Gradient corrections for semiclassical theories of atoms in strong magnetic fields

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Abstract

This paper is divided into two parts. In the first one the von Weizsäcker term is introduced to the Magnetic TF theory and the resulting MTFW functional is mathematically analyzed. In particular, it is shown that the von Weizsäcker term produces the Scott correction up to magnetic fields of order \( B \ll Z^2 \), in accordance with a result of V. Ivrii on the quantum mechanical ground state energy.

The second part is dedicated to gradient corrections for semiclassical theories of atoms restricted to electrons in the lowest Landau band. We consider modifications of the Thomas-Fermi theory for strong magnetic fields (STF), i.e. for \( B \ll Z^3 \). The main modification consists in replacing the integration over the variables perpendicular to the field by an expansion in angular momentum eigenfunctions in the lowest Landau band. This leads to a functional (DSTF) depending on a sequence of one-dimensional densities. For a one-dimensional Fermi gas the analogue of a Weizsäcker correction has a negative sign and we discuss the corresponding modification of the DSTF functional.
1 Introduction

In this paper we study gradient correction terms for semiclassical theories describing the ground state energies of heavy atoms in strong homogeneous magnetic fields. Such an atom, with \(N\) electrons of charge \(-e\) and mass \(m_e\) and nuclear charge \(Ze\) is described by the nonrelativistic Pauli Hamiltonian

\[
H_N = \sum_{1 \leq j \leq N} \left\{ (-i\nabla^{(j)} + \mathbf{A}(x_j)) \cdot \sigma^j \right\}^2 - \frac{Z}{|x_j|} + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|},
\]

(1.1)

acting on the Hilbert space \(\bigwedge_{1 \leq j \leq N} L^2(\mathbb{R}^3, \mathbb{C}^2)\) of electron wave functions. The units are chosen such that \(\hbar = 2m_e = e = 1\). The magnetic field is \(\mathbf{B} = (0, 0, B)\), with vector potential \(\mathbf{A} = \frac{1}{2}B(-x_2, x_1, 0)\), where \(B\) is the magnitude of the field in units of \(B_0 = \frac{m_e^2 e^3}{\hbar^3} = 2.35 \cdot 10^9\) Gauss, the field strength for which the cyclotron radius \(l_B = (\hbar c/(eB))^{1/2}\) is equal to the Bohr radius \(a_0 = \hbar^2/(m_e e^2)\). The ground state energy is

\[
E^Q(N, Z, B) = \inf\{(\psi, H_N \psi) : \psi \in \text{domain } H_N, (\psi, \psi) = 1\}.
\]

(1.2)

In [LSY2] Lieb, Solovej and Yngvason approximated (1.2) by means of the MTF (Magnetic Thomas-Fermi) functional

\[
\mathcal{E}^{MTF}[\rho] = \int \tau_B(\rho) - \int V \rho + D(\rho, \rho),
\]

(1.3)

where \(V(x) = Z/|x|\) and \(D(\rho, \rho) = \frac{1}{2}(\rho, |x|^{-1} \ast \rho)\). The magnetic energy density \(\tau_B\) is, by definition, the Legendre transform of the pressure \(P_B\), i.e.

\[
\tau_B(t) = \sup_{w \geq 0} [tw - P_B(w)],
\]

(1.4)

with

\[
P_B(w) = \frac{B}{3\pi^2}(w^{3/2} - 2 \sum_{i=1}^{\infty} |2iB - w|^{3/2}).
\]

(1.5)

The corresponding energy

\[
E^{MTF}(N, Z, B) = \inf\{\mathcal{E}^{MTF}[\rho] | \rho \geq 0, \rho \in D^{MTF}, \int \rho \leq N\}
\]

(1.6)

was proved by Lieb, Solovej and Yngvason to be asymptotically exact, as shown in the following Theorem:

1.1. THEOREM. ([LSY2] Theorem 5.1) If \(Z \to \infty\) with \(N/Z\) fixed and \(B/Z^3 \to 0\), then

\[
E^Q(N, Z, B)/E^{MTF}(N, Z, B) \to 1.
\]
In the limit $B \to \infty$ the function $\tau_B$ is the kinetic energy describing particles confined to the lowest Landau band, i.e.,

$$\tau_\infty(t) = \frac{4\pi^4}{3} t^3 / B^2,$$

which results in the STF (Strong Thomas-Fermi) functional

$$\mathcal{E}^{\text{STF}}[\rho] = \frac{4\pi^4}{3B^2} \int \rho^3 - \int V\rho + D(\rho, \rho). \quad (1.7)$$

The corresponding energy $E^{\text{STF}}$ is quantum mechanically exact in the limit $Z \to \infty$ for $Z^{4/3} \ll B \ll Z^3$ ([LSY2] Proposition 4.16), which emphasizes the fact ([LSY1] Theorem 1.2) that for $B \gg Z^{4/3}$ the electrons are to leading order confined to the lowest Landau band.

### 1.1 Corrections to the leading order of the full Hamiltonian (1.1)

The best result to date concerning corrections to the leading order of (1.1) is presented by Victor Ivrii in [I], Theorem 0.2:

**1.2. THEOREM.** ([I] Theorem 0.2) Let $B \leq Z^3$ and $N \sim Z$, then

$$|E^Q(N, Z, B) - E^{\text{MTF}}(N, Z, B) - \frac{1}{4}Z^2| \leq R_1 + R_2, \quad (1.8)$$

with

$$R_1 = CZ^{4/3}(N + B)^{1/3} \quad \text{and} \quad R_2 = CZ^{3/5}B^{4/5}. \quad (1.9)$$

Recall the order of the energy, $E^Q \sim Z^{7/3}[1 + B/Z^{4/3}]^{2/5}$.

We make a few comments concerning Ivrii’s proof. Let

$$H_A = [(-i\nabla + A(x)) \cdot \sigma]^2 \quad (1.10)$$

denote the free Pauli-Hamiltonian and

$$\phi^{\text{MTF}} = Z|x|^{-1} - \rho^{\text{MTF}} * |x|^{-1} \quad (1.11)$$

the self consistent magnetic TF potential. The main part of the estimate (1.8) is given by the difference between

$$\text{Tr}[H_A - \phi^{\text{MTF}} + \mu]_-, \quad (1.12)$$

the sum of all negative eigenvalues of the operator $H_A - \phi^{\text{MTF}} + \mu$, and its semiclassical approximation

$$\int P_B(\phi^{\text{MTF}} - \mu). \quad (1.13)$$
For those who are familiar with microlocal analysis we should remark that Ivrii does not really consider $\phi^{MTF}$ but a smooth mollification, which we also denote with $\phi^{MTF}$ for simplicity. In order to derive accurate estimates of

$$\left| \text{Tr}[H_A - \phi^{MTF} + \mu] - \int P_B(\phi^{MTF} - \mu) \right|$$

(1.14)

Ivrii essentially divides the domain into two main zones, for $B \geq Z^{4/3}$, namely

$$\chi_1 = \{ x | 0 \leq |x| \leq B/Z \} \quad \text{and} \quad \chi_2 = \{ x | B/Z \leq |x| \leq r_S = Z^{1/5}B^{-2/5} \}. \quad (1.15)$$

A corresponding partition of unity is given by two function $\varphi_1$ and $\varphi_2$, with $\varphi_1 + \varphi_2 = 1$ on $\chi_1 \cup \chi_2$ and $\varphi_i$ essentially supported in $\chi_i$. Using scaling arguments and semiclassical spectral asymptotics Ivrii treats each zone separately. In the inner zone $\chi_1$, where all Landau levels are taken into account and the MTF potential is very similar to the usual TF potential, he gets

$$\chi_1 : \left| \text{Tr}(\varphi_1[H_A - \phi^{MTF} + \mu] - \int \varphi_1 P_B(\phi^{MTF} - \mu) - \frac{1}{4}Z^2 \right| \leq R_1. \quad (1.16)$$

We see that in $\chi_1$ the Scott correction is recovered. Moreover, we should note that the machinery of semiclassical spectral asymptotics can only be applied to $\chi_1$ under the condition $Z/B \gg 1/Z$ which means that (1.16) is only valid for $B \leq Z^{2-\delta}$, with arbitrary $\delta > 0$. For $B \geq Z^2$ a semiclassical approximation is no longer possible and the terms (1.12) and (1.13) have to be estimated separately. Since $R_2$ overcomes $Z^2$ for $B \geq Z^{7/4}$, we should point out that the Scott correction in (1.8) only provides the next to leading order for $B \ll Z^{7/4}$, but in the domain $\chi_1$ it nevertheless makes sense up to $B \ll Z^2$ according to (1.16).

In the outer zone $\chi_2$ only the lowest Landau band is occupied, which implies that in this region the MTF energy is represented by the STF energy corresponding to the functional (1.7). In $\chi_2$ Ivrii derives the estimate

$$\chi_2 : \left| \text{Tr}(\varphi_2[H_A - \phi^{MTF} + \mu] - \int \varphi_2 P_B(\phi^{MTF} - \mu) \right| \leq R_2, \quad (1.17)$$

where the main contribution of (1.17) really stems from the edge of the STF atom $r_S \sim Z^{1/5}B^{-2/5}$.

For low magnetic fields ($B \leq Z$) V. Ivrii even improves (1.8) and recovers Dirac and Schwinger corrections as well.

1.3. THEOREM. ([I] Theorem 0.3) If $B \leq Z$ then

$$\left| E^{QM}(N, Z, B) - E^{MTF}(N, Z, B) - \frac{1}{4}Z^2 + c_{DS} \int (\rho^{TF})^{4/3} \right| \leq CN^{5/3}((1+B)/N)^{\delta} \quad (1.18)$$

holds with some $\delta > 0$ and an appropriate parameter $c_{DS}.$
1.1.1 The von Weizsäcker term introduced to MTF

The von Weizsäcker correction term was successfully introduced to the TF theory in the sense that it reproduces the Scott correction (rigorously proven in \[SW, H\]), i.e.

\[ E_{\text{TFW}} = E_{\text{TF}} + O(Z^2) + o(Z^2). \] \hspace{1cm} (1.19)

In addition to the \(Z^2\) correction, the TFW theory remedies some defects of the TF theory: The corresponding TFW density is finite at the nuclei, binding of atoms occurs and negative ions are stable, furthermore the density has exponential fall off at infinity, at least for neutral atoms and molecules.

In the limit \(B \to 0\) the function \(\tau_B\) is the kinetic energy density in zero magnetic field, i.e.

\[ \tau_0(t) = \frac{3}{5}(3\pi^2)^{2/3}t^{5/3}. \]

Since for small values of \(B\) the introduction of the von Weizsäcker term to the MTF functional is justified, we will further check up to which values of \(B\) this definition makes sense. We get the functional

\[ E_{\text{MTFW}}[\rho] = A \int |\nabla \rho|^2 + \int \tau_B(\rho) - \int V\rho + D(\rho, \rho), \] \hspace{1cm} (1.20)

with a suitably chosen parameter \(A\). The functional (1.20) can be treated analogously to the usual TFW functional in \[BBL\]. So we will just sketch the proofs of the main propositions.

It turns out that for \(B \ll Z^2\) the von Weizsäcker term still produces the Scott correction, but makes no longer sense for higher magnetic fields. We will derive the following Theorem:

1.4. THEOREM. For all \(B, Z\) and \(N/Z\) fixed

\[ |E_{\text{MTFW}} - E_{\text{MTF}} - O(Z^2)| \leq CB^{4/5}Z^{3/5} + o(Z^2) \] \hspace{1cm} (1.21)

Remark: The estimate (1.21) is clearly useful if \(B \leq Z^{7/4}\). Theorem 1.4 will be proved in Section 2.2.

The Scott correction, just like in TFW theory, comes from distances of order \(1/Z\) near the nucleus, whereas the bound \(CB^{4/5}Z^{3/5}\) comes from the edge of the MTF atom and dominates the Scott correction for \(B \geq Z^{7/4}\). Moreover, (1.21) is in accordance with Theorem 1.2, which justifies a posteriori the introduction of the von Weizsäcker term to the MTF functional.

1.2 Physics in the lowest Landau band

The quantum mechanical ground state energy of particles confined to the lowest Landau band is given by

\[ E_{\text{conf}}^Q(N, Z, B) = \inf_{\|\psi\|_2=1} (\psi, \Pi_0^N H_N \Pi_0^N \psi). \] \hspace{1cm} (1.22)
where $\Pi_0$ represents the projector on the lowest Landau band, given by the kernel

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

where $P_\downarrow$ denotes the projection onto the spin down component, and $\Pi_0^N$ denotes the $N$'th tensorial power of $\Pi_0$. The leading order of $E_\text{conf}^Q$, as $B, Z \to \infty$ with $B \ll Z^3$, is given by $E^{\text{STF}}$, the ground state energy of the functional (1.7). In a companion work we show, what is expected by Ivrii’s Theorem 1.2,

$$
|E_\text{conf}^Q - E^{\text{STF}}| \leq C B^{4/5} Z^{3/5}.
$$

As we have argued above the main contribution to the estimate (1.24) comes from the edge of the STF atom, $r_S \sim Z^{1/5} B^{-2/5}$. Recall the order of $E^{\text{STF}}$, $E^{\text{STF}}[N, Z, B] = Z^3 (B/Z^3)^{2/5} E^{\text{STF}}[N/Z, 1, 1]$, so that the estimate is only of interest for $B \ll Z^3$.

As a better approximation to $E_\text{conf}^Q$, valid also for $B \geq Z^3$, Lieb, Solovej and Yngvason suggested a density matrix functional defined as

$$
\mathcal{E}^{\text{DM}}[\Gamma] = \int_{\mathbb{R}^2} \text{Tr}_{L^2(\mathbb{R})} [-\partial_3^2 \Gamma_{x_\perp}] dx_\perp - Z \int |x|^{-1} \rho_\Gamma(x) + D(\rho_\Gamma, \rho_\Gamma).
$$

Its variable is an operator valued function

$$
\Gamma : x_\perp \to \Gamma_{x_\perp},
$$

where $\Gamma_{x_\perp}$ is an integral operator on $L^2(\mathbb{R})$, given by a kernel $\Gamma_{x_\perp}(x_3, y_3)$ and satisfying

$$
0 \leq \Gamma_{x_\perp} \leq (B/2\pi) I
$$

as an operator on $L^2(\mathbb{R})$. The energy

$$
E^{\text{DM}}(N, Z, B) = \inf \{ \mathcal{E}^{\text{DM}}[\Gamma] | \Gamma \text{ satisfies (1.25) and } \int \rho_\Gamma \leq N \}
$$

turns out to be asymptotically exact for magnetic fields in the following precise sense:

1.5. THEOREM. ([LSY1] Theorem 5.1 and 7.1 and equations 7.3 and 8.5) For some constants, $C_\lambda$ and $C_\lambda'$, we have

$$
R_U \geq E_\text{conf}^Q(N, Z, B) - E^{\text{DM}}(N, Z, B) \geq -R_L,
$$

with

$$
R_L = C_\lambda \min \{ Z^{17/15} B^{2/5}, Z^{8/3} [1 + (\ln(B/Z^3))^2] \}
$$

and

$$
R_U = C_\lambda' \min \{ Z^{5/3} B^{1/3}, Z^{8/3} [1 + \ln(Z) + (\ln(B/Z^3))^2]^{5/6} \}.
$$
We remark that the STF energy is the natural semiclassical approximation of the DM energy. More precisely, the DM energy can be written as

\[
\frac{B}{2\pi} \int d\mathbf{x}_\perp \text{Tr}_{L^2(\mathbb{R})}[-\partial_z^2 - \phi_{\mathbf{x}_\perp}^{\text{DM}} - \mu^{\text{DM}}] - \mu^{\text{DM}} N - D(\rho^{\text{DM}}, \rho^{\text{DM}}),
\]

(1.28)

whereas the STF energy is given by the corresponding semiclassical expression

\[
\frac{B}{2\pi} \int d\mathbf{x}_\perp \int \int dp dz \left[ p^2 - \phi_{\mathbf{x}_\perp}^{\text{STF}} - \mu^{\text{STF}} \right] - \mu^{\text{STF}} N - D(\rho^{\text{STF}}, \rho^{\text{STF}}).
\]

(1.29)

With the decomposition

\[ L^2(\mathbb{R}^3, d\mathbf{x}; \mathbb{C}^2) = L^2(\mathbb{R}^2, d\mathbf{x}_\perp) \otimes L^2(\mathbb{R}, dz) \otimes \mathbb{C}^2 \]

the projector \( \Pi_0 \) can be written as

\[
\Pi_0 = \sum_{m\geq 0} |\phi_m\rangle \langle \phi_m| \otimes 1 \otimes P_\downarrow,
\]

(1.30)

where \( \phi_m \) denotes the function in the lowest Landau band with angular momentum \(-m \leq 0\), i.e., using polar coordinates \((r, \varphi)\),

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

(1.31)

Using this and \( H_A \Phi_m = 0 \), we can write

\[
\Pi_0 H_A \Pi_0 = \sum_{m\geq 0} |\phi_m\rangle \langle \phi_m| \otimes (-\partial_z^2) \otimes P_\downarrow.
\]

(1.32)

Based on this decomposition the author and R. Seiringer introduced in [HS] a natural modification of the DM functional called discrete density matrix functional (DDM)

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

(1.33)

where

\[
\tilde{D}(\rho, \rho) = \frac{1}{2} \sum_{m,n} \int V_{m,n}(z - z') \rho_m(z) \rho_n(z') dz dz',
\]

(1.34)

and the potentials \( V_m \) and \( V_{m,n} \) are given by

\[
V_m(z) = \int \frac{1}{|x|} |\phi_m(\mathbf{x}_\perp)|^2 d\mathbf{x}_\perp,
\]

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

(1.35)
Here $\Gamma$ is a sequence of fermionic density matrices acting on $L^2(\mathbb{R}, dz)$,

$$\Gamma = (\Gamma_m)_{m \in \mathbb{N}_0},$$  \hspace{1cm} (1.36)

with corresponding densities $\rho = (\rho_m)_m$, $\rho_m(z) = \Gamma_m(z, z)$. Note that $E_{B,Z}^{DDM}$ depends on $B$ via the potentials $V_m$ and $V_{m,n}$. The corresponding energy is given by

$$E^{DDM}(N, Z, B) = \inf \left\{ E_{B,Z}^{DDM}[\Gamma] \mid \sum_m \text{Tr}[\Gamma_m] \leq N \right\}. \hspace{1cm} (1.37)$$

It is shown in [HS] that $E^{DDM}$ correctly reproduces the confined ground state energy $E^{Q}_{conf}$ apart from errors due to the indirect part of the Coulomb interaction energy:

**1.6. THEOREM.** ([HS] Theorem 1.2) For some constant $c_{\lambda}$ depending only on $\lambda = N/Z$

$$0 \geq E_{\text{conf}}^{Q}(N, Z, B) - E^{DDM}(N, Z, B) \geq -R_L, \hspace{1cm} (1.38)$$

with

$$R_L = c_{\lambda} \min \left\{ Z^{17/15} B^{2/5}, Z^{8/3}(1 + [\ln(B/Z^4)]^2) \right\}. \hspace{1cm} (1.39)$$

Since the functional (1.33) can also be seen as a reduced Hartree-Fock functional, in the sense of [S], it does not surprise that the upper bound in (1.38) is an improvement to (1.26), the relation between $E^{DDM}$ and $E^{Q}_{conf}$. In addition to better estimates, the DDM theory remedies the defect of the DM theory having a sharply cut ground state density supported in the set $\{ x \mid |x| \leq \sqrt{2N/B} \}$, for the respective three dimensional DDM density,

$$\rho^{DDM}(x) = \sum_m \rho^{DDM}_m(z) \phi_m^2(x_\perp), \hspace{1cm} (1.40)$$

has exponential fall off at infinity. Furthermore, since the DDM energy describes $E^{Q}_{conf}$ correctly apart from errors due to the indirect part of the Coulomb interaction energy, the DDM energy could give rise to even recover the exchange term, by means of an improved lower bound on the two body Coulomb repulsion for particles in the lowest Landau band. For the exchange energy is anticipated to be of order $\ln(B/Z^{4/3})Z^{7/5}B^{1/5}$ for $B \ll Z^3$, which in [HS] by the author and R. Seiringer is conjectured to be given by the term

$$c \ln(B/Z^{4/3}) \sum \int (\rho^{DDM}_i)^2. \hspace{1cm} (1.41)$$

This would lead to the relation

$$E^{Q}_{\text{conf}} = E^{DDM} - c \ln(B/Z^{4/3}) \sum \int (\rho^{DDM}_i)^2 + o(\ln(B/Z^{4/3})Z^{7/5}B^{1/5}), \hspace{1cm} (1.42)$$
with $c$ appropriately chosen.

We have stated above that the STF functional is the natural semiclassical approximation of the DM functional. Hence, we can ask for the natural semiclassical approximation of the DDM functional, of which the answer is given by the so called DSTF functional

$$
\mathcal{E}_{\text{DSTF}}[\rho] = \sum_{m \in \mathbb{N}_0} \left( \kappa \int \rho_m^3(z) - Z \int V_m(z) \rho_m(z) dz \right) + \tilde{D}(\rho, \rho),
$$

where $\rho$ is a sequence of one-dimensional densities, $\rho = (\rho_m)_{m \in \mathbb{N}_0}$, $\kappa = \pi^2/3$, and the respective DSTF energy is defined as

$$
E_{\text{DSTF}}(N, Z, B) = \inf \left\{ \mathcal{E}_{\text{DSTF}}[\rho] \mid \sum_m \int \rho_m \leq N \right\}.
$$

In Section 3.2.2 we will argue that the DSTF functional is even the natural semiclassical approximation of the ground state energy $E_{\text{conf}}$ itself.

1.3 Gradient corrections for semiclassical lowest Landau band theories

1.3.1 The Tomishima-Shinjo correction term

For higher magnetic fields, where only the lowest Landau band has to be taken into account, Tomishima and Shinjo [TS] obtained the gradient correction term

$$
\epsilon_{\text{TS}}[\rho] = \frac{2\pi^4}{B^3} \rho(\nabla_\perp \rho)^2 - \frac{1}{3}(\nabla_\parallel \rho^{1/2})^2,
$$

i.e.

$$
\mathcal{E}_{\text{TS}}[\rho] = \frac{2\pi^4}{B^3} \int \rho(\nabla_\perp \rho)^2 - \frac{1}{3} \int (\nabla_\parallel \rho^{1/2})^2 + \mathcal{E}_{\text{STF}}[\rho],
$$

by perturbation expansion of the canonical density matrix. In 1995 the authors of [MZP] recovered the TS theory within the framework of current density functional theory. Since (1.46) has a negative gradient correction along the magnetic field the TS functional is no longer bounded from below. Hence the corresponding energy cannot, as usual, be defined by minimizing over a suitably domain of definition, but only through the solutions of the corresponding Euler-Lagrange equation under the restriction $\int \rho = N$, i.e.

$$
\frac{4\pi^4}{B^2} \rho^2 - \frac{\pi^4}{B^3} \left( (\nabla_\perp \rho)^2 + 2 \rho \Delta_\perp \rho \right) - \frac{1}{12\rho} \left[ \frac{1}{2\rho} (\nabla_\parallel \rho)^2 - \Delta_\parallel \rho \right] = V - \rho \ast \frac{1}{|x|} - \mu(N).
$$

(1.47)
A direct attack on this complicated equation does not look promising, but a rough estimate of the corrections to STF can be obtained by inserting the density

\[ \rho(r) = \begin{cases} 
\rho_{\text{STF}}(B^{-1/2}) & \text{for } r \leq B^{-1/2}, \\
\rho_{\text{STF}}(r) & \text{for } r \geq B^{-1/2}.
\end{cases} \]  

(1.48)

into (1.46). The negative gradient term gives a correction \(-O(B^{4/5}Z^{3/5})\) coming from the edge of the STF atom. From (1.24) we know that

\[ |E^Q_{\text{conf}} - E^\text{STF}| \leq CB^{4/5}Z^{3/5}, \]

(1.49)

where the main contribution also stems from \(r_S \sim Z^{1/5}B^{-2/5}\), the edge of the STF atom.

On the other hand the positive gradient correction orthogonal to the magnetic field in (1.46) produces a correction \(O(B^{1/4}Z^{3/2})\) at a distance of order \(B^{-1/2}\) from the nucleus. This part of the correction can also be obtained from an isotropic Tomishima functional, defined as

\[ E^{\text{IT}}[\rho] = E^{\text{STF}}[\rho] + \frac{2\pi^4}{B^3} \int \rho(\nabla \rho)^2. \]

(1.50)

The functional (1.50) has all the good properties of the usual TF theories, such as convexity and boundedness from below. The study of this functional, which we do in detail in Section 3.1, should help us to get a deeper understanding of the nature of the positive correction term in (1.46). For the ground state energy of (1.50) we will derive the following theorem.

1.7. THEOREM. For all \(B, Z\) and \(N/Z\) fixed

\[ E^{\text{IT}}(N, Z, B) - E^{\text{STF}}(N, Z, B) = O(B^{1/4}Z^{3/2}) + o(B^{1/4}Z^{3/2}). \]

(1.51)

Furthermore we will argue in Section 3.1 that the \(\rho(\nabla \rho)^2\) term remedies the defect of the STF theory that the full Coulomb potential is used although the particles in the lowest Landau band do not see the full singularity, since they are smeared over a region of radius \(B^{-1/2}\). In contrast to TFW theory, where the maximal number \(N_c\) of electrons that can be bound is strictly larger than \(Z\), it will as a slight surprise turn out that in IT theory \(N_c = Z\), just like in the STF theory itself. Also, the radius of atoms in IT theory is finite, as in STF theory. These features confirm that the \(\rho(\nabla \rho)^2\) term essentially only effects the density close to the nucleus.

1.3.2 Gradient correction for the discrete STF theory

As discussed above, the gradient term \(\sim \rho(\nabla_\perp \rho)^2\) in (1.46) produces essentially a smearing of the Coulomb singularities over a distance of the radius \(B^{-1/2}\). The same effect was obtained by replacing STF by DSTF.
It appears thus natural to look for a negative gradient term that has an analogue effect in DSTF as the negative gradient term in (1.46) has in STF theory, i.e. provides corrections at the edge of the atom.

The DSTF theory is effectively a theory of coupled one-dimensional problems. Analogous arguments as lead to the von Weizsäcker term for a three dimensional Fermi gas give for a one-dimensional Fermi gas a gradient correction $-\frac{1}{3}(\nabla \rho^{1/2})^2$, cf. [Sh]. Hence we suggest the definition of a discrete von Weizsäcker functional:

$$E_{DW}[\rho] = \sum_{m \in \mathbb{N}_0} \left( -\frac{1}{3} \int |\partial_z \sqrt{\rho_m(z)}|^2 + \kappa \int \rho_m^3(z) - Z \int V_m(z) \rho_m(z) \right) + \tilde{D}(\rho, \rho)$$

By denoting $\sqrt{\rho_m} = \psi_m$ we arrive, under the restriction $\sum_m \int \psi_m^2 = N$, at the corresponding TF equation

$$\left(\frac{1}{3}\right) \partial_z^2 \psi_n(z) + 3\kappa \psi_n^5(z) = [\varphi_n(z) - \mu(N)] \psi_n(z) \quad \forall n \in \mathbb{N}_0,$$ \hspace{1cm} (1.53)

with

$$\varphi_n(z) = ZV_n(z) - \sum_m \int \psi_m^2(z') V_{m,n}(z - z')dz'.$$

These coupled equations are probably somewhat easier to deal with than (1.47).

If we reduce (1.52) to the angular momentum channel $m = 0$ and drop the Coulomb repulsion term, we get the one-dimensional functional

$$E_{1DW}[\rho] = -\frac{1}{3} \int |\partial_z \sqrt{\rho(z)}|^2 + \kappa \int \rho^3(z) - Z \int V_0(z) \rho(z).$$ \hspace{1cm} (1.54)

This simplified functional will be studied in Section 3.3.2. In particular, we shall show that the negative gradient term reproduces the right QM correction to the energy without the gradient term.

## 2 The magnetic TFW theory

### 2.1 Mathematical analysis of the MTFW functional

In this section we are going to mathematically analyze the MTFW functional

$$E_{MTFW}[\rho] = A \int |\nabla \sqrt{\rho(z)}|^2 + \int \tau_B(\rho) - \int V \rho + D(\rho, \rho).$$ \hspace{1cm} (2.1)

Since the mathematical propositions do not depend on the parameter $A$, we let $A$ be 1 in this section. The most important features of $\tau_B(t)$ which will be used in our calculations are (compare [LSY2] Lemma 4.1):

$$\tau_B'(t) \leq \kappa_1 t^{2/3} \quad \text{and} \quad \tau_B(t) \leq \frac{3}{5} \kappa_1 t^{5/3},$$ \hspace{1cm} (2.2)
with $\kappa_1 = (4\pi^2)^{2/3}$.

Since the MTFW functional does not differ very much from the functional in [BBL], where the authors used a kinetic energy density $\tau(\rho) = (1/p)\rho^p$, our procedure in analyzing (1.20) will be in analogy to their work. We are thus concerned with the minimizing problem

$$\text{Min}\{E_{\text{MTFW}}[\rho]|\rho \geq 0, \rho \in L^1 \cap L^{5/3}_\text{loc}, \nabla \rho^{1/2} \in L^2 \text{ and } \int \rho = N\},$$

(2.3)

where $N$ is a positive constant, which physically is the total charge number. Our main result is the following:

2.1. THEOREM. There is a critical number $0 < N_c < \infty$, so that

1. if $N \leq N_c$ (2.3) has a unique minimizer,
2. if $N > N_c$ (2.3) has no minimizer,
3. $N_c > Z$.

Similar to [BBL] we first examine the problem

$$\text{Min}\{E_{\text{MTFW}}[\rho]|\rho \in D\}$$

(2.4)

with

$$D = \{\rho|\rho \geq 0, \tau_B(\rho) < \infty, \rho \in L^3, \nabla \rho^{1/2} \in L^2, D(\rho, \rho) < \infty\}$$

(2.5)

and prove the existence of a unique minimizer $\rho_0$. Since $D$ contains the domain of (2.3) we have to show $\rho_0 \in L^1(\mathbb{R}^3)$ in order to guarantee $N_c < \infty$. Furthermore we will derive $N_c > Z$, which shows that this theory allows negative ions. The proofs will be based on the Euler-Lagrange equation for $\psi = \sqrt{\rho_0}$.

First we consider some basic properties of (2.1).

2.2. LEMMA. For $D$ defined in (2.3) we have

$$D \subset \{\rho|\rho \geq 0, \rho \in L^3 \cap L^{5/3}_\text{loc}, \nabla \rho^{1/2} \in L^2, D(\rho, \rho) < \infty\} \equiv \tilde{D}.$$  

(2.6)

Proof. According to [LSY2] (4.19) one gets for all $\Omega \subset \mathbb{R}^3$

$$\int_\Omega \rho(x)^{5/3} dx \leq \frac{1}{\kappa_3} \int_{\Omega_1} \tau_B(\rho(x)) dx + C \text{Vol}(\Omega_2) < \infty$$

with $\Omega = \Omega_1 \cup \Omega_2$. 

2.3. PROPOSITION. The absolute minimum of $E_{\text{MTFW}}[\rho]$ is achieved for a unique $\rho_0 \in \tilde{D}$. 

Proof. (cf. [BBL] Lemmas 2, 3, 4 and 5.) Recall that, by definition (1.4), \( \tau_B(t) \) is strictly convex, hence \( \mathcal{E}^{\text{MTFW}}[\rho] \) is strictly convex.

Let \( \rho_n \) be a minimizing sequence. There exists a constant \( C \) such that

\[
\|\rho_n\|_3 \leq C, \int \tau_B(\rho_n) \leq C, \|\nabla \rho_n^{1/2}\|_2 \leq C, D(\rho_n, \rho_n) \leq C.
\]

By the Banach-Alaoglu theorem we can extract a subsequence, still denoted as \( \rho_n \), with

\[
\rho_n \rightharpoonup \rho_0 \quad \text{weakly in} \quad L^3, \tag{2.7}
\]
\[
\nabla \rho_n^{1/2} \rightharpoonup \nabla \rho_0^{1/2} \quad \text{weakly in} \quad L^2. \tag{2.8}
\]

Since by use of Hölder’s inequality \( \|\rho_n^{1/2}\|_{H^1(\Omega)} \leq C(\Omega) \) and \( H^1(\Omega) \) is relatively compact in \( L^2(\Omega) \), if \( \Omega \) is a bounded smooth domain, \( \rho_n^{1/2} \) has a subsequence converging in \( L^2(\Omega) \). Using Cantor’s diagonal trick on a sequence of increasing \( \Omega \)’s we arrive at

\[
\rho_n^{1/2} \to \rho_0^{1/2} \quad \text{a. e.}. \tag{2.9}
\]

By Fatou’s Lemma we get

\[
\liminf \int \tau_B(\rho_n) \geq \int \tau_B(\rho_0) \quad \text{and} \quad \liminf D(\rho_n, \rho_n) \geq D(\rho_0, \rho_0).
\]

Since \( L^p \) norms are weakly lower semicontinuous,

\[
\liminf \int |\nabla \rho_n^{1/2}|^2 \geq \int |\nabla \rho_0^{1/2}|^2.
\]

Moreover, one can show, in analogy to Proposition 3.3, that

\[
\int V\rho_n \to \int V\rho_0,
\]

so we altogether arrive at

\[
\liminf \mathcal{E}^{\text{MTFW}}[\rho_n] \geq \mathcal{E}^{\text{MTFW}}[\rho_0]. \tag{2.10}
\]

The uniqueness follows from the strict convexity of \( \mathcal{E}^{\text{MTFW}}[\rho] \). \( \square \)

For the minimizing \( \rho_0 \) we now can derive an Euler-Lagrange equation. Denote \( \psi = \sqrt{\rho_0} \).

2.4. PROPOSITION. The minimizing \( \psi^2 = \rho_0 \) satisfies

\[
- \Delta \psi + \tau_B'(\psi^2) \psi = \varphi \psi, \tag{2.11}
\]

in the sense of distributions, with \( \varphi = V - \psi^2 * \frac{1}{|x|} \).
Proof. (cf. [BBL] Lemma 6.) Note that $\psi^2 \in D$ implies $\varphi \psi, \tau'_B(\psi^2) \psi \in L^1_{\text{loc}}$, which gives $\bar{D}$ a meaning in the sense of distributions. Consider the set

$$\bar{D} \equiv \{ \zeta | \zeta \in L^6 \cap L^{10/3}_{\text{loc}}, \nabla \zeta \in L^2 \text{ and } D(\zeta^2, \zeta^2) < \infty \}. \quad (2.12)$$

If $\zeta \in \bar{D}$ then $\rho = \zeta^2 \in D$ and

$$E_{\text{MTFW}}[\rho] = \int |\nabla \zeta|^2 + \int \tau_B(\zeta^2) - \int V \zeta^2 + D(\zeta^2, \zeta^2) \equiv \phi(\zeta).$$

We find $\phi(\psi) \leq \phi(\zeta)$ for all $\zeta \in \bar{D}$. Let $\eta \in C_0^\infty$. Using the fact that $\frac{d}{dt}\phi(\psi + t\eta)|_{t=0} = 0$, we easily arrive at

$$-\int \psi \Delta \eta + \int \tau'_B(\psi^2) \psi \eta = \int \varphi \psi \eta. \quad (2.13)$$

Starting from Equation (2.11) we can now step by step gain several properties for $\psi$.

2.5. LEMMA. $\psi$ is continuous on $\mathbb{R}^3$, more precisely $\psi \in C^{0,\alpha}_{\text{loc}}$ for all $\alpha \leq 1$.

Proof. (cf. [BBL] Lemma 7.) Since (2.11) yields $-\Delta \psi \leq \varphi \psi$, with $\varphi \psi \in L^{2-\delta}_{\text{loc}}$, one gets $\psi \in L^\infty_{\text{loc}}$. Again using (2.11) the proposition follows by means of standard elliptic regularity theory. □

2.6. PROPOSITION. $\psi \in L^2(\mathbb{R}^3)$

Proof. (cf. [BBL] Lemma 8.) Assume, by contradiction, $\int \psi^2 = \infty$. Then we can choose an $r$, such that

$$\int_{|x| \leq r} \psi^2(x) \geq Z + 2\delta,$$

for some $\delta > 0$. Therefore

$$\psi^2 \ast |x|^{-1} \geq \int_{|x| \leq r} \psi^2(x)(|x| + |y|)^{-1} dy \geq (Z + 2\delta) / (|x| + r),$$

which gives us

$$\varphi(x) = V(x) - \psi^2 \ast |x|^{-1} \leq \frac{Z}{|x| - r} - \frac{Z + 2\delta}{|x| + r},$$

with $|x| > r$. Thus there exists an $r_1 > r$, such that for $|x| > r_1$

$$\varphi(x) \leq -\delta|x|^{-1}. \quad (2.14)$$
From (2.11) we get
\[ -\Delta \psi + \delta |x|^{-1} \psi \leq 0, \quad (2.15) \]
for \(|x| > r_1\). Now we choose a comparison density
\[ \tilde{\psi}(x) = Me^{-2(\delta |x|)^{1/2}}, \]
which satisfies
\[ -\Delta \tilde{\psi} + \delta |x|^{-1} \tilde{\psi} \geq 0. \quad (2.16) \]
Hence by (2.15) and (2.16)
\[ -\Delta (\psi - \tilde{\psi}) + \delta |x|^{-1}(\psi - \tilde{\psi}) \leq 0 \]
for \(|x| \geq r_1\). We fix \(M\) such that
\[ \psi(r_1) \leq \tilde{\psi}(r_1). \]
If \(\psi \to 0\) for \(|x| \to \infty\), we immediately get
\[ \psi \leq \tilde{\psi} \quad \text{for} \quad |x| > r_1 \quad (2.17) \]
from the maximum principle. The fact that \(\int \tilde{\psi}^2 < \infty\) and \(\psi \in L_{\text{loc}}^\infty\) contradicts our assumption. Unfortunately, we only know that \(\psi \to \infty\) as \(|x| \to \infty\) in a weak sense, namely \(\psi \in L^6\), so the authors in [BBL] used a variant of Stampaccia’s method to verify the statement of the Lemma, which also works in our case. \(\square\)

Mimicking the proof of [BBL] Lemma 10 and using the fact that \(\tau_B'(\psi^2)\psi - \varphi \psi\) is continuous but not differentiable we get

**2.7. Lemma.** \(\psi > 0\) everywhere and \(\psi \in C^2\), except at \(x = 0\).

Using (2.2) in the proof of [BBL] Lemma 11 and afterwards following the proof of Lemma 13 we additionally get

**2.8. Proposition.** \(N_c = \int \psi^2 > Z\).

Before concluding the proof of Theorem 2.1, we need a final lemma, which is the equivalent to [BBL] Lemma 14.

**2.9. Lemma.** For every \(N > 0\) we have
\[ \inf\{\mathcal{E}^{MTFW}[\rho] | \rho \in \bar{D} \text{ and } \int \rho = N\} = \inf\{\mathcal{E}^{MTFW}[\rho] | \rho \in \bar{D} \text{ and } \int \rho \leq N\}. \]

**Proof of Theorem 2.1:**
For every \(N\) we set
\[ E(N) \equiv \inf\{\mathcal{E}^{MTFW}[\rho] | \rho \in \bar{D} \text{ and } \int \rho \leq N\}. \]
Obviously $E(N)$ is non-increasing and convex. The same proof as in Proposition 2.3 shows that there exists a $\rho_N \in \bar{D}$ with $\int \rho_N \leq N$ and 

$$E^\text{MTFW}[\rho_N] = E(N).$$

With $N_c = \int \psi^2$ it is clear that $E(N)$ is constant for $N > N_c$: $E(N) = E(N_c)$, while $E(N)$ is strictly decreasing on the interval $[0, N_c]$. For $N \leq N_c$ : $\int \rho_N = N$, which implies that (2.3) has a unique solution. On the other hand we deduce from Lemma 2.9 that for $N > N_c$ (2.3) has no solution, which concludes the proof of Theorem 2.1.

After having guaranteed the existence of a minimizing density $\rho_N$ for (2.3), we can derive an Euler-Lagrange equation under the variational restriction $\int \rho = N$.

2.10. PROPOSITION. Denote $\psi = \rho_N^{1/2}$, with $\rho_N$ the minimizing density for 

$$\inf \{E^\text{MTFW}[\rho]|\rho \in \bar{D}, \int \rho = N\}$$

under the restriction $N \leq N_c$. Then we have

$$- \Delta \psi + \tau'_B(\psi^2)\psi - \varphi \psi = \mu(N)\psi, \quad (2.18)$$

where

$$\mu(N) = \frac{d}{dN} E(N). \quad (2.19)$$

Proof. The derivation of (2.18) works analogously to (2.11) apart from the difference that $\mu$ is the Lagrange parameter for the restriction $\int \rho = N$. We can infer

$$\frac{d}{dt} E^\text{MTFW}[t\rho + (1-t)\rho_N] \bigg|_{t=0} = \mu(N) \int (\rho_N - \rho), \quad (2.20)$$

which implies by means of convexity of the functional

$$E^\text{MTFW}[\rho_N] - E^\text{MTFW}[\rho] \geq \mu(N) \int (\rho_N - \rho),$$

or equivalently for every $N'$

$$E(N) - E(N') \geq \mu(N)(N - N'). \quad (2.21)$$

On the other hand we derive from (2.20)

$$E^\text{MTFW}[t\rho + (1-t)\rho_N] - E^\text{MTFW}[\rho_N] = t\mu(N) \int (\rho_N - \rho) + o(t),$$

which yields with $\rho = 2\rho_N$ and $\rho = \frac{1}{2}\rho_N$, respectively,

$$E(N \pm tN) - E(N) \leq \pm \mu(N)tN + o(t). \quad (2.22)$$

Hence (2.21) and (2.22) together imply (2.19).
Next we take a look at the behavior at infinity of the minimizing densities \( \rho_N \). At least for \( N < N_c \) one gets exponential decay.

2.11. PROPOSITION. (a) Let \( \mu < 0 \), which is equivalent to \( N < N_c \), then for every \( \delta > 0 \), with \( \mu < -\delta \), there exists a constant \( M \), such that, for the corresponding minimizer \( \psi = \rho_N^{1/2} \),

\[
\psi \leq Me^{-\delta |x|}. \tag{2.23}
\]

(b) Let \( N = N_c \), then for every \( \delta < N_c - Z \) there is a constant \( M \), such that

\[
\psi \leq Me^{-2(\delta |x|)^{1/2}}. \tag{2.24}
\]

Proof. Note, that we have not yet shown that \( \psi \to 0 \) as \( |x| \to \infty \) in a strong sense, for we only know \( \psi \in L^2 \). From equation (2.18) we derive \(-\Delta \psi \leq V \psi \), which implies \((-\Delta + I)\psi \leq (V + I)\psi \). Since we know \((V + I)\psi \in L^2 \), recall that \((V + I) \in L^2 + L^\infty \) and \( \psi \in L^2 \cap L^\infty \), we conclude from

\[
\psi \leq (-\Delta + I)^{-1}[(V + I)\psi], \tag{2.25}
\]

that \( \psi \to 0 \) at infinity, e.g. from the well known fact ([LS] Lemma II.25) that the convolution \( f * g \) of two functions \( f \in L^p, g \in L^q \), with \( 1/p + 1/q = 1 \), goes to 0 at infinity.

(a) (cf. [L1] Theorem 7.24.) Let \( \delta < -\mu \). From (2.18) we get

\[
(-\Delta + \delta)\psi = [-\tau'_B(\psi^2) + \varphi + \mu + \delta]\psi \tag{2.26}
\]

and

\[
\psi = (-\Delta + \delta)^{-1}[-\tau'_B(\psi^2) + \varphi + \mu + \delta]\psi. \tag{2.27}
\]

Since \( V, \psi \to 0 \) as \( |x| \to \infty \), there is a \( r_1 \), such that \([-\tau'_B(\psi^2) + \varphi + \mu + \delta] < 0 \) for \( |x| > r_1 \). This implies

\[
\psi(x) \leq \int_{|y| \leq r_1} (4\pi|x - y|)^{-1}e^{-\delta^{1/2}|x-y|}([-\tau'_B(\psi^2) + \varphi + \mu + \delta]\psi(y)dy < \infty, \tag{2.28}
\]

and (2.23) with

\[
M = \sup_x e^{\delta^{1/2}r_1} \int_{|y| \leq r_1} (4\pi|x - y|)^{-1}([-\tau'_B(\psi^2) + \varphi + \mu + \delta]\psi(y)dy, \tag{2.29}
\]

(b) This follows directly from (2.17) and the fact that \( \psi \to 0 \) as \( |x| \to \infty \). \( \square \)

We state a final proposition concerning the behavior of the chemical potential at \( N = 0 \) (which is \(-\infty \) in the usual TF theory), because of the simple and illuminating proof.
2.12. PROPOSITION. Let $e_0 = -\frac{1}{4}Z^2$ be the smallest eigenvalue of the Schrödinger operator $-\Delta - Z/|x|$. Then

$$\mu(0) = \frac{d}{dN}E(N)\bigg|_{N=0} = e_0. \quad (2.30)$$

Proof. (cf. [BBL] Lemma 15.) Let $\varphi(x)$ be the normalized eigenvector of $-\Delta - Z/|x|$ belonging to the lowest eigenvalue $e_0 = -\frac{1}{4}Z^2$ and let $\rho_N = N\varphi(x)^2$. Then

$$E(N) \leq E_{\text{MTFW}}(\rho_N) = \int |\nabla \rho_N^{1/2}|^2 - \int V \rho_N + \int \tau_B(\rho_N) + D(\rho_N, \rho_N)$$

$$= N[(\varphi, -\Delta \varphi) - Z(\varphi, |x|^{-1}\varphi)] + \int \tau_B(\rho_N) + D(\rho_N, \rho_N)$$

$$\leq Ne_0 + C_1 N^{5/3} + C_2 N^2.$$

On the other hand we have

$$E(N) \geq \inf \int \rho = N \inf \text{spec} \{-\Delta - Z|x|^{-1}\} = Ne_0,$$

which altogether implies

$$\lim_{N \to +0} \frac{E(N)}{N} = e_0.$$

Taking into account that $E(0) = 0$ this is equivalent to $\text{(2.30)}$. \hfill \square

2.2 The Scott correction

If one takes a look at Lieb's proof [L1] that in the usual TF theory without magnetic fields the von Weizsäcker term produces the Scott correction, one realizes that the main correction comes from distances of order $Z^{-1}$ from the nucleus. It is thus reasonable to guess that in the MTF theory the von Weizsäcker term produces the Scott correction as long as $\rho_{\text{MTF}}$, the density corresponding to the MTF energy (1.6), is well approximated by the usual TF density $\rho_{\text{TF}}$ up to distances of order $Z^{-1}$ from the nucleus. This condition is equivalent to the demand that $\tau_B'(\rho)$ is proportional to $\rho^{2/3}$ for $r \sim Z^{-1}$ and this is the case for $B \ll Z^2$.

In other words, for $B \ll Z^2$ the von Weizsäcker term produces a $Z^2$ correction at the distance of order $Z^{-1}$ from the nucleus. At the edge of the MTF atom, the radius is known [LSY2] to be proportional to $Z^{1/5}B^{-2/5}$ and the lowest Landau band is occupied, which leads to $\tau_B'(\rho_{\text{MTF}}) = 4\pi B^{-2}(\rho_{\text{MTF}})^2$ in the outer region. Hence, one computes very easily, by using $\rho_{\text{MTF}}$ as comparison density, that the correction coming from the edge of the atom is of order $B^{4/5}Z^{3/5}$.

Thus, for $B \geq Z^{7/4}$ the correction from the edge of the atom overcomes the Scott correction and Theorem 1.4 follows by using the variational density (2.35).
So it suffices to prove Theorem 1.4 for $B \leq Z^{7/4}$.

*Proof of Theorem 1.4:*  
First of all notice that there is an $r_B$, such that for $r \geq r_B$ the density $\rho_{\text{MTF}}$ corresponds to the lowest Landau band, i.e.

$$
\tau'_B(\rho_{\text{MTF}}(r)) = \frac{4\pi^4}{B^2}(\rho_{\text{MTF}}(r))^2 \quad \text{for} \quad r \geq r_B, 
$$

and for $r \leq r_B$ we have

$$
\kappa_3(\rho_{\text{MTF}}(r))^{2/3} \leq \tau'_B(\rho_{\text{MTF}}(r)) \leq \kappa_1(\rho_{\text{MTF}}(r))^{2/3},
$$
with $\kappa_3 = 0.83(3\pi^2)^{2/3}$. Using (2.31) and (2.32) one realizes that if one fixes any $\varepsilon > 0$ with $B \leq Z^{2-\varepsilon}$ there is a $\delta > 0$ such that $r_B \geq Z^{\delta-1}$.

**Lower bound:**  
We know from Section 2.1 that there exists a $\rho_0$ satisfying

$$
E_{\text{MTFW}}^{\rho_0} = \mathcal{E}_{\text{MTFW}}[\rho_0] = \int \tau_B(\rho_0) + \int |\nabla \rho_0^{1/2}|^2 - \int V \rho_0 + D(\rho_0, \rho_0). 
$$

Denote $Z|x|^{-1} = V = \tilde{V} + H$, with

- $H = Z/r - Z^2/b$ for $r < b/Z$ and 0 otherwise,
- $\tilde{V} = Z^2/b$ for $r < b/Z$ and $Z/r$ otherwise.

Now let us rewrite the energy functional in the following way:

$$
\mathcal{E}_{\text{MTFW}}[\rho_0] = \int \tau_B(\rho_0) - \int \rho_0^{1/2} \Delta \rho_0^{1/2} - \int \rho_0^{1/2} \tilde{V} \rho_0^{1/2} - \int H \rho_0 + D(\rho_0, \rho_0)
$$

Observe that $-\Delta - H \geq \inf_\rho \{(\nabla \rho^{1/2}, \nabla \rho^{1/2}) - (\rho^{1/2}, H \rho^{1/2})\}$, which by using Sobolev’s inequality can be bounded from below by

$$
-\Delta - H \geq \inf_\rho \{ || \rho ||_3^3 - || \rho ||_3 || H ||_{3/2} \}.
$$

Since $|| H ||_{3/2} \sim b$ we can guarantee $-\Delta - H \geq 0$ with $b$ small enough. Choosing such a $b$ we derive

$$
E_{\text{MTFW}} \geq \mathcal{E}_{\text{MTFW}}[\rho_0, \tilde{V}] \geq E_{\text{MTFW}}[\tilde{V}] = \int \tau(\tilde{\rho}) - \int \tilde{\rho} \tilde{V} + D(\tilde{\rho}, \tilde{\rho}) \geq E_{\text{MTFW}}[V] + \int H \tilde{\rho}.
$$
The density $\tilde{\rho}$ minimizes $E_{MTF}[\rho, \tilde{V}]$ and therefore fulfills the TF equation:

$$\tau'_B(\tilde{\rho}) = \tilde{V} - \tilde{\rho} \ast |x|^{-1}.$$ 

By means of (2.32) we get that $\int H\tilde{\rho} = O(Z^2)$ for $B \leq Z^{7/4}$ which yields

$$E_{MTFW} \geq E_{MTF} + O(Z^2).$$  \hspace{1cm} (2.34)

**Upper bound:**

In order to get an upper bound we use a variational density $\rho$ in the following way:

$$\rho(r) = \begin{cases} 
\tilde{\rho}_{TF}^{MTF}(Z^{-1}) & \text{for } r < Z^{-1}, \\
\tilde{\rho}_{TF}^{MTF}(r) & \text{for } Z^{-1} \leq r \leq r_B, \\
\rho^{MTF}(r) & \text{for } r \geq r_B,
\end{cases}$$  \hspace{1cm} (2.35)

where $\rho_{TF}^{MTF}$ indicates that we essentially use the usual TF density $\rho_{TF}^{TF}$. Only in the region $\varepsilon Z/B \leq r \leq r_B$ we eventually have to modify $\rho_{TF}^{TF}$, such that

$$|E_{MTF} - E_{MTF}[\rho]| \leq O(Z^2).$$

(This e.g. can be done by following the way of [I] and taking the $C^\infty$ modification $W$ of the effective potential $\phi_{MTF}$ and defining $4\pi\tilde{\rho}_{TF} = \Delta(W - Z|x|^{-1}).$) By means of our variational density $\rho$ we get

$$\int_{r \leq r_B} |\nabla \rho^{1/2}|^2 = O(Z^2),$$  \hspace{1cm} (2.36)

$$\int_{r \geq r_B} |\nabla \rho^{1/2}|^2 = O(B^{4/5}Z^{3/5}).$$  \hspace{1cm} (2.37)

For $B \leq Z^{7/4}$ this leads to

$$E_{MTFW} \leq E_{MTF} + O(Z^2),$$

which together with (2.34) completes the proof of Theorem 1.4.  \hspace{1cm} $\square$

### 3 Gradient corrections for STF type theories

#### 3.1 The functional (1.50)

Starting point in this section is the functional

$$E_{IT}[\rho] = \frac{1}{B^2} \int \rho^3 + \frac{1}{B^3} \int (\nabla \rho^{3/2})^2 - \int V\rho + D(\rho, \rho),$$  \hspace{1cm} (3.1)

with $V$ and $D(\rho, \rho)$ defined as in (1.3). Compared to (1.50) we rewrite

$$\frac{1}{B^3} \int \rho(\nabla \rho)^2 = \frac{4}{9B^3} \int (\nabla \rho^{3/2})^2,$$
and for simplicity forget about the numerical constant, which does not effect any mathematical statements. The corresponding energy is defined as

$$E(N, Z, B) = \inf \{ \mathcal{E}^{IT}[\rho] | \rho \in \tilde{D}, \int \rho \leq N \},$$

(3.2)

where the domain $\tilde{D}$ is given by

$$\tilde{D} = \{ \rho | \rho \geq 0, \rho \in L^1 \cap L^3, \nabla \rho^{3/2} \in L^2 \}.$$

In analogy to Section 2 we first consider the problem

$$\text{Min} \{ \mathcal{E}^{IT}[\rho] | \rho \in D \},$$

(3.3)

with

$$D = \{ \rho | \rho \geq 0, \rho \in L^3, \nabla \rho^{3/2} \in L^2, D(\rho, \rho) < \infty \}$$

(3.4)

and show that the minimum is achieved for a unique $\rho_0$. By means of the corresponding Euler-Lagrange equation we shall deduce that $\rho_0$ is in $L^1(\mathbb{R}^3)$, more precisely $\int \rho_0 = Z$.

First of all, we collect some properties of (3.1).

3.1. **Lemma.** There are positive constants $\alpha, C$, so that

$$\mathcal{E}^{IT}[\rho] \geq \alpha(\|\rho\|_3 + \int \tau_B(\rho) + \|\nabla \rho^{1/2}\|_2^2 + D(\rho, \rho)) - C,$$

(3.5)

Proof. This is a consequence of Lemma 2 in [BBL], which tells us that for every $\varepsilon > 0$ there exists a constant $C_\varepsilon$ so that

$$\int V \rho \leq \varepsilon \|\rho\|_3 + C_\varepsilon D(\rho, \rho)^{1/2}$$

for every $\rho \geq 0$. \hfill \Box

3.2. **Lemma.** $\mathcal{E}^{IT}[\rho]$ is strictly convex in $\rho$.

Proof. This follows immediately from the strict convexity of $(\nabla \rho^{3/2})^2$ and $\mathcal{E}^{\text{STF}}$. \hfill \Box

By means of these Lemmas we can prove the existence of a unique minimizer in $\tilde{D}$.

3.3. **Proposition.** The Minimum of $\mathcal{E}^{IT}[\rho]$ is achieved by a unique $\rho_0 \in \tilde{D}$. 
Proof. The proof is similar to that of Proposition 2.3. Let \( \rho_n \) be a minimizing sequence. By Lemma 3.1 we have

\[
\|\rho_n\|_3^3 \leq C, \quad \|\nabla \rho_n^{3/2}\|_2^2 \leq C, \quad D(\rho_n, \rho_n) \leq C. \tag{3.6}
\]

With Banach-Alaoglu theorem we therefore extract a subsequence, still denoted by \( \rho_n \), such that

\[
\rho_n \rightharpoonup \rho_0 \quad \text{weakly in } L^3, \tag{3.7}
\]

\[
\nabla \rho_n^{3/2} \rightharpoonup \nabla \rho_0^{3/2} \quad \text{weakly in } L^2. \tag{3.8}
\]

Furthermore \( \rho_n^{3/2} \) is bounded in \( H^1 \), which implies that there exists a further subsequence, again denoted as \( \rho_n \), with

\[
\rho_n^{3/2} \rightarrow \rho_0^{3/2} \quad \text{a. e.} \]

(This relies on the fact that for a smooth bounded domain \( \Omega \), \( H^1(\Omega) \) is relatively compact in \( L^2(\Omega) \).) Hence, using Fatou’s Lemma we get

\[
\liminf D(\rho_n, \rho_n) \geq D(\rho_0, \rho_0),
\]

and by the weak lower semicontinuity of \( L^p \)-norms we deduce

\[
\liminf \int (\nabla \rho_n^{3/2})^2 \geq \int (\nabla \rho_0^{3/2})^2, \\
\liminf \int \rho_n^3 \geq \int \rho_0^3.
\]

In order to prove \( \int V \rho_n \rightarrow \int V \rho_0 \), we decompose \( V = V_1 + V_2 \) such that both functions are in \( C^\infty \). With \( V_1 \in L^{3/2}, \ (3.7) \) implies

\[
\int V_1 \rho_n \rightarrow \int V_1 \rho_0.
\]

On the other hand \( V_2 \) fulfills

\[
\int V_2 \rho_n = \int V_2 [-\Delta (\rho_n * |x|^{-1})] = \int (-\Delta V_2) (\rho_n * |x|^{-1}),
\]

which converges to

\[
\int (-\Delta V_2) (\rho_0 * |x|^{-1}) = \int V_2 \rho_0,
\]

for \( -\Delta V_2 \in L^{6/5} \) and \( \| \rho_n * |x|^{-1} \|_6 \) is bounded.

Thus

\[
\liminf E[\rho_n] \geq E[\rho_0].
\]

The uniqueness is an immediate consequence of the strict convexity of the functional. \( \square \)
For this minimizing $\rho_0$ we can derive an Euler-Lagrange equation.

3.4. PROPOSITION. The minimizing $\psi^{2/3} = \rho_0^{3/2}$ satisfies

$$( -\Delta + B )\psi = \frac{B^3}{3} \varphi \psi^{-1/3},$$

with $\varphi = V - \psi^{3/2} * \frac{1}{|x|}$, in the sense of distributions, on the set where $\psi > 0$.

Proof. The uniqueness of the minimum, the spherical symmetry of the functional (3.3) and the fact that $\psi \in H^1$ implies the continuity of $\psi$ away from the origin. With $\varphi \in L^2_{\text{loc}}$ the Equation (3.9) has a meaning in the sense of distributions on the domain $\{ x | \psi(x) > 0 \}$. Consider the set

$$\bar{D} = \{ \eta | \eta \in H^1, D(\eta^{2/3}, \eta^{2/3}) < \infty \}.$$ 

If $\eta \in \bar{D}$, then $\rho = (\eta^{2})^{1/3} \in D$ and

$$E^{IT}[\rho] = \frac{1}{B^2} \int \eta^2 + \frac{1}{B^3} \int (\nabla \eta)^2 - \int V \eta^{2/3} + D(\eta^{2/3}, \eta^{2/3}) \equiv \phi(\eta).$$

For all $\eta \in \bar{D}$ we find $\phi(\psi) \leq \phi(\eta)$.

Let $\xi \in C_0^\infty$, then using $\frac{d}{dt} \phi(\psi + t\xi)|_{t=0} = 0$ we infer

$$- \int \psi \Delta \xi + B \int \psi \xi = \frac{B^3}{3} \int \varphi \psi^{-1/3} \xi.$$ 

3.5. PROPOSITION. $\psi$ is bounded and $\psi$ is in $C^\infty$ away from the origin and eventual points with $\psi(x) = 0$.

Proof. Denote

$$\Omega_\epsilon = \{ x | \psi(x) \geq \epsilon \}.$$

On this domain we have

$$(-\Delta + B)\psi = f,$$

with $f \in L^2_{\text{loc}}$, since $\varphi \in L^2_{\text{loc}}$. So we conclude from standard elliptic arguments (e.g. [LL] Section 10) that $\psi$ is bounded, hence continuous everywhere. From

$$\Delta \varphi = 4\pi (\psi^{2/3}(x) - Z\delta(x))$$

we get the two times differentiability of $\varphi$ away from the origin and as long as $\psi > 0$. By means of (3.9) and a standard bootstrap argument we conclude $\psi \in C^\infty$.  

□
3.6. PROPOSITION. $\int \psi^{2/3} = Z$.

Proof. Suppose by contradiction $\int \psi^{2/3} = \lambda \neq Z$. We do not assume $\lambda$ to be finite. Then, as in (2.14), we get that there is some $r_1$ and an $\epsilon > 0$, such that

$$|\varphi(x)| \geq \epsilon/r,$$

(3.10)

for $|x| \geq r_1$. Since $\psi \in L^2$, we conclude $\psi < M/r^{3/2}$ for $r$ large enough. Hence, from (3.9) we get

$$|(-\Delta + B)\psi| = |\varphi\psi^{-1/3}| \geq \epsilon r^{-1/2},$$

which is a contradiction to $\psi \in H^1$.

3.7. Remark. The Proposition 3.6 is interesting, since gradient corrections usually give rise to binding of additional electrons. The reason that this is not the case in 3.6 relies on the negative potent of $\psi$ on the right side of (3.9). This fact forces the potential $\varphi$ to fall off much faster than $O(1/r)$.

Since we only consider atoms with a point nucleus, we get the following remark for the minimizing $\rho_0$.

3.8. PROPOSITION. $\rho_0$ is a symmetric non increasing function of $|x|$.

Proof. As we have already argued above, the symmetry of $\rho_0$ follows from the symmetry of the functional and the uniqueness of $\rho_0$.

Denote $\rho_0^*$ the non increasing rearrangement of $\rho_0$. (For definition see e.g. [LL] Section 3.3.) From the fact that $\int \rho_0 \leq Z$ and [L1] Theorem 2.12 we get

$${\mathcal E}_{\text{STF}}[\rho_0^*] \leq {\mathcal E}_{\text{STF}}[\rho_0].$$

[LL] Lemma 7.17 implies

$$\int |\nabla (\rho_0^{3/2})^*|^2 \geq \int |\nabla (\rho_0^{3/2})|^2$$

(3.11)

and again from [LL] 3.3 (v) we get $(\rho_0^{3/2})^* = (\rho_0^*)^{3/2}$, which proves the statement.

3.9. PROPOSITION. $\psi$ has compact support.

Proof. Inserting $\Delta \varphi = \psi^{2/3}$ into (3.9) yields the following equation for the potential, away from the origin:

$$(\Delta \varphi)^{1/2}[\Delta(\Delta \varphi)^{3/2}] = (\Delta \varphi)^2 - \varphi,$$

(3.12)

where we replaced the constants by one. Since $\varphi$ is spherical symmetric we can use the ansatz $\varphi = \frac{1}{r^{\lambda}}(r)$ and obtain by (3.12) the following fourth order equation:
\[
2\left[\frac{1}{r^2} \chi''^2 - \frac{2}{r^3} \chi'' \chi''' + \frac{1}{r^4} \chi''''^2 \right] + \left[\frac{1}{r^2} \chi''^2 - \frac{2}{r^3} \chi'' \chi''' + \frac{1}{r^4} \chi''''^2 \right] \\
= \frac{4}{9} \frac{1}{r^2} \chi^2 - \frac{2}{r^3} \chi \chi'' + \left(\frac{1}{r^4} \chi''''\right)
\]

(3.13)

We can see that in the surrounding of each point \( r_0 > 0 \) there exists a local solution

\[
\chi = a_6 (r - r_0)^6 + O((r - r_0)^7),
\]

with \( a_6 = (\text{const.}) r_0^2 \). Since \( \chi \equiv 0 \) is also a solution of (3.13), every composed function

\[
\chi = a_6 (r - r_0)^6 + O((r - r_0)^7) \quad \text{for} \quad r \leq r_0 \quad \text{and} \quad \chi \equiv 0 \quad \text{for} \quad r > r_0
\]
is a local solution around \( r_0 \).

Away from 0 the solutions can be uniquely continued up to \( r = 0 \). Hence, there exists a solution \( \chi \) and a \( r_1 > 0 \), such that \( \chi(0) = Z \) and \( \text{supp} \chi = [0, r_1] \).

Repeating the argument of [L1] Theorem 2.6, one can show that a solution of (3.3), with \( \psi \in H^1 \) and \( \int \psi^{2/3} < \infty, (\psi^2)^{1/3} \) uniquely determines the minimum of the functional (3.1). Therefore \( \chi(r) \) uniquely determines the selfconsistent potential \( \phi = \chi/r \), which implies that \( \psi = \rho^{3/2}_0 = (\Delta \phi)^{3/2} \) has compact support, too. \( \square \)

3.10. Remark. The preceding three propositions are equivalent to those for the STF theory. This confirms that the \( \rho (\nabla \rho)^2 \) term only amounts to changes close to the nucleus.

By the convexity of the functional (3.1) one easily derives the following properties for the energy \( E^{\text{IT}}(N, Z, B) \):

3.11. PROPOSITION. \( E^{\text{IT}}(N, Z, B) \) is convex as a function of \( N \) and strictly monoton decreasing on the interval \([0, Z]\). For \( N > Z \) we get \( E^{\text{IT}}(N, Z, B) = E^{\text{IT}}(Z, Z, B) \).

Next we prove Theorem 1.7.

Proof of Theorem 1.7: Upper bound:

We use the comparison density \( \bar{\rho} \), with

\[
\bar{\rho}(r) = \begin{cases} 
\rho^{\text{STF}}(l_B) & \text{for } r \leq l_B = B^{-1/2} \\
\rho^{\text{STF}}(r) & \text{otherwise}
\end{cases}
\]

(3.14)

and immediately get

\[
E^{\text{IT}} \leq E^{\text{STF}} + O(Z^{3/2} B^{1/4}).
\]
Lower bound:
Let $\rho$ be the minimizer of the energy (3.2), for given $B, Z, N$. We can rewrite
\[
E^{\text{IT}} = E^{\text{IT}}[\rho] = \frac{\kappa}{B^2} \int \rho^3 + \frac{1}{B^3} \int |\nabla \rho^{3/2}|^2 - \int \tilde{H} \rho - \int \tilde{V} \rho + D(\rho, \rho),
\]
where $\tilde{H} = \frac{Z}{r} - \frac{B^{1/2}Z}{b}$ for $r \leq b l_B$ and 0 otherwise, $\tilde{V} = \frac{B^{1/2}Z}{b}$ for $r \leq b l_B$ and $Z/r$ otherwise. Looking at the term
\[
\frac{1}{B^3} \int |\nabla \rho^{3/2}|^2 - \int \tilde{H} \rho,
\]
we infer by means of the Sobolev inequality the estimate
\[
\frac{1}{B^3} \int |\nabla \rho^{3/2}|^2 - \int \tilde{H} \rho \geq \frac{4}{9B^3} \| \rho \|_9^3 - \| \tilde{H} \|_{9/8} \| \rho \|_{9/8}. \tag{3.15}
\]
Since $\| \tilde{H} \|_{9/8} \sim b^{15/9}$ we can choose $b$ such that (3.15) $> 0$. Hence
\[
E^{\text{IT}} \geq \frac{\kappa}{B^2} \int \rho^3 - \int \tilde{V} \rho + D(\rho, \rho)
\geq E^{\text{STF}}[\tilde{V}] = E^{\text{STF}}[\tilde{V}, \tilde{\rho}]
\geq E^{\text{STF}} + \int \tilde{\rho} \tilde{H}.
\]
Since $\int \tilde{\rho} \tilde{H} = O(Z^{3/2}B^{1/4})$ we prove the proposition. \hfill \Box

We see that the main contribution of the correction (1.50) comes from the radius $l_B = B^{-1/2}$, in other words the gradient correction repairs the infinity of the STF density at a distance $B^{-1/2}$ from the nucleus. This infinity stems from the fact that in the STF theory the full $|x|^{-1}$ potential is involved, although particles in the lowest Landau band, which are smeared over a radius of at least $B^{-1/2}$, never see the full Coulomb singularity.

Moreover, the Tomishima-Shinjo correction (1.46) orthogonal to the magnetic field remedies the singularity of the Coulomb potential in a similar way as the isotropic gradient term. We will see that the same effect, as caused by (1.1) and (1.46), is also naturally obtained by using the DSTF functional.

3.2 A discrete von Weizsäcker functional

3.2.1 The DSTF functional

First of all we are going to collect some information about the DSTF functional (which are rigorously proved in a companion work). The DSTF functional
\[
E^{\text{DSTF}}[\rho] = \sum_{m \in \mathbb{N}_0} \left( \kappa \int \rho_m^3(z) - \int V_m(z) \rho_m(z) dz \right) + \tilde{D}(\rho, \rho), \tag{3.16}
\]
with \( V_n \) and \( V_{m,n} \) as in (1.35), is defined on the domain

\[
D = \{ \rho \mid \sum_m \int \rho_m^3 < \infty, \sum_m \int \rho_m < \infty, \tilde{D}(\rho, \rho) < \infty \} \tag{3.17}
\]

with corresponding energy

\[
E_{\text{DSTF}}(N, Z, B) = \inf \left\{ \mathcal{E}_{\text{DSTF}}[^\rho] \mid \rho \in D \text{ and } \sum_m \int \rho_m \leq N \right\}. \tag{3.18}
\]

Following the considerations of [LSY2] one can easily see that (3.16) is convex and bounded from below on \( D^N = \{ \rho \mid \rho \in D, \sum_m \int \rho_m \leq N \} \) and derive the following Theorem:

**3.12. THEOREM.** With \( N \leq Z \) fixed there exists a unique minimizer \( \rho^N \) for \( E_{\text{DSTF}} \), under the restriction \( \sum_m \int \rho_m \leq N \), i.e. \( E_{\text{DSTF}}(N, Z, B) = \mathcal{E}_{\text{DSTF}}[\rho^N] \). Moreover, \( \rho^N \) satisfies \( \sum_m \int \rho^N_m = N \).

Furthermore each minimizer \( \rho^N \) obeys the coupled TF equations

\[
3\kappa(\rho^N_m(z))^2 = [ZV_m(z) - \sum_n \int V_{m,n}(z - z')\rho^N_n(z') + \mu(N)]_+ \quad \forall (m \in \mathbb{N}_0), \tag{3.19}
\]

where \( \mu(N) \) is the Lagrange parameter belonging to the restriction \( \sum_m \int \rho_m = N \) and \([t]_+ = t \) for \( t \geq 0 \) and \([t]_+ = 0 \) otherwise, corresponds to the fact that the functional is only varied over positive functions, i.e. \( \rho_n \geq 0 \) \( \forall n \in \mathbb{N}_0 \).

By means of the notation

\[
ZV_m(z) - \sum_n \int V_{m,n}(z - z')\rho^N_n(z') + \mu(N) = \varphi^{(m)}_{\text{eff}}(z) \tag{3.20}
\]

and inserting in the TF equation we can rewrite the energy \( E_{\text{DSTF}}(N, Z, B) = \mathcal{E}_{\text{DSTF}}[\rho^N] \) as

\[
E_{\text{DSTF}}(N, Z, B) = \sum_m \int \int \left[p^2 - \varphi^{(m)}_{\text{eff}}(z)\right] - \frac{dpdz}{2\pi} + N\mu - \tilde{D}(\rho^N, \rho^N). \tag{3.21}
\]

### 3.2.2 Semiclassical approximation of \( E_{\text{conf}}^Q \)

First of all we want to state a useful theorem concerning the sum of the negative eigenvalues of the one-particle operator \( \Pi_0[H_A + \varphi]\Pi_0 \), where \( H_A = ((-i\nabla + A(x)) \cdot \sigma)^2 \) and \( \varphi \) is an axially symmetric potential \( \varphi(r, z) \) with \( r = |x_\perp| \).
3.13. THEOREM. Let $\varphi = \varphi(r, z)$ be axially symmetric. Then one can write the trace of the negative part of the operator $\Pi_0[H_A + \varphi]\Pi_0$ as the sum of one-dimensional traces, i.e.

$$\text{Tr}[\Pi_0[H_A + \varphi]\Pi_0]_-= \sum_{m \in \mathbb{N}_0} \text{Tr}_{L^2(\mathbb{R})}[-\partial_z^2 + \varphi^{(m)}(z)]_-, \quad (3.22)$$

with

$$\varphi^{(m)}(z) = \int \varphi(x)|\phi_m(x_\perp)|^2dx_\perp. \quad (3.23)$$

Proof. Let $L_z$ denote the angular momentum operator parallel to the magnetic field. Since $\varphi = \varphi(r, z)$, we have

$$[\Pi_0[H_A + \varphi]\Pi_0, L_z] = 0, \quad (3.24)$$

which implies that the eigenvectors of the operator $\Pi_0[H_A + \varphi]\Pi_0$ are of the form $|m, i\rangle = \Phi_m(x_\perp)f^i_m(z)$. Hence we can write the sum of the negative eigenvalues as

$$\text{Tr}[\Pi_0[H_A + \varphi]\Pi_0]_- = \sum_{m,i} \langle m, i|\Pi_0[H_A + \varphi]\Pi_0|m, i\rangle$$

$$= \sum_m \left( \sum_i (f^i_m, [-\partial_z^2 + \varphi^{(m)}(z)]f^i_m) \right), \quad (3.25)$$

showing that the $f^i_m$'s are the eigenvectors of the one-dimensional operator $-\partial_z^2 + \varphi^{(m)}(z)$. $\square$

3.14. PROPOSITION. Let $N, Z, B$ be fixed. Then

$$E_{\text{conf}}^Q(N, Z, B) \leq E_{\text{DSTF}}^Q(N, Z, B) + R_1 + R_2 + R_3, \quad (3.26)$$

$$E_{\text{conf}}^Q(N, Z, B) \geq E_{\text{DSTF}}^Q(N, Z, B) - R_1 - C \int \rho^{4/3}_\psi, \quad (3.27)$$

with

$$R_1 = \left| \sum_{m \in \mathbb{N}_0} \left( \text{Tr}_{L^2(\mathbb{R})}[-\partial_z^2 - \varphi^{(m)}_{\text{eff}}(z)]_-- \int \int [p^2 - \varphi^{(m)}_{\text{eff}}(z)]_-\frac{dpdz}{2\pi} \right) \right| \quad (3.28)$$

$$R_2 = D(\rho_\psi - \tilde{\rho}, \rho_\psi - \tilde{\rho}), \quad (3.29)$$

$$R_3 = \sum_{\lambda_N < \lambda_i < \mu(N)} (\lambda_i - \mu(N)), \quad (3.30)$$

where $\lambda_i$ and $\tilde{\rho}$ are defined in the proof.
Proof. Upper bound:
First of all we note that for any comparison wave function \( \psi \) and fixed integer \( N \) we get
\[
E_{\text{conf}}^Q \leq \sum_{i=1}^{N} (\psi, \Pi_0^N[H_A(x_i) - Z|x_i|^{-1}]\Pi_0^N\psi) + D(\rho_\psi, \rho_\psi),
\]
with
\[
\rho_\psi(x) = N \sum_s \int \psi(x, x_2, \ldots, x_N; s_1, \ldots, s_N)^2 dx_2 \ldots dx_N.
\]
If we set \( \tilde{\rho}(x) = \sum_m |\phi_m(x_\perp)|^2 \rho_m(z) \) and add and subtract \( \tilde{\rho} * |x|^{-1} - \mu(N) \) in the scalar product and use \( \psi = \frac{1}{\sqrt{N!}} \phi_1 \wedge \ldots \wedge \phi_N \), where \( \phi_i \) is the eigenvector corresponding to the \( i \)-th lowest eigenvalue \( \lambda_i \) of the one-particle operator
\[
\Pi_0(H_A - Z|x|^{-1} + \tilde{\rho} * |x|^{-1} - \mu(N))\Pi_0,
\]
as comparison wave function, (3.31) reads
\[
E_{\text{conf}}^Q \leq \text{Tr}[\Pi_0(H_A - Z|x|^{-1} + \tilde{\rho} * |x|^{-1} - \mu(N))\Pi_0] - 2D(\rho_\psi, \tilde{\rho}) + D(\rho_\psi, \rho_\psi) + N\mu(N) + \sum_{\lambda_N < \lambda_i < \mu(N)} (\lambda_i - \mu(N)).
\]
Applying Theorem 3.13 and (3.21) to the inequality above, we finally arrive at the upper bound (3.31).

Lower bound:
Let \( \psi \) denote the minimizer of (1.22), i.e. \( \psi = \psi_{\text{conf}} \). So after again adding and subtracting \( \tilde{\rho} * |x|^{-1} - \mu(N) \) and using the Lieb-Oxford inequality [LO], we can write the lower bound on \( E_{\text{conf}}^Q \) as follows:
\[
E_{\text{conf}}^Q = (\psi, \Pi_0^N H_N\Pi_0^N)
\geq \sum_{i=1}^{N} (\psi, \Pi_0^N[H_A(x_i) - Z|x_i|^{-1} + \tilde{\rho} * |x_i|^{-1} - \mu(N)]\Pi_0^N\psi)
\geq \text{Tr}[\Pi_0(H_A - Z|x|^{-1} + \tilde{\rho} * |x|^{-1} - \mu(N))\Pi_0] + N\mu
\geq \text{Tr}[\Pi_0(H_A - Z|x|^{-1} + \tilde{\rho} * |x|^{-1} - \mu(N))\Pi_0] - C \int \rho_\psi^{4/3}
\geq \text{Tr}[\Pi_0(H_A - Z|x|^{-1} + \tilde{\rho} * |x|^{-1} - \mu(N))\Pi_0] + N\mu
\geq -D(\tilde{\rho}, \tilde{\rho}) - C \int \rho_\psi^{4/3}
\]
Using (3.21) we arrive at (3.27).
3.15. Remark. Due to (3.26) and (3.27) the main contribution to the difference between $E_{\text{conf}}^Q$ and $E_{\text{DSTF}}$ is given by

$$R_1 = \left| \sum_{m \in \mathbb{N}_0} \left( \text{Tr}_{L^2(\mathbb{R})} [-\partial_z^2 - \varphi^{(m)}_{\text{eff}}(z)] - \int \int [p^2 - \varphi^{(m)}_{\text{eff}}(z)] \frac{dpdz}{2\pi} \right) \right|,$$  \hspace{1cm} (3.35)

which, by definition, shows that $E_{\text{DSTF}}$ is the natural semiclassical approximation of $E_{\text{conf}}^Q$.

As a corollary, for example by following the way of [LSY2] and using coherent states and the above estimates, or simply by estimating the difference between $E_{\text{DSTF}}$ and $E_{\text{STF}}$ one gets

3.16. COROLLARY. If $Z \to \infty$ with $N/Z$ fixed and $B/Z^3 \to 0$, then

$$E_{\text{conf}}^Q(N, Z, B)/E_{\text{DSTF}}(N, Z, B) \to 1.$$  

The DSTF theory is equivalent to a three dimensional functional using modified Coulomb potentials,

$$V_\chi(x) = \sum_n \chi^n(x_\perp)V_n(z)$$  \hspace{1cm} (3.36)

replacing the attractive Coulomb potential and

$$V_{n,m}(z - z')\chi_n(x_\perp)\chi_m(x'_\perp)$$  \hspace{1cm} (3.37)

replacing the Coulomb repulsion, with

$$\chi^n(x_\perp) = \begin{cases} 1 & \text{for } \sqrt{(2n)/B} \leq |x_\perp| \leq \sqrt{2(n+1)/B} \\
0 & \text{otherwise.} \end{cases}$$  \hspace{1cm} (3.38)

I.e., for the respective minimizing density of a resulting MSTF functional, we have $\rho_{\text{MSTF}}(x) = B \sum_m \rho^{\text{MSTF}}_{m}(z)\chi_m(x_\perp)$ as well as $E_{\text{MSTF}} = E_{\text{DSTF}}$ for the energy.

Since $V_\chi(0) \sim B^{1/2}$, $V_\chi(x)$ can be regarded as a cut off Coulomb potential

$$\bar{V}(x) = \begin{cases} B^{1/2} & \text{for } |x| \leq B^{-1/2}, \\
|x|^{-1} & \text{for } |x| \geq B^{-1/2}. \end{cases}$$  \hspace{1cm} (3.39)

Hence, it is obvious that the main contribution to the difference $E_{\text{DSTF}} - E_{\text{STF}}$ stems from the Coulomb potential in the region $r \leq B^{-1/2}$, given by the term

$$B \int_{0 \leq r \leq B^{-1/2}} |\phi_{\text{STF}}|^{3/2} = O(B^{1/4}Z^{3/2}),$$  \hspace{1cm} (3.40)

which leads to the relation

$$E_{\text{DSTF}}(N, Z, B) - E_{\text{STF}}(N, Z, B) = O(B^{1/4}Z^{3/2}).$$  \hspace{1cm} (3.41)

The comparison with Theorem [1.7] shows that the DSTF theory has the same effect as the introduction of the gradient correction in (1.50) as well as in (1.40).
3.3 The discrete von Weizsäcker functional

The variable of the DSTF functional is given by a sum of one dimensional densities, emphasizing the character of lowest Landau band particles, whose positions orthogonal to the magnetic field are “frozen” and they therefore only move parallel to the magnetic field. Now taking into account the result (cf. e.g. Shao) that the first order correction to the semiclassical description of the one-dimensional free Fermi gas is given by $-\frac{1}{3}\int (\partial_z\sqrt{\rho(z)})^2$, we are motivated to propose the already mentioned discrete von Weizsäcker functional

$$E_{DW}[\rho] = \sum_{m \in \mathbb{N}_0} \left(-\frac{1}{3}\int |\partial_z\sqrt{\rho_m(z)}|^2 + \kappa \int \rho_m^3(z) - Z \int V_m(z)\rho_m(z)\right) + \tilde{D}(\rho,\rho).$$

(3.42)

Since the von Weizsäcker term appears with negative sign, (3.42) has the same defects as the Tomishima-Shinjo functional (1.46), i.e. it is not bounded from below and not convex. Precisely these two features (boundedness and convexity) of the semiclassical TF functionals, as well the (M)TFW functional, provided not only the existence of a minimizer but the existence of a solution of the corresponding TF equation.

As a way out of this problem we can define the energy corresponding to (3.42) by means of stationary solutions $\rho^N$, whose variational derivative vanish under the restriction $\sum_m \int \rho_m = N$ and $\rho \geq 0$. In order to avoid the assumption of positivity we concentrate on real functions $\psi$, with $\psi^2 = \rho$ and consider the functional

$$E[\psi] = \sum_{m \in \mathbb{N}_0} \left(-\frac{1}{3}\int |\partial_z\psi_m(z)|^2 + \kappa \int \psi_m^6(z) - Z \int V_m(z)\psi_m^2(z)\right) + \tilde{D}(\psi^2,\psi^2).$$

(3.43)

Let

$$D = \{\psi| \sum_m \int \psi_m^2 < \infty, \sum\int \psi_m^6 < \infty, \text{ and } \sum_m \int (\partial_z\psi_m)^2 < \infty\}$$

(3.44)

be the domain of (3.43). The question for stationary points in $D$, under the restriction $\sum_m \int \psi_m^2 = N$, is equivalent to the existence of a Lagrange parameter $\mu(N)$ and a $\psi^N$, so that

$$\frac{d}{dt} \left( E[\psi^N + t\eta] + \mu(N) \int (\psi^N + t\eta)^2 \right) \bigg|_{t=0} = 0,$$

(3.45)

for each $\eta \in D$. (3.45) yields the Euler-Lagrange equation, denoting $\psi^N = \psi$,

$$\frac{1}{3}\partial_z^2\psi_m(z) + 3\kappa\psi_m^5(z) = [\varphi_{eff}^{(m)}(z) - \mu(N)]\psi_m(z) \quad \forall m \in \mathbb{N}_0.$$

(3.46)

Starting from (3.43), (3.46) a priori only exists in the sense of distributions, but if there is a solution for (3.43) then one can conclude that it is even in $C^\infty(\mathbb{R}\setminus\{0\})$. 
If there is a solution $\psi^N$ for $N \in [0, N_c]$, with $N_c \geq Z$, then we can define the corresponding energy by

$$E_{\text{DW}}(N, Z, B) = \mathcal{E}[\psi^N] = \mathcal{E}_{\text{DW}}[(\psi^N)^2]. \quad (3.47)$$

### 3.3.1 Recovering the exchange term

Now we even go a step further. Following the reflections of Section 1.3.1 concerning the magnitude of the negative von Weizsäcker term we guess that $\mathcal{E}_{\text{DW}}$ is equivalent to the DDM functional ([L33]) for $B \ll Z^3$. Hence looking at ([L42]) we suggest another functional,

$$\mathcal{E}_{\text{DWHF}}[\rho] = \sum_{m \in \mathbb{N}_0} \left( -(1/3) \int |\partial_z \sqrt{\rho_m(z)}|^2 + \kappa \int \rho_m^3(z) - Z \int V_m(z) \rho_m(z) - c \ln(B/Z^{4/3}) \int \rho_m^2(z) + \tilde{D}(\rho, \rho) \right), \quad (3.48)$$

where we recover the exchange energy, which could be compared with the Thomas-Fermi-Dirac-von Weizsäcker functional ([L1]) in the $B = 0$ case.

### 3.3.2 The one-dimensional DW functional

In this section we study a toy model obtained by reducing ([L52]) to a one-dimensional functional and dropping the Coulomb repulsion, which leads to the functional

$$\mathcal{E}^{1\text{DW}}[\rho] = -\frac{1}{3} \int |\partial_z \sqrt{\rho(z)}|^2 + \kappa \int \rho^3(z) - Z \int V_0(z) \rho(z). \quad (3.49)$$

First of all we consider the corresponding TF functional

$$\mathcal{E}^{1\text{D}}_{B, Z}[\rho] = \kappa \int \rho^3(z) - Z \int V_0(z) \rho(z), \quad (3.50)$$

for which we easily get the following lemma:

**3.17. Lemma.** $\mathcal{E}^{1\text{D}}_{B, Z}[\rho]$, with $\rho \in L^3(\mathbb{R})$, is bounded from below, and there exists a unique minimizing density $\rho_0 \in L^3$, with $\mathcal{E}^{1\text{D}}_{B, Z}[\rho_0] = E^{1\text{D}}(Z, B)$.

*Proof.* Since $\int V_0 \rho \leq \|V_0\|_{3/2} \|\rho\|_3$, we get

$$\mathcal{E}^{1\text{D}}_{B, Z}[\rho] \geq \|\rho\|^3_3 - \|V_0\|^3_{3/2} \|\rho\|_3. \quad (3.51)$$

Minimizing over $\|\rho\|_3$, we get the first part of the lemma. The proof of second part works analogously to Propositions 3.2 and 3.3. \qed
For the minimizing density $\rho_0$ we get the simple TF equation
\[ 3\kappa \rho_0^2(z) = ZV_0(z). \] (3.52)
By the definition (1.33) one easily sees the relation
\[ V_0(z) \equiv V_0^B(z) = B^{1/2}V_0^1(B^{1/2}z), \] (3.53)
which implies an interesting scaling relation for the energy $E^{1D}(Z,B)$:

3.18. LEMMA.
\[ E^{1D}(Z,B) = Z^{3/2}B^{1/4}E^{1D}(1,1). \] (3.54)

Proof. Using the scaling relation (3.53) and defining
\[ \rho(z) = B^{1/4}Z^{1/2}\bar{\rho}(B^{1/2}z), \] (3.55)
we get
\[ \mathcal{E}_{B,Z}^{1D}[\rho] = B^{1/4}Z^{3/2}\mathcal{E}_{1,1}^{1D}[\bar{\rho}]. \] (3.56)

In the next Theorem we point out that for $B \ll Z^2$, the energy (3.54) is the semiclassical approximation of $\text{Tr}[-\partial_z^2 - ZV_0(z)]_-$, the sum of all negative eigenvalues of $-\partial_z^2 - ZV_0(z)$.

3.19. THEOREM. Let $B \leq Z^2$ and $\psi \in C_0^\infty(B(0,B^{-1/2}))$. Then
\[ \text{Tr}(\psi[-\partial_z^2 - ZV_0(z)]_-) = Z^{3/2}B^{1/4} \int \int \frac{dzdp}{2\pi} \psi[p^2 - V_0^1(z)]_- - O(B^{3/4}Z^{1/2}), \] (3.57)
and there is a constant $C$, such that
\[ |\text{Tr}[-\partial_z^2 - ZV_0(z)]_- - Z^{3/2}B^{1/4}E^{1D}(1,1)| \leq CB^{3/4}Z^{1/2}. \] (3.58)

Proof. Let us rewrite
\[ -\partial_z^2 - ZV_0^B(z) = B^{1/2}Z[-(B^{1/2}Z)^{-1}\partial_z^2 - V_0^1(B^{1/2}z)] \] (3.59)
and define the unitary operator
\[ (U(l)\psi)(z) = l^{1/2}\psi(lz). \] (3.60)
With $l = B^{-1/2}$ and the fact that unitary transformations do not change traces we derive
\[ \text{Tr}[-\partial_z^2 - ZV_0^B(z)]_- = B^{1/2}Z\text{Tr}[-h^2\partial_z^2 - V_0^1(z)]_- , \] (3.61)
where
\[ h = B^{1/4}Z^{-1/2}. \] (3.62)
So we have the self-adjoint Schrödinger operator
\[ H = -\hbar^2 \partial_z^2 - V_0^l(z), \] (3.63)
and its symbol
\[ h(z, p) = p^2 - V_0^l(z). \] (3.64)
Using the relation
\[ |\partial^\nu V_0^l(z)| \leq C^\nu \text{ on } B(0, 2) = \{ z | |z| < 2 \} \] (3.65)
and by means of some cut off function \( \psi \in C_0^\infty \), Theorem 6.1 yields
\[ \text{Tr}(\psi[z\phi V_0^l(z)]) = h^{-1} \int \int \frac{dpdz}{2\pi} \psi(z)[p^2 - V_0^l(z)] - O(h), \] (3.66)
which together with (3.61) and (3.62) immediately implies (3.57).

Recall, that by \( |t| = t \) for \( t \leq 0 \) and 0 otherwise.

In order to tackle the outer zone \( \{ z | 1 \leq |z| \leq \infty \} \), we note that the potential fulfills
\[ |\partial^\nu V_0^l(z)| \leq C^\nu |z|^{-\nu} \text{ for } |z| \geq 1. \] (3.67)
So by definition of the scaling functions \( l(z) = |z| \) and \( f(z) = 1 \), we can use Theorem 7.1, which states that with a cut off function \( \psi \in C^\infty(B(1, \infty)) \), we get
\[ \left| \text{Tr}[h^2 \partial_z^2 - V_0^l(z)] - h^{-1} \int \int \frac{dpdz}{2\pi} \psi[p^2 - V_0^l(z)] \right| \leq h \int_1^\infty dzl^{-2} \leq h. \] (3.68)
Combining (3.66) and (3.68) together with (3.61) and (3.62) completes the proof of Theorem 3.19.

Turning back to the functional (3.49), we recall that the corresponding energy has to be defined by means of the solution of the TF equation
\[ \partial_z^2 \psi(z) + 3\kappa\psi^5(z) - ZV_0^B(z)\psi(z) = 0. \] (3.69)
Introducing the scaling relations
\[ \psi(z) = B^{1/8}Z^{1/4} \varphi(zB^{1/2}), \quad z \rightarrow zB^{1/2}, \] (3.70)
(3.69) can be written as
\[ \frac{B^{1/2}}{Z} \partial_z^2 \varphi(z) + 3\kappa\varphi^5(z) - V_0^l(z) = 0. \] (3.71)
We set \( \varepsilon \equiv B^{1/2}/Z \ll 1 \) and make the ansatz \( \varphi = \varphi_0 + \varepsilon \varphi_1 \) to get an approximate solution of (3.71). Rescaling and inserting into (3.49) yields
\[ E^{IDW} = E^{IDW}[\psi^2] = Z^{3/2}B^{1/4}E^{ID}(1, 1) - O(B^{3/4}Z^{1/2}), \] (3.72)
which is in accordance with (3.57) and justifies a posteriori the introduction of the negative von Weizsäcker term in (1.52) and (3.49).
4 Some concluding remarks

Throughout this paper we have studied, among others, two functionals, the MTFW, which represents an approximation to the full quantum mechanical energy $E^Q$, and the DW functional, which should approximate the ground state energy $E^Q_{\text{conf}}$ of particles in the lowest Landau band. Now we can ask for the magnitude of $B$, for which the use of DW becomes more reasonable than MTFW. This question is connected with the estimation of

$$|E^Q(N, Z, B) - E^Q_{\text{conf}}(N, Z, B)|.$$ (4.1)

For $B \ll Z^3$ this can be compared with the difference of the corresponding semiclassical approximations

$$
B \int |\phi^{MTF}(x)|^{3/2}_+ dx + 2B \sum_{i \geq 1} \int |\phi^{MTF}(x) - 2iB|^{3/2}_+ dx - B \int |\phi^{STF}(x)|^{3/2}_+ dx
\leq C \int |Z|^{-1} - 2B |^{3/2}_+ dx \leq CZ^3 / B^{1/2}. \tag{4.2}
$$

From the preceding sections we guess, on the one hand,

$$|E^{\text{DW}} - E^Q_{\text{conf}}| \leq o(B^{4/5}Z^{3/5}), \tag{4.3}$$

and on the other hand we know

$$|E^{\text{MTFW}} - E^Q| \leq O(Z^2) + O(B^{4/5}Z^{3/5}). \tag{4.4}$$

Hence, one might expect the DW theory to give the better description of the quantum mechanical energy, if $Z^3 / B^{1/2} \leq B^{4/5}Z^{3/5}$, or, in other words, $B \geq Z^{24/13}$.

Summing up, we suggest to use MTFW theory for $B \leq Z^{24/13}$ and DW for $Z^{24/13} \leq B \ll Z^3$.

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