The magnetisation of large atoms in strong magnetic fields.

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Abstract

In this paper we study the asymptotic form of the magnetisation and current of large atoms in strong constant magnetic fields. We prove that the Magnetic Thomas-Fermi theory gives the right magnetisation/current for magnetic field strengths which satisfy $B \leq Z^{4/3}$.

Contents

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1 Introduction

Starting with the pioneering work of Lieb and Simon [LS77] the ground state properties of large atoms, the asymptotic exactness of approximating density functional theories and the corrections thereto have received a lot of attention. For atoms without magnetic fields Lieb and Simon proved that Thomas-Fermi theory gives the energy correctly to highest order. This started an enormous development which so far has resulted in the proof of a three term asymptotic expansion of the energy (Thomas-Fermi, Scott and Dirac-Schwinger terms) given in the monumental work [FS94].

For the case of atoms in strong, constant magnetic fields, it was proved in [LSY94] that a modified Thomas-Fermi theory - *Magnetic Thomas-Fermi theory* (MTF-theory) - gives the correct energy to highest order, when $B \ll Z^3$. The result has been generalized to non-constant magnetic fields in [ES97] (for $B \ll Z^2$). The convergence of the energy combined with a variational argument gives immediately that the ground state density is also given (to highest order) by MTF-theory.

In the presence of magnetic fields another quantity - the *magnetisation* - is as natural and important as the density, but till now it has not been established, whether MTF-theory also gives the right (asymptotic) answer for this quantity. The reason for this is that the asymptotic form of the magnetisation can not be derived directly from that of the energy, as is the case for the density.

In this paper, we prove that MTF-theory does indeed give the correct asymptotic magnetisation - at least for $B \leq CZ^{4/3}$. The proof of this statement relies on a novel commutator formula for the magnetisation (current) operator.

In this paper we study properties of the ground state of an atom. It is a standing hypothesis throughout the paper that this ground state exists. The proof of the asymptotics for the current is *not* valid for approximate ground states. This is similar to the situation in a non-interacting electron gas. Here it can be proved (see [Fou00]) that an approximate ground state does not necessarily have (approximately) the right current.

We will fix $\vec{A} = 1/2(-x^{(2)}, x^{(1)}, 0)$ as a vector field which generates a constant magnetic field of unit strength $\mathrm{rot}\vec{A} = (0,0,1)$. Now we introduce a parameter $B = |\vec{B}|$ measuring the strength of the magnetic field $\vec{B}$, and therefore we get the slightly odd relation: $\vec{B} = B\mathrm{rot}\vec{A}$. The Hamiltonian for a non-relativistic atom with N electrons and nuclear charge Z in the magnetic field $\vec{B}$ is:

$$H(N,Z,\vec{B}) = \sum_{j=1}^{N} \left[(\vec{p}_j + B\vec{A}(x_j))^2 + \vec{\sigma}_j \cdot \vec{B}(x_j) - \frac{Z}{|x_j|} \right] + \sum_{1 \le j < k \le N} \frac{1}{|x_j - x_k|}.$$

where $\vec{p} = -i\nabla$ and $\vec{\sigma}$ is the vector of Pauli spin matrices. The configuration space is the fermionic Hilbert space $\wedge_{j=1}^{N} L^2(\mathbb{R}^3, \mathbb{C}^2)$. We apply the convention that an index j on an operator means that it acts in the j-th electron space, i.e.

$$\begin{aligned} & (\vec{p}_j + B\vec{A}(x_j))^2 \psi_1(x_1) \otimes \ldots \otimes \psi_N(x_N) \\ \equiv \;& \psi_1(x_1) \otimes \ldots \otimes [(\vec{p}_j + B\vec{A}(x_j))^2 \psi_j(x_j)] \otimes \ldots \otimes \psi_N(x_N). \end{aligned}$$

1.1 The current/magnetisation

Let Ψ be the ground state of $H(N,Z,\vec{B})$ and let $\vec{a} \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$, then the *current* $\vec{j}$ is the distribution

$$\frac{d}{dt}|_{t=0} E(N,Z,\vec{B} + t\mathrm{rot}\vec{a}) = \int_{\mathbb{R}^3} \vec{a} \cdot \vec{j}\, dx,$$

if the derivative on the left hand side exists. It is easy to see, by the variational characterisation of the energy, that

$$\begin{aligned} & \frac{d}{dt}|_{t=0} E(N,Z,\vec{B} + t\mathrm{rot}\vec{a}) \\ = \;& \langle \Psi | J_N(\vec{B}, \vec{a}) | \Psi \rangle, \end{aligned}$$

if the derivative exists, where

$$J_N(\vec{B}, \vec{a}) = \sum_{j=1}^{N} \left(\vec{a}(x_j) \cdot (\vec{p}_j + B\vec{A}(x_j)) + (\vec{p}_j + B\vec{A}(x_j) \cdot \vec{a}(x_j)) + \vec{\sigma}_j \cdot \vec{b}(x_j) \right).$$

Here $\vec{b} = \mathrm{rot}\vec{a}$ is the magnetic field generated by $\vec{a}$. So we may *define* the current for all $\vec{a} \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$ by

$$\int_{\mathbb{R}^3} \vec{a} \cdot \vec{j}\, dx = \langle \Psi | J_N(\vec{B}, \vec{a}) | \Psi \rangle.$$

Since the energy does not depend on the choice of $\vec{a}$ - only on the magnetic field generated by $\vec{a}$ (gauge invariance) - we may write the derivative as

$$\frac{d}{dt}|_{t=0} E(N, Z, \vec{B} + t\vec{b}) = \int_{\mathbb{R}^3} \vec{b} \cdot \vec{M}\, dx,$$

where $\vec{M}$ by definition is the *magnetisation*. It is easy to see (by integration by parts) that $\mathrm{rot}\vec{M} = \vec{j}$.

1.2 Statement of the results

For matter in magnetic fields the correct Thomas-Fermi theory is the following *Magnetic Thomas-Fermi theory* (MTF theory). See [LSY94] for a discussion and further references.

$$\mathcal{E}_{MTF}[\rho; \vec{B}, V] = \int_{\mathbb{R}^3} \tau_{B(x)}(\rho(x))\, dx + \int_{\mathbb{R}^3} V(x)\rho(x)\, dx + D(\rho, \rho),$$

where $D(f, g) = \frac{1}{2} \iint f(x)|x - y|^{-1} g(y)\, dxdy$, $\tau_b(t) = \sup_{w \geq 0}[tw - P_B(w)]$, and $P_B(w) = \frac{B}{3\pi^2}\left(w^{3/2} + 2\sum_{\nu=1}^{\infty} |2\nu B - w|_-^{3/2}\right)$.

The MTF-energy $E_{MTF}(V, \vec{B})$ is the minimum of this functional on the natural domain. It is proved that there is a unique minimizer. Essentially, the result on the correctness of MTF-theory states that if $BZ^{-3} \to 0$ as $Z \to \infty$, with N/Z fixed, then

$$|E(N, Z, \vec{B}) - E_{MTF}(V, \vec{B})| = o(E_{MTF}(V, \vec{B}).$$

Asymptotically,

$$E_{MTF} \approx \left\{ \begin{array}{cl} Z^{7/3} & \text{for } B \leq CZ^{4/3} \\ Z^{7/3}(B/Z^{4/3})^{2/5} & \text{for } B/Z^{4/3} \to \infty \end{array} \right. .$$

Now we can state the result of the paper:

Theorem 1.1. *Let* $\vec{a}_0 = (a^{(1)}, a^{(2)}, 0) \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$*, and define* $\vec{a}(x) = l\vec{a}_0(x/l)$*, where* $l = Z^{-1/3}(1 + B/Z^{4/3})^{-2/5}$*. Let us assume that* $BZ^{-4/3} \leq C$ *for some constant* $C \in \mathbb{R}_+$*, and that* $\lambda = N/Z$ *is held fixed as* $Z \to \infty$*. Suppose finally that* Ψ *is a ground state for* $H(N, Z, \vec{B})$*, then*

$$\langle \Psi | J_N(\vec{B}, \vec{a}) | \Psi \rangle = \frac{d}{dt}|_{t=0} E_{MTF}(V, \vec{B} + t\mathrm{rot}\vec{a}) + o(Z^{7/3}),$$

as $Z \to \infty$*.*

A more precise result will be given in Thm 1.9 below.

Remark 1.2. Of course, the natural thing is to choose $\vec{a}(x/l)$ in such a way that the magnetic field generated is of the same order of magnitude as B. Thus we choose a test function $\vec{a} \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$ and look at $Bl\vec{a}(x/l)$. Notice, that Theorem 1.1 is not affected by scaling factors, since the current is linear in $\vec{a}$.

Remark 1.3. As will be seen below, it is important for the proof that Ψ is an eigenvector of $H(N, Z, \vec{B})$ - an approximate ground state does not necessarily have the right current. However, Ψ may be *any* ground state - uniqueness of the ground state is not assumed.

In the theorem above we only calculate the current perpendicular to the magnetic field. Notice, that the MTF energy only depends on the magnitude of the magnetic field - not on the direction of it. Therefore the MTF current, $\frac{d}{dt}|_{t=0} E_{MTF}(V, \vec{B} + t\mathrm{rot}\vec{a})$, does not depend on $a^{(3)}$, since the third component of $\vec{a}$ does not contribute to the first order change in $|\vec{B} + t\mathrm{rot}\vec{a}|$.

In order to include the parallel current in the result we will exploit a symmetry of the atomic Hamiltonian:

Let $\mathbb{P}$ be the unitary transformation that changes sign on the third component of all the electron coordinates i.e. $\mathbb{P} = P_1 \otimes \ldots \otimes P_N$, where

$$(P\psi)(x^{(1)}, x^{(2)}, x^{(3)}) = \psi(x^{(1)}, x^{(2)}, -x^{(3)}).$$

This operation leaves the Hamiltonian invariant and therefore we can impose on eigenstates for $H(N, Z, \vec{B})$ that they also be eigenfunctions of $\mathbb{P}$. This leads to the result on the parallel current:

Theorem 1.4. *Let the assumptions be as in Thm 1.1 except that* $\vec{a}_0 = (a^{(1)}, a^{(2)}, a^{(3)})$ *(i.e. the third component does not necessarily vanish) and that* Ψ *is an eigenfunction for* $\mathbb{P}$ *(i.e* $\mathbb{P}\Psi = \pm\Psi$*). Then*

$$\langle \Psi | J_N(\vec{B}, \vec{a}) | \Psi \rangle = \frac{d}{dt}|_{t=0} E_{MTF}(V, \vec{B} + t\mathrm{rot}\vec{a}) + o(Z^{7/3}),$$

as $Z \to \infty$*.*

In the rest of this introduction we will fix some notation and make a simple preliminary analysis which will permit us to state a more precise version of the main theorem.

1.3 The parallel current

Let us choose $\vec{a} = (0, 0, a^{(3)})$. It turns out that these particular test functions are difficult to handle in the theory, so we will use this subsection to reduce the calculation of the current to the calculation of the current perpendicular to the magnetic field.

The current $\int \vec{j} \cdot \vec{a}$ only depends on the magnetic field generated by $\vec{a}$ (gauge invariance) so we can start by asking when there exists an $\tilde{a} = (\tilde{a}^{(1)}, \tilde{a}^{(2)}, 0) \in C_0^\infty(\mathbb{R}^3)$ (notice: compact support) such that $\mathrm{rot}\tilde{a} = \mathrm{rot}\vec{a}$. It turns out to be the case if

$$\int_{-\infty}^{\infty} a^{(3)}(x^{(1)}, x^{(2)}, x^{(3)})\, dx^{(3)} = 0$$

for all $x^{(1)}, x^{(2)}$. In particular, this is the case if $a^{(3)}$ is an odd function in $x^{(3)}$. So we need only deal with even functions $a^{(3)}$:

Lemma 1.5. *Let* $\vec{a} = (0, 0, a^{(3)})$*, where* $a^{(3)} \in C_0^\infty(\mathbb{R}^3)$ *satisfies* $a^{(3)}(x^{(1)}, x^{(2)}, -x^{(3)}) = a^{(3)}(x^{(1)}, x^{(2)}, x^{(3)})$*, and let* Ψ *satisfy* $\mathbb{P}\Psi = \pm\Psi$*, then*

$$\langle \Psi | J_N(\vec{B}, \vec{a}) | \Psi \rangle = 0.$$

Remark 1.6. Notice that in this lemma we do not need Ψ to be an eigenfunction for the Hamiltonian.

Proof. We get

$$\langle \Psi | J_N(\vec{B}, \vec{a}) | \Psi \rangle = \langle \mathbb{P}\Psi | J_N(\vec{B}, \vec{a}) | \mathbb{P}\Psi \rangle = -\langle \Psi | J_N(\vec{B}, \vec{a}) | \Psi \rangle.$$

□

1.4 Scaling

It will be convenient for us to change to the natural length scale l of the atom. Therefore, we perform the following unitary transformation:

Let U_l be the unitary operator

$$(U_l\psi)(x_1,\dots,x_N) = l^{-3N/2}\psi(l^{-1}x_1,\dots,l^{-1}x_N),$$

where $l = Z^{-1/3}(1+\beta)^{-2/5}$, $\beta = (B/Z^{4/3})$. Then

$$U_l^{-1}H(N,Z,\vec{B})U_l = Zl^{-1}H_N(h,\mu)$$

and

$$U_l^{-1}J_N(\vec{B},Bl\vec{a}(x/l))U_l = Zl^{-1}\tilde{J}_N(h,\mu,\mu\vec{a}),$$

where

$$H_N(h,\mu) = \sum_{j=1}^{N}\left[(h\vec{p}_j+\mu\vec{A}(x_j))^2 + h\mu\vec{\sigma}_3 - \frac{1}{|x_j|}\right] + Z^{-1}\sum_{1\le j<k\le N}\frac{1}{|x_j-x_k|},$$

$$\begin{aligned}&\tilde{J}_N(h,\mu,\vec{a})\\ =&\sum_{j=1}^{N}\left[\vec{a}(x_j)\cdot(h\vec{p}_j+\mu\vec{A}(x_j)) + (h\vec{p}_j+\mu\vec{A}(x_j))\cdot\vec{a}(x_j) + h\mu\sigma_3 b^{(3)}(x_j)\right],\end{aligned}$$

$h = l^{-1/2}Z^{-1/2}$, $\mu = Bl^{3/2}Z^{-1/2}$. Notice that $h\to 0$ iff $BZ^{-3}\to 0$. In the rest of the paper Ψ_{scaled} will always denote a ground state of $H_N(h,\mu)$, which exists by assumption.

1.5 Commutator formula

Let us take an $\vec{a} = (a^{(1)},a^{(2)},0)\in C_0^\infty(\mathbb{R}^3)$, and define $\tilde{a} = (-a^{(2)},a^{(1)},0)$. We can now calculate the commutator

$$[H_N(h,\mu),\sum_{j=1}^{N}\tilde{a}(x_j)\cdot(h\vec{p}_j+\mu\vec{A}(x_j)) + (h\vec{p}_j+\mu\vec{A}(x_j))\cdot\tilde{a}(x_j)],$$

using the commutator formula from Section 2 below. Thereby we will find, using the virial theorem, that

$$\langle\Psi_{scaled}|J_N(h,\mu,\mu\vec{a})|\Psi_{scaled}\rangle = \langle\Psi_{scaled}|\tilde{J}_N(h,\mu,\tilde{a})|\Psi_{scaled}\rangle,$$

where

$$
\begin{aligned}
&\tilde{J}_N(h,\mu,\tilde{a}) = \\
&-\sum_{j=1}^{N}(h\vec{p}_j + \mu\vec{A}(x_j))(D\tilde{a}(x_j) + (D\tilde{a}(x_j))^T)(h\vec{p}_j + \mu\vec{A}(x_j)) - h\mu\sigma_3 b^{(3)}(x_j) \\
&-Z^{-1}\sum_{1\leq j<k\leq N}\frac{(x_j - x_k)\cdot(\tilde{a}(x_j) - \tilde{a}(x_k))}{|x_j - x_k|^3} \\
&+\sum_{j=1}^{N}\left(\frac{\tilde{a}(x_j)\cdot x_j}{|x_j|^3} - \frac{1}{2}h^2\Delta\mathrm{div}\tilde{a}(x_j)\right).
\end{aligned}
$$

Let us denote the terms on the right $\tilde{J}_{N,KIN}(\tilde{a})$, $\tilde{J}_{N,INT}(\tilde{a})$ and $\tilde{J}_{N,DENS}(\tilde{a})$ respectively.

From the convergence of the quantum mechanical density to the MTF-density (see [LSY94]), we easily get:

Theorem 1.7.

$$
\langle\Psi_{scaled}|\tilde{J}_{N,DENS}(h,\mu,\tilde{a})|\Psi_{scaled}\rangle \to Z\int\frac{\tilde{a}(x)\cdot x}{|x|^3}\rho_{\lambda,\beta}(x)\,dx,
$$

as $Z\to\infty$. Here $\rho_{\lambda,\beta}$ is the unique minimizer in scaled MTF-theory - see Section 3 below.

In the rest of the paper we will calculate the other two contributions to the current. The result is summarized in the following theorem:

Theorem 1.8. *Suppose there exists $C<\infty$ such that $\mu h\leq C$, then as $h\to 0$ we get*

$$
\begin{aligned}
&\langle\Psi_{scaled}|\tilde{J}_{N,KIN}(h,\mu,\tilde{a})|\Psi_{scaled}\rangle \\
=\;& -\frac{3}{2}Z\int(\partial_{x_1}a_2 - \partial_{x_2}a_1)\hat{P}_\beta(|v_{eff}|_-)\,dx \\
&-Z\int(\partial_{x_1}a_2 - \partial_{x_2}a_1)v_{eff}\rho_{\lambda,\beta}\,dx + o(Z),
\end{aligned}
$$

and

$$
\begin{aligned}
&\langle\Psi_{scaled}|\tilde{J}_{N,INT}(h,\mu,\tilde{a})|\Psi_{scaled}\rangle \\
=\;& Z\frac{1}{2}\iint\rho_{\lambda,\beta}(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho_{\lambda,\beta}(y)\,dxdy + o(Z).
\end{aligned}
$$

Here $\rho_{\lambda,\beta}$ is the unique minimizer in scaled MTF-theory (see Section 3 below) and $v_{eff} = -|x|^{-1} + \rho_{\lambda,\beta} * |x|^{-1} + \nu(\lambda,\beta)$, is the effective potential (also from scaled MTF-theory).

Using the results above it is easy to prove (see Section 3) the following theorem:

Theorem 1.9. *Let $\vec{a} = (a^{(1)}, a^{(2)}, 0) \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$ and let $\tilde{a} = (-a^{(2)}, a^{(1)}, 0)$, $b^{(3)} = \partial_{x^{(1)}} a^{(2)} - \partial_{x^{(2)}} a^{(1)}$. Suppose there exists $C < \infty$ such that $\mu h \le C$, then as $h \to 0$ (or equivalently $Z \to \infty$)*

$$\begin{aligned} &\langle \Psi_{scaled} | \tilde{J}_N(h,\mu,\tilde{a}) | \Psi_{scaled} \rangle \\ = \; & Z\frac{5}{2} \int b^{(3)}(x) \left(\hat{\tau}_\beta(\rho_{\lambda,\beta}(x)) + \frac{3}{5}\rho_{\lambda,\beta}(x) v_{eff}(x) \right) dx + o(Z). \end{aligned}$$

Here the term on the right hand side is exactly the current obtained in scaled MTF theory.

This is the desired more precise version of Thm 1.1. The rest of the paper will be devoted to its proof: In Section 2 we state the commutator formula used in the discussion above. Then in Section 3 we discuss MTF-theory and calculate the current in MTF-theory.
The term $\langle \Psi_{scaled} | \tilde{J}_{N,INT}(h,\mu,\tilde{a}) | \Psi_{scaled} \rangle$ can be seen as a new electron-electron interaction. This makes it look complicated at first sight, but it turns out to be fairly easy to include it in the MTF-theory and apply the ideas from [LSY94] to calculate the corresponding current. This is the subject of Sections 4 and 5. In order to see that this term can be reduced to a new term in the density functional theory we need to prove an inequality of Lieb-Oxford type. This is done in Appendix 6.
Finally, $J_{N,KIN}$: this operator is a one-particle operator and it is therefore only necessary to modify the semiclassical analysis in order to calculate the corresponding current. This is also done in Section 5. It is, however, this term which forces us to limit ourselves to the case $\mu h \le C$ (or $B \le CZ^{4/3}$), for a further discussion of this see [Fou00].

2 A commutator formula for the current

In this section we will violate slightly the conventions on the notation, since here we will let $\vec{A}$ be an arbitrary vector potential and thus $\vec{B} = \mathrm{rot}\vec{A}$ will not necessarily be constant in space.

Let us assume $|\vec{B}(x)| \neq 0$ for all x. Define

$$H = (-ih\nabla + \mu\vec{A})^2 + V(x),$$

and write $J_p(\vec{a}) = \vec{a} \cdot (-ih\nabla + \mu\vec{A}) + (-ih\nabla + \mu\vec{A}) \cdot \vec{a}$. Let furthermore

$$\begin{aligned} \tilde{a} &= \frac{\vec{B} \times \vec{a}}{|\vec{B}|^2}, \\ \mathbb{B} &= \begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix} = \{\partial_{x_j} A_k - \partial_{x_k} A_j\}_{j,k}. \end{aligned}$$

If now $\vec{a}(x) \cdot \vec{B}(x) = 0$ for all x, then $\mathbb{B}\tilde{a} = \vec{a}$.

Remark 2.1. Notice, that if $\vec{B} = (1, 0, 0)$ and $\vec{a} = (a_1, a_2, 0)$ then $\tilde{a} = (-a_2, a_1, 0)$.

Let us denote by $(;)$ the inner product in $\mathbb{R}^3$ and by $\langle ; \rangle$ the inner product in $L^2(\mathbb{R}^3)$. Let us finally write the magnetic momentum operator as $p_{\vec{A}} = (-ih\nabla + \mu\vec{A})$. Then we get:

Lemma 2.2. *If $|\vec{B}(x)| \neq 0$ and $\vec{a}(x) \cdot \vec{B}(x) = 0$ for all x, then*

$$\begin{aligned} [H, J_p(\tilde{a})] &= 2ih\tilde{a} \cdot \nabla V - 2ih\mu J_p(\vec{a}) \\ &\quad -2ih(p_{\vec{A}}; (D\tilde{a} + (D\tilde{a})^t)p_{\vec{A}}) - ih^3\Delta \mathrm{div}(\tilde{a}). \end{aligned}$$

Proof. The proof of Lemma 2.2 is essentially just a calculation. □

Corollary 2.3. *Let ϕ be an eigenfunction for H, i.e. $H\phi = \lambda\phi$, then*

$$\begin{aligned} \mu\langle \phi; J_p(\vec{a})\phi \rangle &= +\langle \phi; \tilde{a} \cdot \nabla V \phi \rangle \\ &\quad -\langle \phi; (p_{\vec{A}}; ((D\tilde{a} + (D\tilde{a})^t)p_{\vec{A}})\phi \rangle - \frac{1}{2}h^2\langle \phi; \Delta \mathrm{div}(\tilde{a})\phi \rangle. \end{aligned}$$

Proof. This follows from the virial theorem and the lemma above. □

3 Magnetisation in MTF-theory

The correct Thomas-Fermi-like theory for matter in magnetic fields is the following functional:

$$\mathcal{E}_{MTF}[\rho; \vec{B}, V] = \int_{\mathbb{R}^3} \tau_{B(x)}(\rho(x))\, dx + \int_{\mathbb{R}^3} V(x)\rho(x)\, dx + D(\rho,\rho),$$

where $D(f,g) = \frac{1}{2}\iint f(x)|x-y|^{-1}g(y)\, dxdy$, $\tau_B(t) = \sup_{w\geq 0}[tw - P_B(w)]$, and $P_B(w) = \frac{B}{3\pi^2}\left(w^{3/2} + 2\sum_{\nu=1}^{\infty}|2\nu B - w|_-^{3/2}\right)$.

The functional should be seen as giving the (MTF-) energy $\mathcal{E}_{MTF}$ as a function of the density $\rho(x) = |\psi(x)|^2$. The three terms in the functional represent the kinetic energy, the direct potential energy and the electronic repulsion, respectively.

In our case, we have $B(x) = B = const$ and $V(x) = -Z/|x|$. The domain of the functional is:

$$\mathcal{C}_B = \{\rho : \rho \geq 0, \int \rho(x)\, dx < +\infty, \int \tau_B(\rho(x))\, dx < +\infty, D(\rho,\rho) < +\infty\}.$$

We will restrict attention to the subset of $\mathcal{C}_B$ where the electron number is fixed, i.e.

$$\mathcal{C}_{B,N} = \{\rho \in \mathcal{C}_B | \int \rho = N\}.$$

In [LSY94] the existence of a unique minimizer was established:

Theorem 3.1. *There is a unique $\rho = \rho_{N,B,V} \in \mathcal{C}_{B,N}$ such that*

$$E(N,B,V) \stackrel{def}{=} \inf_{\eta \in \mathcal{C}_{B,N}} \mathcal{E}_{MTF}[\eta; \vec{B}, V] = \mathcal{E}_{MTF}[\rho; \vec{B}, V].$$

The minimizer satisfies the Thomas-Fermi equation:

$$\tau_B'(\rho(x)) = |V(x) + \rho * |x|^{-1} + \nu|_-,$$

for some (unique) $\nu = \nu(N,B,V)$.

This defines $V_{eff}(x) = V(x) + \rho * |x|^{-1} + \nu$.

Remark 3.2. We will also state some consequences of the Thomas-Fermi equation. From the definition of τ_B and P_B, we see that the inverse function of τ_B' is P_B', and therefore

$$\rho_{N,B,V}(x) = P_B'(|V_{eff}(x)|_-),$$

which again implies that

$$\tau_B(\rho_{N,B,V}(x)) = \rho_{N,B,V}(x)|V_{eff}(x)|_- - P_B(|V_{eff}(x)|_-).$$

From the Thomas-Fermi equation we get: $V_{eff}(x) \geq 0 \Rightarrow \rho_{N,B,V}(x) = 0$, and therefore the equation above can be written

$$-P_B(|V_{eff}(x)|_-) = \tau_B(\rho_{N,B,V}(x)) + V_{eff}(x)\rho_{N,B,V}(x).$$

We will also need the following results from MTF theory:

Proposition 3.3. *1.* $\frac{d}{dB}\tau_B(t) = \frac{5}{2B}\left(\tau_B(t) - \frac{3}{5}t\tau_B'(t)\right).$

2. $\tau_B'(t) \leq \kappa_1 t^{2/3}$, $\tau_B(t) \leq \frac{3}{5}\kappa_1 t^{5/3}$, *with* $\kappa_1 = (4\pi^2)^{2/3}$.

3. If $|\vec{B}(\cdot)| \to |\vec{B}_0(\cdot)|$ *in* $L^\infty_{loc}(\mathbb{R}^3)$*, then* $\rho_{N,\vec{B},V} \to \rho_{N,\vec{B}_0,V}$ *weakly in* $L^{5/3}_{loc}(\mathbb{R}^3)$.

Using this proposition we can prove that the MTF-energy is differentiable in the magnetic field:

Lemma 3.4.
- *Let* $\vec{a} \in C_0^\infty(\mathbb{R}^3)$ *and write* $\vec{b} = \mathrm{rot}\vec{a}$*, then the map* $t \mapsto E_{MTF}(N, \vec{B} + t\vec{b}, V)$ *is differentiable at* $t = 0$.
- *Let the distribution* $\vec{j}_{MTF}$ *be defined as*

$$\int \vec{j}_{MTF} \cdot \vec{a} = \frac{d}{dt}|_{t=0} E(N, \vec{B} + t\mathrm{rot}\vec{a}, V),$$

then

$$\int \vec{j}_{MTF} \cdot \vec{a} = \frac{5}{2}\int \frac{\vec{B} \cdot \mathrm{rot}\vec{a}}{B^2}[\tau_B(\rho) + \frac{3}{5}\rho V_{eff}]\, dx.$$

Proof. Denote by ρ_t the minimizer of $\mathcal{E}_{MTF}(\cdot, \vec{B}+t\vec{b}, V)$. Using the minimizing property we easily get:

$$\begin{aligned}
\int \tau_{|\vec{B}+t\vec{b}|}(\rho_t(x)) - \tau_{|\vec{B}|}(\rho_t(x))\,dx &= \mathcal{E}_{MTF}(\rho_t, \vec{B}+t\vec{b}, V) - \mathcal{E}_{MTF}(\rho_t, \vec{B}, V) \\
&\leq E_{MTF}(N, \vec{B}+t\vec{b}, V) - E_{MTF}(N, \vec{B}, V) \\
&\leq \mathcal{E}_{MTF}(\rho_0, \vec{B}+t\vec{b}, V) - \mathcal{E}_{MTF}(\rho_0, \vec{B}, V) \\
&= \int \tau_{|\vec{B}+t\vec{b}|}(\rho_0(x)) - \tau_{|\vec{B}|}(\rho_0(x))\,dx.
\end{aligned}$$

We will prove that $t^{-1}\int \tau_{|\vec{B}+t\vec{b}|}(\rho_t(x)) - \tau_{|\vec{B}|}(\rho_t(x))\,dx \to \int \frac{d}{dt}|_{t=0}\tau_{|\vec{B}+t\vec{b}|}(\rho_0(x))\,dx$ as $t \to 0$.

Let us choose $R > 0$ such that $\operatorname{supp}\vec{b} \subset B(0,R)$, where $B(0,R)$ denotes the ball of radius R around the origin. Using the proposition above and the compact support of $\vec{b}$ we get

$$\begin{aligned}
& \int \tau_{|\vec{B}+t\vec{b}|}(\rho_t(x)) - \tau_{|\vec{B}|}(\rho_t(x))\,dx \\
={}& \int_{B(0,R)} \tau_{|\vec{B}+t\vec{b}|}(\rho_t(x)) - \tau_{|\vec{B}|}(\rho_t(x))\,dx \\
={}& \int_{B(0,R)} \int_{|\vec{B}|}^{|\vec{B}+t\vec{b}|} \frac{5}{2\tilde{B}} \left(\tau_{\tilde{B}}(\rho_t) - \frac{3}{5}\rho_t\tau'_{\tilde{B}}(\rho_t)\right) d\tilde{B}dx \\
={}& \int_{|\vec{B}|}^{|\vec{B}+t\vec{b}|} \int_{B(0,R)} \frac{5}{2\tilde{B}} \left(\tau_{\tilde{B}}(\rho_0) - \frac{3}{5}\rho_0\tau'_{\tilde{B}}(\rho_0)\right) dxd\tilde{B} + o(t),
\end{aligned}$$

where we used the bounds on τ, τ' and the weak convergence in $L^{5/3}$ to get the last equality. This proves the differentiability and the formula

$$\frac{d}{dt}|_{t=0}E(N, \vec{B}+t\operatorname{rot}\vec{a}, V) = \int \frac{5}{2B}[\tau_B(\rho) - \frac{3}{5}\rho\tau'_B(\rho)]\,dx.$$

If we apply the Thomas-Fermi equation we get:

$$\int j_{MTF}\cdot\vec{a} = \frac{5}{2}\int \frac{\vec{B}\cdot\operatorname{rot}\vec{a}}{B^2}[\tau_B(\rho) + \frac{3}{5}\rho V_{eff}]\,dx.$$

Now it only remains to notice, from the Thomas-Fermi equation, that $\rho(x) = 0$ if $V_{eff}(x) > 0$. $\square$

3.1 A useful relation

When we calculate the limit of the current in quantum mechanics we will get a term which looks like

$$\iint \rho(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho(y)\,dxdy.$$

We will now use the minimizing property of the MTF-density ρ to obtain an equality for this term:

Lemma 3.5. *Let ρ be the minimizer in MTF-theory and let $\tilde{a} \in C_0^\infty(\mathbb{R}^3)$. Then*

$$\int \rho\tilde{a}\cdot\nabla V+\frac{1}{2}\iint \rho(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho(y)\,dxdy = \int \mathrm{tr}(D\tilde{a})P_B(|V_{eff}|_-).$$

Proof. Let us define $\rho_t(x) = \Lambda_t(x)\rho(x+t\tilde{a}(x))$ for small t, where $\Lambda_t(x) = |\det(I+tD\tilde{a}(x))| = 1+t\mathrm{tr}(D\tilde{a}(x))+O(t^2)$. Notice, that for small t we may write $x = \phi_t(x+t\tilde{a}(x))$, where $\phi_t(y) = y - t\tilde{a}(y)+O(t^2)$.

Now

$$\begin{aligned}
\mathcal{E}_{MTF}[\rho_t] &= \int \tau_B(\Lambda_t(\phi_t(y))\rho(y))\frac{dy}{\Lambda_t(\phi_t(y))} + \int V(\phi_t(y))\rho(y)\,dy \\
&\quad +\frac{1}{2}\iint \rho(x)\frac{1}{|\phi_t(x)-\phi_t(y)|}\rho(y)\,dxdy.
\end{aligned}$$

Using the minimizing property of ρ we get:

$$\begin{aligned}
0 &= \frac{d}{dt}|_{t=0}\mathcal{E}_{MTF}[\rho_t] \\
&= \int (\tau_B'(\rho)\rho\mathrm{tr}(D\tilde{a}) - \tau_B(\rho)\mathrm{tr}(D\tilde{a})) - \int \rho\nabla V\cdot\tilde{a} \\
&\quad -\frac{1}{2}\iint \rho(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho(y)\,dxdy.
\end{aligned}$$

Thus,

$$\begin{aligned}
&\int \rho\tilde{a}\cdot\nabla V + \frac{1}{2}\iint \rho(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho(y)\,dxdy \\
&= -\int \mathrm{tr}(D\tilde{a})(\tau_B(\rho)+\rho V_{eff}) \\
&= \int \mathrm{tr}(D\tilde{a})P_B(|V_{eff}|_-).
\end{aligned}$$

□

3.2 Scaling in MTF-theory

When $V(x) = \frac{-Z}{|x|}$ and $\vec{B} = B(1,0,0)$, we may define a scaled functional

$$\hat{\mathcal{E}}_\beta[\rho] = \int \hat{\tau}_\beta(\rho(x))\,dx + \int \frac{-\rho(x)}{|x|}\,dx + D(\rho,\rho),$$

where $\hat{\tau}_\beta(t) = (1+\beta)^{-8/5}\tau_\beta((1+\beta)^{6/5}t)$. The corresponding energy is

$$\begin{aligned}\hat{E}(\lambda,\beta) &= \inf\{\hat{\mathcal{E}}_\beta[\rho] | \rho \in L^1 \cap L^{5/3}, \rho \geq 0, \int \rho \leq \lambda\} \\ &= Z^{-7/3}(1+\beta)^{-2/5}E^{MTF}(N,B,Z),\end{aligned}$$

and the minimizing densities ρ^{MTF} and $\rho_{\lambda,\beta}$ are related by

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

Let us state the TF-equation:

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

or

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

Here $\hat{P}_\beta(w) = (1+\beta)^{-8/5}P_\beta((1+\beta)^{2/5}w)$, and $v_{eff}(x) = \frac{-1}{|x|} + \rho_{\lambda,\beta} * \frac{1}{|x|} + \nu(\lambda,\beta)$.

Notice also that

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

Using the identity from Lemma 3.5 we can prove the Theorem 1.9 - assuming the validity of Theorem 1.8:

Proof. From Theorem 1.8 and Theorem 1.7 we get that the quantum mechanical current in the limit behaves like:

$$\begin{aligned} & Z\int \frac{\tilde{a}(x)\cdot x}{|x|^3}\rho_{\lambda,\beta}(x)\,dx \\ - & \frac{3}{2}Z\int (\partial_{x_1}a_2 - \partial_{x_2}a_1)\hat{P}_\beta(|v_{eff}|_-)\,dx \\ & -Z\int (\partial_{x_1}a_2 - \partial_{x_2}a_1)v_{eff}\rho_{\lambda,\beta}\,dx \\ + & Z\frac{1}{2}\iint \rho_{\lambda,\beta}(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho_{\lambda,\beta}(y)\,dxdy.\end{aligned}$$

If we use the identity above on the first and the last term we get:

$$\begin{aligned} &= -\frac{5}{2}Z\int(\partial_{x_1}a_2-\partial_{x_2}a_1)\hat{P}_\beta(|v_{eff}|_-)\,dx \\ &\quad -Z\int(\partial_{x_1}a_2-\partial_{x_2}a_1)v_{eff}\rho_{\lambda,\beta}\,dx \\ &= \frac{5}{2}Z\int(\partial_{x_1}a_2-\partial_{x_2}a_1)\hat{\tau}_\beta(\rho_{\lambda,\beta})\,dx \\ &\quad +\frac{3}{2}Z\int(\partial_{x_1}a_2-\partial_{x_2}a_1)v_{eff}\rho_{\lambda,\beta}\,dx, \end{aligned}$$

which is exactly the result from MTF-theory. □

4 MTF-theory with a current term

In order to calculate the current we need to introduce a perturbed MTF-functional with a current term. We want to stress that this functional is not meant to have anything to do with the so-called *current density functional theories* appearing in the physics litterature. This functional is still a functional of the density alone, but it will enable us to calculate a part of the current.

The functional is:

$$\mathcal{E}_{C-MTF,t}[\rho;\vec{B},V,\tilde{a}] = \int_{\mathbb{R}^3}\tau_{B(x)}(\rho(x))\,dx + \int_{\mathbb{R}^3}V(x)\rho(x)\,dx + \tilde{D}_t(\rho,\rho),$$

where $\tilde{D}_t(f,g) = \frac{1}{2}\iint f(x)\frac{(x-y)\cdot(x-y+t(\tilde{a}(x)-\tilde{a}(y)))}{|x-y|^3}g(y)\,dxdy$, and where the other terms are as in standard MTF-theory.

It is easy to see that

$$(1-tc)D(\rho,\rho) \le \tilde{D}_t(\rho,\rho) \le (1+tc)D(\rho,\rho),$$

where c only depends on $\|D\tilde{a}\|_\infty$. We will assume t so small that the constants $1-tc$ and $1+tc$, appearing in the inequality above, can be bounded below resp. above by $1/2$ resp. $3/2$. Therefore the proofs of the main theorems in MTF-theory apply to C-MTF-theory essentially without change so we only state the following conclusion:

Theorem 4.1. *For sufficiently small (depending only on $\|D\tilde{a}\|_\infty$) t we have: There is a unique minimizer $\rho_t \in \mathcal{C}_{B,N}$ of $\mathcal{E}_{C-MTF}$. This ρ_t satisfies the Thomas-Fermi equation:*

$$\tau_B'(\rho_t(x)) = |V_{eff,t}|_-,$$

where $V_{eff,t} = V(x) + \int \frac{(x-y)\cdot(x-y+t(\tilde{a}(x)-\tilde{a}(y)))}{|x-y|^3}\rho_t(y)\,dy + \nu$. The Thomas-Fermi equation can also be formulated:

$$-P_B(|V_{eff,t}(x)|_-) = \tau_B(\rho_t(x)) + V_{eff,t}\rho_t(x).$$

The energy $E_{C-MTF,t}(N, \vec{B}, Z)$ is differentiable in t at $t = 0$ and satisfies

$$\frac{d}{dt}E_{C-MTF,t}(N, \vec{B}, Z) = \frac{1}{2}\int \rho_0(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho_0(y)\,dxdy.$$

4.1 Scaled C-MTF-theory

Suppose now $\tilde{a}(x) = l\tilde{a}_0(x/l)$ and define $\hat{\tau}_\beta(t) = (1+\beta)^{-8/5}\tau_\beta((1+\beta)^{6/5}t) = (1+\beta)^{2/5}\tau_{\beta(1+\beta)^{-4/5}}(t)$. Define furthermore,

$$\hat{\mathcal{E}}_{\beta,t}[\rho] = \int \hat{\tau}_\beta(\rho(x))\,dx + \int \frac{-1}{|x|}\rho(x)\,dx + D_t(\rho,\rho),$$

where $D_t(f,g) = \frac{1}{2}\iint f(x)\frac{(x-y)\cdot(x-y+t(\tilde{a}_0(x)-\tilde{a}_0(y)))}{|x-y|^3}g(y)\,dxdy$. Then the energy corresponding to $\hat{\mathcal{E}}_{\beta,t}$:

$$\hat{E}_{C-MTF,t}(\lambda,\beta) = \inf\{\hat{\mathcal{E}}_{\beta,t}[\rho] | \rho \in L^1 \cap L^{5/3}, \rho \geq 0, \int \rho \leq \lambda\},$$

satisfies

$$E_{C-MTF,t}(N,B,Z) = Z^2 l^{-1}\hat{E}_{C-MTF,t}(\lambda,\beta),$$

with $\lambda = N/Z$ and the minimizers $\rho = \rho_{C-MTF,t}(N,B,Z)$ and $\rho_{\lambda,\beta,t}$ of $\hat{\mathcal{E}}_{\beta,t}$ satisfy

$$\rho(x) = Zl^{-3}\rho_{\lambda,\beta,t}(x/l).$$

5 A lower bound on the perturbed quantum energy

In this section we will prove Theorem 1.8.

Lemma 5.1. *Suppose there exists $C < \infty$ such that $\mu h \leq C$, then as $h \to 0$ we get*

$$\begin{aligned} &\langle \Psi_{scaled} | \tilde{J}_{N,KIN}(h,\mu,\tilde{a}) | \Psi_{scaled} \rangle \\ \approx\; & -\frac{3}{2} Z \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) \hat{P}_\beta(|v_{eff}|_-)\, dx \\ & -Z \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) v_{eff} \rho_{\lambda,\beta}\, dx, \end{aligned}$$

and

$$\begin{aligned} &\langle \Psi_{scaled} | \tilde{J}_{N,INT}(h,\mu,\tilde{a}) | \Psi_{scaled} \rangle \\ \approx\; & Z \iint \rho_{\lambda,\beta}(x) \frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3} \rho_{\lambda,\beta}(y)\, dxdy. \end{aligned}$$

In the proof we will use the semiclassical lower bound from [Fou00]:

Lemma 5.2. *Let $v_{eff,t} = -|x|^{-1} + \int \frac{(x-y)\cdot(x-y+t(\tilde{a}(x)-\tilde{a}(y)))}{|x-y|^3} \rho_t(y)\, dy + \nu(\lambda,\beta)$, and*

$$H_N^0(t,h,\mu,v_{eff,t}) = \sum_{j=1}^N (p_{\vec{A}})_j \cdot S_t(x_j)(p_{\vec{A}})_j - \mu h(1+tb^{(3)}(x_j)) + v_{eff,t}(x_j),$$

where $S_t(x) = 1 + tM(x)$, $M(x) = -\left(D\tilde{a}(x) + (D\tilde{a}(x))^T\right)$. Then

$$\inf \operatorname{Spec} H_N^0(t,h,\mu,v_{eff,t}) \geq E_{scl}(t,h,\mu,v_{eff,t}) + o(h^{-3} + \mu h^{-2}),$$

where

$$\begin{aligned} &E_{scl}(t,h,\mu,v_{eff,t}) \\ =\; & \frac{\mu}{h^2} \sum_{\nu=0}^{\infty} d_\nu \int \frac{4b_{u,t}}{6\pi\Lambda_{u,t}} \left[(2\nu+1)\mu h b_{u,t} - \mu h(1+tb_3(u)) + v_{eff,t}(u)\right]_-^{3/2} du, \end{aligned}$$

where $b_{u,t} = |\mathrm{rot}_x \sqrt{1+tM(u)}\vec{A}(\sqrt{1+tM(u)}x)|$, $\Lambda_{u,t} = |\det\sqrt{1+tM(u)}|$ and $d_0 = \frac{1}{2\pi}$, $d_\nu = \frac{1}{\pi}$ for $\nu \geq 1$.

Remark 5.3. Notice, that the bound above only was proved for a fixed (independent of h) v. In the present case $v_{eff,t}$ depends on h. It is, however, easy (see [LSY94, p.99]) to see that the proof of the bound holds in our case as well.

Proof. Define $H_N(t,h,\mu) = H_N(h,\mu) + t(\tilde{J}_{N,KIN}(h,\mu,\tilde{a}) + \tilde{J}_{N,INT}(h,\mu,\tilde{a}))$. We seek a lower bound on

$$E_N(t,h,\mu) = \inf_{\|\psi\|=1} \langle \psi | H_N(t,h,\mu) | \psi \rangle.$$

Lower bound Let $\psi \in \wedge_{j=1}^N L^2(\mathbb{R}^3, \mathbb{C}^2)$, and let $\rho_t = \rho_{t,\lambda,\beta}$ be the minimizer of scaled C-MTF theory, then

$$\begin{aligned}
& \langle \psi | H_N(h,\mu) + t\tilde{J}_N(h,\mu) | \psi \rangle \\
\geq\ & \inf \operatorname{Spec} H_N^0(t,h,\mu,v_{eff,t}) \\
& + Z^{-1} \langle \psi | \sum_{j<k} \frac{(x_j - x_k) \cdot (x_j - x_k - t(\tilde{a}(x_j) - \tilde{a}(x_k)))}{|x_j - x_k|^3} | \psi \rangle \\
& - 2\tilde{D}_t(\rho_{t,\lambda,\beta}, \rho_\psi) - \nu N.
\end{aligned}$$

We can now use the bound given in the lemma above. The important thing about this bound is that we may write it as

$$E_{scl}(0,h,\mu,v_{eff,t}) + t\epsilon(t,h,\mu,v_{eff,t}),$$

by a Taylor expansion to zeroth order.

Finally, we integrate the Thomas-Fermi equation to get:

$$E_{scl}(0,h,\mu,v_{eff,t}) = Z\left(\hat{E}_{C-MTF,t}(\lambda,\beta) + \tilde{D}_t(\rho_{t,\lambda,\beta}, \rho_{t,\lambda,\beta}) + \mu \min(\lambda, \lambda_c)\right).$$

Using the modified Lieb-Oxford inequality and "completing the square" in $\tilde{D}_t$ we get

$$E_N(t,h,\mu) \geq Z\hat{E}_{C-MTF,t}(\lambda,\beta) + t\epsilon(t,h,\mu,v_{eff,t}) + Zo(\hat{E}_{C-MTF}(\lambda,\beta)).$$

Differentiation

By using Ψ_{scaled} in the variational principle for $E_N(t,h,\mu)$ we get

$$t\langle \Psi_{scaled} | \tilde{J}_{N,KIN}(h,\mu,\tilde{a}) + \tilde{J}_{N,INT}(h,\mu,\tilde{a}) | \Psi_{scaled} \rangle \geq E_N(t,h,\mu) - E_N(0,h,\mu).$$

We have from above and from the result

$$|E_N(t=0,h,\mu) - Z\hat{E}_{C-MTF}(t=0,\lambda,\beta)| = Zo(\hat{E}_{C-MTF}),$$

that

$$\begin{aligned} E_N(t,h,\mu) - E_N(t=0,h,\mu) \quad &\geq \quad Z\hat{E}_{C-MTF}(t,\lambda,\beta) - Z\hat{E}_{C-MTF}(t=0,\lambda,\beta) \\ &\quad +t\epsilon(t,h,\mu,v_{eff,t}) + Zo(\hat{E}_{C-MTF}(\lambda,\beta)). \end{aligned}$$

If we divide by t on both sides, multiply by Z^{-1}, let $Z \to \infty$ and afterwards let $t \to 0$ we get

$$\begin{aligned} &\langle \Psi_{scaled} | \tilde{J}_{N,KIN}(h,\mu,\tilde{a}) + \tilde{J}_{N,INT}(h,\mu,\tilde{a}) | \Psi_{scaled} \rangle \\ = \quad & Z\frac{d}{dt}|_{t=0}\hat{E}_{C-MTF}(t,\lambda,\beta) + \epsilon(0,h,\mu,v_{eff}), \end{aligned}$$

where

$$\begin{aligned} &\epsilon(0,h,\mu,v_{eff}) \\ = \quad & \frac{\mu}{h^2} 2 \sum_{\nu=0}^{\infty} \frac{2\nu\mu h}{2\pi^2} \int (\partial_{x_1} a_2 - \partial_{x_2} a_1)[2\nu\mu h - |v_{eff}|_-]_-^{1/2}\, dx \\ = \quad & -\frac{3}{2}h^{-3} \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) P_{h\mu}(|v_{eff}|_-)\, dx \\ & +h^{-3} \int (\partial_{x_1} a_2 - \partial_{x_2} a_1)|v_{eff}|_- P'_{h\mu}(|v_{eff}|_-)\, dx \\ = \quad & -\frac{3}{2}Z \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) \hat{P}_\beta(|v_{eff}|_-)\, dx \\ & +Z \int (\partial_{x_1} a_2 - \partial_{x_2} a_1)|v_{eff}|_- \hat{P}'_\beta(|v_{eff}|_-)\, dx. \end{aligned}$$

Using the TF-equation we get:

$$\begin{aligned} &\langle \Psi_{scaled} | \tilde{J}_{N,KIN}(h,\mu,\tilde{a}) | \Psi_{scaled} \rangle \\ \approx \quad & -\frac{3}{2}Z \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) \hat{P}_\beta(|v_{eff}|_-)\, dx \\ & -Z \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) v_{eff} \rho_{\lambda,\beta}\, dx, \end{aligned}$$

and

$$\begin{aligned}
&\langle \Psi_{scaled}|\tilde{J}_{N,INT}(h,\mu,\tilde{a})|\Psi_{scaled}\rangle \\
\approx\ & Z \iint \rho_{\lambda,\beta}(x) \frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3} \rho_{\lambda,\beta}(y)\, dxdy.
\end{aligned}$$

□

6 A modified Lieb-Oxford inequality

The original current operator is a sum of one-particle operators, but after application of the commutator formula we get a term of the form:

$$\sum_{j<k} \frac{(x_j-x_k)\cdot(\tilde{a}(x_j)-\tilde{a}(x_k))}{|x_j-x_k|^3}.$$

We want to replace $\langle\psi|\sum_{j<k}\frac{(x_j-x_k)\cdot(\tilde{a}(x_j)-\tilde{a}(x_k))}{|x_j-x_k|^3}|\psi\rangle$ by the direct interaction part $\iint \rho_\psi(x)\frac{(x-y)\cdot(\tilde{a}(x)-\tilde{a}(y))}{|x-y|^3}\rho_\psi(y)\, dxdy$. In this section we prove a lemma which will allow us to do so.

Let us recall the Lieb-Oxford inequality [LO81]:

Lemma 6.1. *Let $\psi \in \wedge_{j=1}^N L^2(\mathbb{R}^3)$ be normalized and let $\rho_\psi \in L^1(\mathbb{R}^3)$ be the corresponding density. Then the following inequality holds with a (negative) constant C independent of ψ:*

$$\langle\psi|\sum_{j<k}\frac{1}{|x_j-x_k|}|\psi\rangle \geq D(\rho_\psi,\rho_\psi) + C\int \rho_\psi^{4/3},$$

where $D(f,g) = \frac{1}{2}\iint \frac{f(x)g(y)}{|x-y|}\, dxdy$.

Here we want to modify the inequality above to accommodate the extra term we have from the current:

Lemma 6.2. *Let $\psi \in \wedge_{j=1}^N L^2(\mathbb{R}^3)$ be normalized and let $\rho_\psi \in L^1(\mathbb{R}^3)$ be the corresponding density. Let $\tilde{a} \in C_0^\infty(\mathbb{R}^3)$. Then the following inequality holds for sufficiently small (depending only on $\tilde{a}$) t with constants C_1, C_2 independent of ψ:*

$$\begin{aligned}
&\langle\psi|\sum_{j<k}\frac{(x_j-x_k)\cdot(x_j-x_k+t(\tilde{a}(x_j)-\tilde{a}(x_k)))}{|x_j-x_k|^3}|\psi\rangle \\
\geq\ & (1-C_1t^2)\tilde{D}_t(\rho_\psi,\rho_\psi) + C_2\int \rho_\psi^{4/3},
\end{aligned}$$

where $\tilde{D}_t(f,g) = \frac{1}{2}\iint f(x)\frac{(x-y)\cdot(x-y+t(\tilde{a}(x)-\tilde{a}(y)))}{|x-y|^3}g(y)\,dxdy$.

Proof. Let us pick a normalized $\psi \in \wedge_{j=1}^N L^2(\mathbb{R}^3)$ and let $\psi_t(x_1,\cdots,x_N) = \Lambda_t^{1/2}(x_1)\cdots\Lambda_t^{1/2}(x_N)\psi(x_1+t\tilde{a}(x_1),\cdots,x_N+t\tilde{a}(x_N))$, where $\Lambda_t(x) = \det(I+tD\tilde{a}(x))$. Then also $\psi_t \in \wedge_{j=1}^N L^2(\mathbb{R}^3)$ is normalized. Let us choose $\phi_t(y) = y - t\tilde{a}(y) + O(t^2)$ such that

$$\phi_t(x+t\tilde{a}(x)) = x.$$

Then we have

$$\langle\psi_t|\sum_{j<k}\frac{1}{|x_j-x_k|}|\psi_t\rangle = \langle\psi|\sum_{j<k}\frac{1}{|\phi_t(x_j)-\phi_t(x_k)|}|\psi\rangle,$$

so we get from the Lieb-Oxford inequality, applied to ψ_t:

$$\begin{aligned}
&\langle\psi|\sum_{j<k}\frac{1}{|\phi_t(x_j)-\phi_t(x_k)|}|\psi\rangle\\
\geq\;& D(\rho_{\psi_t},\rho_{\psi_t}) + C\int\rho_{\psi_t}^{4/3}\\
=\;& \frac{1}{2}\iint\rho_\psi(x)\frac{1}{|\phi_t(x)-\phi_t(y)|}\rho_\psi(y)\,dxdy + C\int\rho_\psi^{4/3}.
\end{aligned}$$

Now we notice that $\exists C$ only depending on $\tilde{a}$ such that

$$\begin{aligned}
&\frac{(x-y)\cdot(x-y+t(\tilde{a}(x)-\tilde{a}(y)))}{|x-y|^3} - Ct^2\frac{1}{|x-y|}\\
\leq\;& \frac{1}{|\phi_t(x)-\phi_t(y)|}\\
\leq\;& \frac{(x-y)\cdot(x-y+t(\tilde{a}(x)-\tilde{a}(y)))}{|x-y|^3} + Ct^2\frac{1}{|x-y|}.
\end{aligned}$$

This finishes the proof. □

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