in \bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$. We define

$$E^Q(N, B, Z) = \inf_{\|\psi\|=1} \langle \psi | H_{N,B,Z} | \psi \rangle . \tag{5.2}$$

Clearly $E^Q = 0$ if $v \geqq 0$, and therefore we assume henceforth that $v < 0$ on a set of positive measure. Then $E^{\mathrm{MTF}}(N, B, Z) < 0$ by (4.56) and (4.49). Our main goal in this section is the following theorem.

**5.1 Theorem (Energy Asymptotics in Regions 1, 2, 3).** *If $Z \to \infty$ with $\lambda = N/Z$ fixed and $B/Z^3 \to 0$, then*

$$E^Q(N, B, Z)/E^{\mathrm{MTF}}(N, B, Z) \to 1 .$$

*Proof. Step 1* (*Scaling*). In order to move the scaling factors from the potential to the kinetic energy term in (5.1) we define a unitary operator $U_\ell$ on the wave functions by

$$(U_\ell \psi)(x_1, \ldots, x_N) = \ell^{-3N/2} \psi(\ell^{-1}x_1, \ldots, \ell^{-1}x_N) \tag{5.3}$$

with $\ell = Z^{-1/3}(1 + \beta)^{-2/5}$ as in (4.41). We have

$$U_\ell^{-1} H_{N,B,Z} U_\ell = Z\ell^{-1} H_N(h, b, v) , \tag{5.4}$$

where

$$H_N(h, b, v) := \sum_{i=1}^{N} \{[\boldsymbol{\sigma}_i \cdot (h\mathbf{p}_i + b\mathbf{a}(x_i))]^2 + v(x_i)\} + Z^{-1} \sum_{i<j}^{N} |x_i - x_j|^{-1} \tag{5.5}$$

with

$$h = \ell^{-1/2} Z^{1/2} = Z^{-1/3}(1 + \beta)^{1/5} \approx \begin{cases} Z^{-1/3} & \text{for } B \ll Z^{4/3} \\ (B/Z^3)^{1/5} & \text{for } B \gg Z^{4/3} \end{cases}, \tag{5.6}$$

$$b = B\ell^{3/2} Z^{-1/2} = Z^{1/3} \beta (1 + \beta)^{-3/5} \approx \begin{cases} B/Z & \text{for } B \ll Z^{4/3} \\ (B^2/Z)^{1/5} & \text{for } B \gg Z^{4/3} \end{cases} \tag{5.7}$$

Note also that

$$hb = \beta(1 + \beta)^{-2/5}, \quad h^{-3} = Z(1 + \beta)^{-3/5} \quad \text{and} \quad h^{-2}b = Z\beta(1 + \beta)^{-1} . \tag{5.8}$$

By (5.4) the ground state energy $E_N(h, b, v)$ of $H_N(h, b, v)$ is related to $E^Q(N, B, Z)$ by the scaling

$$E^Q(N, B, Z) = Z\ell^{-1} E_N(h, b, v) , \tag{5.9}$$

whereas according to (4.49)

$$E^{\mathrm{MTF}}(N, B, Z) = Z^2 \ell^{-1} \hat{E}(\lambda, \beta) .$$

The task is thus to show that for each fixed $\lambda$

$$E_N(h, b, v)/Z\hat{E}(\lambda, \beta) \to 1 \tag{5.10}$$

uniformly in $\beta$ as $h = Z^{-1/3}(1+\beta)^{1/5} \to 0$, with $b = Z^{1/3}\beta(1+\beta)^{-2/5}$. Note that the condition $h \to 0$ is equivalent to $Z \to \infty$ and $B/Z^3 \to 0$.

*Step 2* (*Semiclassics related to* MTF). Define $v_{\mathrm{eff}}$ as in (4.54), i.e.

$$v_{\mathrm{eff}}(x) = v(x) + \rho_{\lambda,\beta} * |x|^{-1} + \mu(\lambda, \beta) ,$$

where $\rho_{\lambda,\beta}$ is the minimizer of (4.46) with $\int \rho_{\lambda,\beta} \leqq \lambda$. We can then write

$$H_N(h, b, v) = H_N^0(h, b, v_{\mathrm{eff}}) - \sum_{i=1}^{N} \rho_{\lambda,\beta} * |x_i|^{-1} + Z^{-1} \sum_{i<j}^{N} |x_i - x_j|^{-1} - \mu N \tag{5.11}$$

with

$$H_N^0(h, b, v_{\mathrm{eff}}) := \sum_{i=1}^{N} [\boldsymbol{\sigma}_i \cdot (h\mathbf{p}_i + b\mathbf{a}(x_i))]^2 + v_{\mathrm{eff}}(x_i) . \tag{5.12}$$

$H_N^0$ is a sum of $N$ copies of the single-particle Hamiltonian $H_1^0 = H(h, b, v_{\mathrm{eff}})$, in the notation of Sect. III. To relate the semiclassical energy $E_{\mathrm{scl}}(h, b, v_{\mathrm{eff}})$ to $\hat{E}(\lambda, \beta)$, we use the TF equation in the form (4.55):

$$-\hat{P}_\beta(|v_{\mathrm{eff}}|_-) = \hat{\tau}_\beta(\rho_{\lambda,\beta}) + v_{\mathrm{eff}}\, \rho_{\lambda,\beta} .$$

By (5.8) and (4.6) we have $\hat{P}_\beta(w) = Z^{-1}h^{-3}P_{hb}(w)$, so integration over $x$ gives

$$E_{\mathrm{scl}}(h, b, v_{\mathrm{eff}}) = Z\{\hat{E}(\lambda, \beta) + D(\rho_{\lambda,\beta}, \rho_{\lambda,\beta}) + \mu \min\{\lambda, \lambda_c\}\} . \tag{5.13}$$

*Step 3* (*Upper bound*). We use the variational principle [16] and the semiclassical upper bound on $H_1^0$ from Sect. III to bound the ground state energy of the Hamiltonian $H_N(h, b, v)$ from above by the Thomas–Fermi energy $Z\hat{E}(\lambda, \beta)$ plus an error term of lower order. Notice that the semiclassical Theorem 3.1 is applicable by the Remark following Theorem 3.1 because of Proposition 4.19. We test the Hamiltonian with a density matrix $\gamma$ as in (3.26) with $V$ replaced by $v_{\mathrm{eff}}$. This time, however, it is not necessary to cut at a finite radius $R$, for $P'(|v_{\mathrm{eff}}(u)|_-)$ is integrable over all of $\mathbf{R}^3$. In fact,

$$P'(|v_{\mathrm{eff}}(u)|_-) = Z\hat{P}'_\beta(|v_{\mathrm{eff}}(u)|_-) = Z\rho_{\lambda,\beta}(u) ,$$

where we have used (4.51), (5.8) and (4.53). (Recall that $P(w) = h^{-3}P_{hb}(w)$.) In the estimate (3.27) we can therefore take $R = \infty$, and (3.29) and (3.30) become superfluous. By (3.26) and (3.28) the density associated with $\gamma$ is

$$\rho_\gamma(x) := \gamma(x, x) = Z\rho_{\lambda,\beta} * g_r^2(x) .$$

In particular,

$$\operatorname{Tr}\gamma = Z\int \rho_{\lambda,\beta} * g_r^2 = \min\{N, N_c\} \leqq N .$$

Since $v \to 0$ at $\infty$, $\gamma$ is thus an acceptable density matrix for the variational principle [16], which for $H_N$ as in (5.11) implies that

$$\inf\operatorname{spec} H_N(h, b, v) \leqq \operatorname{Tr}(\gamma H_1^0) - \operatorname{Tr}(\gamma\, \rho_{\lambda,\beta} * |x|^{-1}) + Z^{-1}D(\rho_\gamma, \rho_\gamma) - \mu \min\{N, N_c\} .$$

By the semiclassical upper bound in the proof of Theorem 3.1, and Eqs. (5.8) and (5.13), we have for $h = Z^{-1/3}(1+\beta)^{1/5} \to 0$:

$$\begin{aligned}\mathrm{Tr}(\gamma H_1^0) &= E_{\mathrm{scl}}(h, b, v_{\mathrm{eff}}) + o(h^{-3} + h^{-2}b) \\ &= Z\hat{E}(\lambda, \beta) + ZD(\rho_{\lambda,\beta}, \rho_{\lambda,\beta}) + \mu \min\{N, N_c\} + o(Z)\,.\end{aligned}$$

Because $|\hat{E}(\lambda, \beta)| \geqq c_\lambda > 0$ by (4.56), the error term is of lower order than $Z\hat{E}(\lambda, \beta)$. Moreover,

$$\mathrm{Tr}(\gamma\, \rho_{\lambda,\beta} * |x|^{-1}) = 2ZD(\rho_{\lambda,\beta} * g_r^2, \rho_{\lambda,\beta})$$

and

$$Z^{-1}D(\rho_\gamma, \rho_\gamma) = ZD(\rho_{\lambda,\beta} * g_r^2, \rho_{\lambda,\beta} * g_r^2)\,.$$

Hence

$$E_N(h, b, v) \leqq Z\hat{E}(\lambda, \beta) + ZD(\rho_{\lambda,\beta} - \rho_{\lambda,\beta} * g_r^2, \rho_{\lambda,\beta} - \rho_{\lambda,\beta} * g_r^2) + o(Z)\,, \quad (5.14)$$

and $D(\rho_{\lambda,\beta} - \rho_{\lambda,\beta} * g_r^2, \rho_{\lambda,\beta} - \rho_{\lambda,\beta} * g_r^2) \to 0$ as $r \to 0$ by Proposition 4.18.

*Step 4* (*Lower bound*). For any normalized $\psi \in \bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$ we have by (5.11),

$$\begin{aligned}\langle\psi|H_N(h, b, v)|\psi\rangle \geqq{} & \inf\mathrm{spec}\, H_N^0(h, b, v_{\mathrm{eff}}) \\ & + Z^{-1}\langle\psi|\sum_{i<j}|x_i - x_j|^{-1}|\psi\rangle - 2D(\rho_{\lambda,\beta}, \rho_\psi) - \mu N.\end{aligned}$$

From the semiclassical lower bound for $H_N^0$ and Eq. (5.13) it follows that we only have to consider the terms

$$ZD(\rho_{\lambda,\beta}, \rho_{\lambda,\beta}) + Z^{-1}\langle\psi|\sum_{i<j}|x_i - x_j|^{-1}|\psi\rangle - 2D(\rho_{\lambda,\beta}, \rho_\psi) =: \mathscr{R}\,.$$

Note that the terms proportional to $\mu$ cancel, because $\mu = 0$ if $N > N_c$.

Using the Lieb–Oxford inequality [17] we have

$$\mathscr{R} \geqq Z[D(\rho_{\lambda,\beta}, \rho_{\lambda,\beta}) + D(\tilde{\rho}_\psi, \tilde{\rho}_\psi) - 2D(\rho_{\lambda,\beta}, \tilde{\rho}_\psi)] - (\mathrm{const.})Z^{-1}\int\rho_\psi^{4/3}\,,$$

where we have put $\tilde{\rho}_\psi = Z^{-1}\rho_\psi$. The term in square brackets is $\geqq 0$. Hence it remains only to show that $Z^{-1}\int\rho_\psi^{4/3}$ is of lower order than $Z\hat{E}(\lambda, \beta)$, if $\psi$ is approximately a ground state of $H_N(h, b, v)$. Note first that $Z^{-1}\int\rho_\psi^{4/3} \leqq Z^{-1}(\int\rho_\psi^{5/3})^{1/2}(\int\rho_\psi)^{1/2}$. To estimate $\int\rho_\psi^{5/3}$ we use Corollary 2.2. The function $F_B$ introduced in (2.6) satisfies the bound $\min\{t^{5/3}, B^{-2}t^3\} \leqq (\mathrm{const.})\, F_B(t)$. Hence for any $\rho \in L^1 \cap L^{5/3}$, $\rho \geqq 0$, we have in the same way as in (4.20),

$$\begin{aligned}\int\rho^{5/3} &\leqq \left(\int_{\rho^3 \leqq B^2\rho^{5/3}} \rho^3\right)^{1/3} \left(\int\rho\right)^{2/3} + \int_{\rho^3 \geqq B^2\rho^{5/3}} \rho^{5/3} \\ &\leqq (\mathrm{const.})\left[B^{2/3}\left(\int F_B(\rho)\right)^{1/3}\left(\int\rho\right)^{2/3} + \int F_B(\rho)\right]\,. \end{aligned} \quad (5.15)$$

We now apply Corollary 2.2 to the function $U_\ell\psi$ with $U_\ell$ as in (5.3). Its density is $\rho_{U_\ell\psi}(x) = \ell^{-3}\rho_\psi(\ell^{-1}x)$, and from Corollary 2.2 we obtain

$$\int F_B(\rho_{U_\ell\psi}) \leqq \langle U_\ell\psi|\sum_{i=1}^N [\sigma_i\cdot(\mathbf{p}_i + \mathbf{A}(x_i))]^2|U_\ell\psi\rangle\,. \quad (5.16)$$

If $\psi$ is an approximate ground state for $H_N(h, b, v)$, then, by the upper bound (5.14) and (4.56), we may assume that $\langle\psi|H_N(h, b, v)|\psi\rangle \leqq 0$. Hence $\langle U_\ell\psi|\tilde{H}_{N,B,Z}|U_\ell\psi\rangle \leqq 0$, where $\tilde{H}_{N,B,Z}$, defined in (2.44), is $H_{N,B,Z}$ without the electronic repulsion. Combining (5.15) and (5.16) with Corollary 2.9, we obtain

$$\int \rho_\psi^{5/3} = \ell^2 \int \rho_{U_\ell \psi}^{5/3} \leqq (\text{const.})\{ZN^{2/3}(\beta(\beta+1)^{-1})^{2/3} + Z^{5/3}(1+\beta)^{-2/5}\}.$$

We remark that this estimate is analogous to the estimate (4.58) in Thomas–Fermi theory. Returning to the estimate on $Z^{-1}\int\rho^{4/3}$ we finally obtain

$$Z^{-1}\int \rho^{4/3} \leqq (\text{const.})\, Z^{-1}N^{1/2}(ZN^{2/3} + Z^{5/3})^{1/2} \leqq (\text{const.})\,\lambda(1+\lambda^{1/3})\, Z^{1/3},$$

which for fixed $\lambda$ is smaller than $Z\hat{E}(\lambda, \beta)$ by a factor $(\text{const.})Z^{-2/3}$. ∎

Combining Theorem 5.1 with Proposition 4.17 we obtain as an immediate corollary:

**5.2 Theorem (Energy Asymptotics in Regions 1 and 3).** (i) *If $Z \to \infty$ with $\lambda = N/Z$ fixed and $B/Z^{4/3} \to 0$, then*

$$E^Q(N, B, Z)/E^{\mathrm{TF}}(N, Z) \to 1.$$

(ii) *If $Z \to \infty$ with $\lambda = N/Z$ fixed and $B/Z^3 \to 0$, but $B/Z^{4/3} \to \infty$, then*

$$E^Q(N, B, Z)/E^{\mathrm{STF}}(N, B, Z) \to 1.$$

Theorem 5.1 can also be stated in another way. We denote as before the scaled Thomas–Fermi energy (4.48) by $\hat{E}(\lambda, \beta)$ with $0 \leqq \beta \leqq \infty$ and recall that $\hat{E}(\lambda, 0) = E^{\mathrm{TF}}(\lambda, 1)$ and $\hat{E}(\lambda, \infty) = E^{\mathrm{STF}}(\lambda, 1, 1)$. Because of Proposition 4.17, Theorem 5.1 is equivalent to the following statement: If $Z \to \infty$, $B/Z^3 \to 0$ and $B/Z^{4/3} \to \beta$, $0 \leqq \beta \leqq \infty$ with $\lambda = N/Z$ fixed, then

$$Z^{-7/3}(1 + B/Z^{4/3})^{-2/5} E^Q(N, B, Z) \to \hat{E}(\lambda, \beta). \tag{5.17}$$

Theorem 5.1 implies also that the quantum ground state density

$$\rho^Q_{N,B,Z}(x) := N \sum_{s_i = \pm 1/2} \int |\psi(x, x_2, \ldots, x_N; s_1, \ldots, s_N)|^2 dx_1 \cdots dx_N, \tag{5.18}$$

where $\psi$ is a ground state[8] of $H_{N,B,Z}$, converges, suitably scaled, to the Thomas–Fermi density $\rho_{\lambda,\beta}$. Given Theorem 5.1, the proof is analogous to the proof of the corresponding statement in Proposition 4.14, cf. also [42].

**5.3 Theorem (Density Asymptotics in Regions 1, 2 and 3).** *If $Z \to \infty$, $B/Z^3 \to 0$ and $B/Z^{4/3} \to \beta$, $0 \leqq \beta \leqq \infty$, with $\lambda = N/Z$ fixed, then*

$$Z^{-2}(1 + B/Z^{4/3})^{-6/5} \rho^Q_{N,B,Z}(Z^{-1/3}(1 + B/Z^{4/3})^{-2/5} x) \rightharpoonup \rho_{\lambda,\beta}(x)$$

*weakly in $L^{5/3}_{\mathrm{loc}}$.*

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[8] As in Theorem III.1 in [42] $\psi$ can be replaced by a sequence of approximate ground states

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