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Abstract

In this talk I will discuss recent results on the magnetisation/current of large atoms in strong magnetic fields. It is known from the work of Lieb, Solovej and Yngvason [LSY94] that the energy and density of atoms in strong magnetic fields are given to highest order by a Magnetic Thomas Fermi theory (MTF-theory) when the magnetic field strength B and nuclear charge Z satisfy $BZ^{-3} \to 0$. It is, however, equally interesting to establish whether MTF-theory also gives the right asymptotic current. In this talk we will prove that this is indeed the case, at least for moderate magnetic fields. However, we will also prove that approximate ground states do not in general give the right asymptotics for the current.

1. Introduction

Let us consider a large neutral atom with nuclear charge Z in a strong magnetic field $\vec{B} = B(0,0,1)$. In a quantum mechanical description the dynamics of the atom is governed by the (Pauli-) Hamiltonian:

$$H(\vec{B}, V_Z) = \sum_{j=1}^{Z} \left\{ (-i\nabla_j + \vec{A}(x_j))^2 + \vec{B}(x_j) \cdot \vec{\sigma_j} + V_Z(x_j) \right\} + \sum_{1 \leq j < k \leq Z} \frac{1}{|x_j - x_k|},$$

Here $\vec{A}(x) = B/2(-x^{(2)}, x^{(1)}, 0)$, $V_Z(x) = \frac{-Z}{|x|}$ and $\vec{\sigma}$ is the vector of Pauli spin matrices. The unbounded, self-adjoint operator H acts on the Hilbert space $\mathcal{H} = \wedge^Z L^2(\mathbb{R}^3; \mathbb{C}^2)$. We have applied the convention that a suffix on a one particle operator means that the corresponding operator acts on the j'th electron i.e.

$$A_j \phi_1 \otimes \cdots \otimes \phi_Z = \phi_1 \otimes \cdots \otimes A\phi_j \otimes \cdots \otimes \phi_Z.$$

We will be interested in obtaining approximations for the energy, density and current of the atom in the case where B, Z are large i.e. we will let B, Z tend to infinity.

Part of the work presented in this article was done during the author's stay at the ESI in Vienna, fall 1999. He wishes to express his gratitude to Thomas and Maria Hoffmann-Ostenhof for giving him the opportunity to go there, and to Thomas Østergaard Sørensen for many discussions on this subject.

1.1. Basic notions

The (ground state) energy of the atom is defined by the variational principle:

$$E(\vec{B}, V_Z) = \inf_{\Psi \in \mathcal{H}, \|\Psi\|=1} \langle \Psi | H(\vec{B}, V_Z) | \Psi \rangle.$$

From the work of [AHS] it is known that the ground state energy is actually an eigenvalue, so we can let Ψ_0 denote a (not necessarily unique) ground state of $H(\vec{B}, V_Z)$.

The *density* ρ of the atom is defined as the distribution $\frac{\delta E}{\delta V}$ i.e.

$$\frac{d}{dt}|_{t=0} E(\vec{B}, V_Z + t\phi) = \int \rho\phi \, dx,$$

for all $\phi \in C_0^\infty(\mathbb{R}^3)$. By the variational principle it is easy to see that, if the derivative exists, we get:

$$\int \rho\phi \, dx = \langle \Psi_0 | \sum_{j=1}^{Z} \phi(x_j) | \Psi_0 \rangle,$$

or

$$\rho(x) = Z \int |\Psi_0(x, x_2, \cdots, x_Z)|^2 dx_2 \cdots dx_Z.$$

Here we used the symmetry properties of the space $\mathcal{H}$.

In the same way the *current* $\vec{j}$ is defined as the distribution $\frac{\delta E}{\delta \vec{A}}$ i.e. for all $\vec{a} \in C_0^\infty(\mathbb{R}^3; \mathbb{R}^3)$ we have

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

if the derivative on the left hand side exists. Using again the variational principle we get:

$$\int_{\mathbb{R}^3} \vec{a} \cdot \vec{j} \, dx, = \langle \Psi_0 | J_Z(\vec{B}, \vec{a}) | \Psi_0 \rangle,$$

if the derivative exists, where

$$J_Z(\vec{B}, \vec{a}) = \sum_{j=1}^{Z} \left(\vec{a}(x_j) \cdot (-i\nabla_j + B\vec{A}(x_j)) + (-i\nabla_j + B\vec{A}(x_j) \cdot \vec{a}(x_j)) + \vec{\sigma}_j \cdot \vec{b}(x_j) \right).$$

Here $\vec{b} = \text{curl}\vec{a}$ is the magnetic field generated by $\vec{a}$.

Remark 1.1. Notice that even if the ground state is degenerate the above formulas hold for *any* ground state wave function Ψ_0.

We may *define* the current for all $\vec{a} \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$ by

$$\int_{\mathbb{R}^3} \vec{a} \cdot \vec{j} \, dx = \langle \Psi_0 | J_Z(\vec{B}, \vec{a}) | \Psi_0 \rangle.$$

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 curl$\vec{M} = \vec{j}$.

1.2. Magnetic Thomas-Fermi theory

It is known from the work of Lieb, Solovej and Yngvason that the energy of the atom can be approximated by a functional of the density alone. Let us introduce a bit of notation:

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

where $D(f,g) = \frac{1}{2}\int f(x)|x-y|^{-1}g(y)\,dxdy$, $\tau_B(t) = \sup_{w\geq 0}[tw - P_B(w)]$, 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 ρ. The three terms in the functional represent the kinetic energy[1] , the direct potential energy and the electronic repulsion, respectively.

We define the MTF-energy as the minimum of the above functional:

$$E_{MTF}(\vec{B},V) = \inf_{\rho\in\mathcal{C}_{\vec{B},V}} \mathcal{E}_{MTF}[\rho;\vec{B},V],$$

where the domain $\mathcal{C}_{\vec{B},V}$ is given by:

$$\mathcal{C}_{\vec{B},V} = \{\rho|\rho\geq 0, \int\rho = Z, \int\tau_{B(x)}(\rho(x))dx < \infty, D(\rho,\rho)<\infty\}.$$

It can be proved, that there is a unique minimizing density ρ_{MTF} of the functional.

The MTF-theory is meant as a simpler, approximate theory of large atoms, and indeed we find:

Theorem 1.2 ([LSY94] Convergence of the energy). *Let $V(x) = Zl^{-1}v(x/l)$ where $v\in L^{5/2}+L^{\infty}$, $v(x)\to 0$ as $|x|\to\infty$ and where $l = Z^{-1/3}(1+\beta)^{-2/5}$, with $\beta = B/Z^{4/3}$. Then*

$$\frac{E(\vec{B},V)}{E_{MTF}(\vec{B},V)} \to 1,$$

as $B,Z\to\infty$ with $B/Z^3\to 0$.

Remark 1.3. By a study of the scaling behaviour of $\mathcal{E}_{MTF}$ we get that both energies have the following order :

$$E(\vec{B},V_Z) \approx Z^{7/3}(1+\beta)^{2/5}.$$

[1] In Thomas-Fermi theory without magnetic fields, the kinetic energy $\tau(\rho)$ is taken as $\tau(\rho) = c_{TF}\rho^{5/3}$.

Remark 1.4. The result above has been generalised to nonconstant magnetic fields by [ES97].

By a variational argument (see below) the convergence of the energy gives immediately the convergence of the density.

Theorem 1.5 (Convergence of the density [LSY94]). *Let ρ be the minimizer of $\mathcal{E}_{MTF}$ and define $\rho_\beta(x)$ by $\rho(x) = Zl^{-3}\rho_\beta(x/l)$. Let ρ^Q be the quantum mechanical density. If $Z \to \infty$, $B/Z^3 \to 0$ and $B/Z^{4/3} \to \beta$, $0 \leq \beta \leq \infty$, then*

$$Z^{-2}(1 + B/Z^{4/3})^{-6/5}\rho^Q(x/l) \to \rho_\beta,$$

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

One would now naturally suppose that MTF-theory also gives the right current. Notice that it is quite easy to calculate the MTF-current:

Lemma 1.6.

- *Let $\vec{a} \in C_0^\infty(\mathbb{R}^3)$ and write $\vec{b} = \mathrm{curl}\vec{a}$, 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*

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

then

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

where ρ is the unique minimizer of $\mathcal{E}_{MTF}$, and $V_{eff} = V + \rho * |x|^{-1} + \mu_0$ is the effective potential.

It will indeed turn out, that we can prove the following theorem:

Theorem 1.7 (Convergence of the current [Fou00a]). *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 $C \in \mathbb{R}_+$. Suppose finally that Ψ is a ground state for $H(\vec{B}, V_Z)$, then*

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

as $Z \to \infty$.

In the rest of this paper we will discuss why it is correct, though maybe a little surprising that MTF-theory gives the right current of the atom.

Let us first discuss why MTF-theory might *not* give the right current. In order to do that let us look a bit at the proof that MTF-theory gives the right *density*:

1.3. The convergence argument for the density

We immediately get, by using Ψ_0 in the variational principle for $E(\vec{B}, V_Z + t\phi)$ and $E(\vec{B}, V)$, the following inequality:

$$E(\vec{B}, V_Z + t\phi) - E(\vec{B}, V_Z) \leq \langle \Psi_0 | t \sum_{j=1}^{Z} \phi(x_j) | \Psi_0 \rangle,$$

where Ψ_0 is a ground state for $H(\vec{B}, V_Z)$. If we know that $E(\vec{B}, V_Z + t\phi) = E_{MTF}(\vec{B}, V_Z + t\phi) + o(E_{MTF}(\vec{B}, V_Z + t\phi))$, then we can let Z, B tend to infinity in the above inequality, then divide by t and let t tend to zero. Thereby we get[2]:

$$\langle \Psi_0 | \sum_{j=1}^{Z} \phi(x_j) | \Psi_0 \rangle = \frac{d}{dt}|_{t=0} E_{MTF}(\vec{B}, V_Z + t\phi) + o(E_{MTF}(\vec{B}, V_Z)).$$

The derivative on the right does exist and gives exactly the MTF-density.

Unfortunately, the above argument does not work for the current as the following calculation shows:

Let us define

$$H(t) = H(\vec{B}, V_Z) + t J_Z(\vec{B}, B\vec{a}),$$

in order to try the plan of attack above. But now,

$$H(t) = H(\vec{B} + tB\text{curl}\vec{a}, V_Z) - B^2 t^2 \sum_{j=1}^{Z} \vec{a}^2(x_j),$$

and $E(\vec{B} + tB\text{curl}\vec{a}, V_Z) \approx E(\vec{B}, V_Z)$ but

$$\begin{aligned} \langle \Psi_0 | B^2 t^2 \sum_{j=1}^{Z} \vec{a}^2(x_j) | \Psi_0 \rangle &= t^2 B^2 \int \rho(x) \vec{a}^2(x)\, dx \\ &\approx B^2 t^2 E(\vec{B}, V_Z), \end{aligned}$$

where $a \approx b$ means that a, b have the same order of magnitude in Z, B.

Therefore, this second term, which is of second order in t and thus vanishes upon taking t to zero, is of too high order in the parameters B, Z and spoils the picture.

The above only shows that the method of proof for the density does not carry over directly to the case of the current. Worse is that we can in fact show that "approximate ground states" do not necessarily give the right current i.e. it is possible to construct sequences of functions $\Psi_{Z,B}$ such that

$$\langle \Psi_{Z,B} | H(\vec{B}, V_Z) | \Psi_{Z,B} \rangle = E_{MTF}(\vec{B}, V_Z) + o(E(\vec{B}, V_Z)),$$

but

$$\langle \Psi_{Z,B} | J_Z(\vec{B}, B\vec{a}) | \Psi_{Z,B} \rangle \neq J_{MTF}(\vec{B}, V_Z) + o(E(\vec{B}, V_Z)).$$

This is in sharp contrast to the case of the density, where all approximate ground states give the right density to highest order.

In the next section (Section 2) we will give a semiclassical example of what can go wrong with approximate ground states. Then in Section 3 we will explain the main ingredient of the proof of Theorem 1.7.

[2]We get two inequalities since t can take both positive and negative values.

2. A density matrix with too high current

In order to illustrate that the current can, in fact, be orders of magnitude too big, let us go to a semiclassical picture. For simplicity, let us look at a two-dimensional situation:

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

acting on $L^2(\mathbb{R}^2)$. We suppose $\vec{A} = 1/2(-x_2, x_1)$, $\mu h = 1$ and let $h \to 0$. This describes a non-interacting electron gas in the external magnetic field of strength μ and electric potential V. The energy of the gas is

$$\begin{aligned} E(h,\mu,V) &= \operatorname{tr}[H 1_{(-\infty;0]}(H)] \\ &= -\frac{\mu}{h}\int \frac{1}{2\pi}\left([V]_- + 2\sum_{\nu=1}^{\infty}[2\nu + V]_-\right) dx + o(\frac{\mu}{h}) \\ &= \frac{\mu}{h}E_{scl}(V) + o(\mu/h). \end{aligned}$$

The density is given by

$$\begin{aligned} \int \rho\phi\, dx &= \operatorname{tr}[\phi 1_{(-\infty;0]}(H)] \\ &\stackrel{def}{=} \frac{\mu}{h}\frac{d}{dt}|_{t=0} E_{scl}(V + t\phi) + o(\mu/h), \end{aligned}$$

and the current by

$$\int \vec{j}\cdot\mu\vec{a}\, dx = \operatorname{tr}[J(\mu\vec{a})1_{(-\infty;0]}(H)],$$

where

$$J(\mu\vec{a}) = \mu\vec{a}\cdot(-ih\nabla + \mu\vec{A}(x)) + (-ih\nabla + \mu\vec{A}(x))\cdot\mu\vec{a} - \mu h(\partial_{x_1}a_2 - \partial_{x_2}a_1).$$

In order to simplify some expressions we will write $\vec{p_{\vec{A}}} = (-ih\nabla + \mu\vec{A}(x))$.

We want to prove that it is necessary to use something like our commutator argument below (see Section 4) in order to calculate the current. Therefore we will produce an example of a density matrix γ that gives the right energy to highest order - but gives a current of too high order.

Lemma 2.1. *There exists a potential $V(x) \in C_0^\infty(\mathbb{R}^2)$ and a test function $\vec{\phi} = (\phi_1, \phi_2) \in C_0^\infty(\mathbb{R}^2)$ together with a density matrix i.e. an operator γ satisfying $0 \leq \gamma \leq 1$ such that*

$$\operatorname{tr}[H\gamma] = \frac{\mu}{h}E_{scl}(V) + o(\frac{\mu}{h}),$$

and

$$\frac{h}{\mu}|\operatorname{tr}[J(\mu\phi)\gamma]| \to \infty,$$

as $h \to 0$.

Thus the lemma says that a density matrix that gives the right energy does *not* necessarily give the right current. This is unlike the situation for the density, since it is easy to prove that a density matrix that gives the right energy also gives the right density.

The key to the construction is the following: The current operator - as opposed to the energy operator (the Hamiltonian) - mixes the Landau levels. In fact, the main part of the current operator does not respect the Landau levels - the part that does is much smaller[3]. Thus, a density matrix that gives the right energy but contains a small part which mixes neighboring Landau levels should have too large a current. As the proof below shows this turns out to be the case.

Proof. We will construct our density matrix as a small perturbation of a density matrix which respects the Landau levels and gives the right energy.
Let us choose $V \in C_0^\infty(\mathbb{R}^2)$, which satisfies $[V(x)]_- = 10$ for all $x \in B(0,2)$ ($=\{y \in \mathbb{R}^2 \,|\, |y| < 2\}$). We will choose a test vector $\vec{\phi} = (\phi_1, \phi_2)$, which is supported in $B(0,1)$.

The density matrix γ' which gives the correct energy is:

$$\gamma' = \sum_{\nu=1}^{\infty} \frac{1}{2\pi} \int M(\nu,u)\Pi(\nu,u)\, du,$$

where $M(\nu,u)$ is the characteristic function of the set (in $(\mathbb{N}_+ \cup \{0\}) \times \mathbb{R}_u^2$)

$$\{(\nu,u) | 2\nu\mu h + V(u) \leq 0\},$$

and where $\Pi(\nu,u)$ is an operator with kernel

$$\Pi(\nu,u)(x,y) = g_r(x-u)\Pi_\nu^{(2)}(x,y)g_r(y-u).$$

In this last expression g_r is a localisation function $g_r(x) = r^{-1}g(x/r)$, $0 \leq g \in C_0^\infty(\mathbb{R}^2)$, $\int g^2 = 1$ and $r = h^{1-\alpha}$ for some $0 < \alpha < 1$. Furthermore, $\Pi_\nu^{(2)}(x,y)$ is the integral kernel of the projection to the ν-th Landau level:

$$\Pi_\nu^{(2)}(x,y) = \frac{\mu}{2\pi h} \exp\{i(x_1y_2 - x_2y_1)\frac{\mu}{2h} - |x-y|^2\frac{\mu}{4h}\}L_\nu(|x-y|^2\frac{\mu}{2h}),$$

where L_ν are Laguerre polynomials normalised by $L_\nu(0) = 1$.
We will not prove here that γ' gives the right energy to highest order. This will follow from calculations similar to those below (or see [LSY94]).

Let now $\tilde{M}$ be the characteristic function of $B(0,1)_u$, and write

$$\tilde{\gamma} = \epsilon \int \tilde{M}(u)\tilde{\Pi}(u)\, du,$$

where $\epsilon \to 0$ as $h \to 0$ and where

$$\tilde{\Pi}(u)(x,y) = g_r(x-u)P(x,y)g_r(y-u).$$

[3] This can be seen explicitly from the commutator formula in Section 4.

In this final expression P is the operator

$$P = \Pi_1^{(2)} a^* \Pi_0^{(2)} + \Pi_0^{(2)} a \Pi_1^{(2)},$$

with $a = p_{\vec{A},1} - ip_{\vec{A},2}, a^* = p_{\vec{A},1} + ip_{\vec{A},2}$ being the raising and lowering operators that define the Landau levels.

We finally define $\gamma = \gamma' + \tilde{\gamma}$. Since the operator P satisfies (remember $\mu h = 1$)

$$-c(\Pi_0^{(2)} + \Pi_1^{(2)}) \leq P \leq c(\Pi_0^{(2)} + \Pi_1^{(2)}),$$

it is easy to see that $0 \leq \gamma$ for sufficiently small ϵ. In order to get $\gamma \leq 1$ we should multiply by a factor $\frac{1}{1+\delta}$, where $\delta \to 0$ as $h \to 0$. We will not do this, since it will not affect order of magnitude estimates and only obscure notation.

We need to calculate

$$\mathrm{tr}[H\gamma] = \frac{\mu}{h} E_{scl} + \mathrm{tr}[H\tilde{\gamma}] + o(\mu/h),$$

and

$$\mathrm{tr}[h^{-1} J_p(\vec{\phi})\gamma],$$

with $J_p(\vec{\phi}) = \vec{\phi} \cdot \vec{p}_{\vec{A}} + \vec{p}_{\vec{A}} \cdot \vec{\phi}$. Notice that since γ gives the right *density* to highest order, we do not need to calculate the spin current i.e. $\mathrm{tr}[\mu h(\partial_{x_1}\phi_2 - \partial_{x_2}\phi_1)\gamma]$, since we know this to be of order $\frac{\mu}{h}$ once we have proved that γ gives the right energy. Furthermore, we may assume that γ' does *not* satisfy the requirements of Lemma 2.1 - if it does we do not have to construct anything.

The energy: Using linearity, we write,

$$\mathrm{tr}[H\tilde{\gamma}] = \epsilon \int \tilde{M}(u) \mathrm{tr}[H\tilde{\Pi}(u)]\, du,$$

and then we use the AMS-localisation formula:

$$2gp_{\vec{A}}^2 g - (p_{\vec{A}}^2 g^2 + g^2 p_{\vec{A}}^2) = [[g, p_{\vec{A}}^2], g].$$

Let us first look at the potential energy:

$$\mathrm{tr}[V\tilde{\Pi}(u)] = \mathrm{tr}[g_r^2(\cdot - u)VP].$$

This is small (i.e $o(\mu)$) since $\Pi_1^{(2)} f \Pi_0^{(2)}$ is small for $f \in C_0^\infty$ (see Lemma 2.2 below). For the kinetic energy term we get:

$$\begin{aligned}
&\mathrm{tr}[(p_{\vec{A}}^2 - \mu h)\tilde{\Pi}(u)] \\
&= \frac{1}{2}\mathrm{tr}\left((p_{\vec{A}}^2 g_r^2(\cdot - u) + g_r^2(\cdot - u)p_{\vec{A}}^2 - 2\mu h)P + 2[[g_r(\cdot - u), p_{\vec{A}}^2], g_r(\cdot - u)]P\right) \\
&= \frac{1}{2}\mathrm{tr}\left(2\mu h g_r^2(\cdot - u)P + 2h^2(\nabla g_r(\cdot - u))^2 P\right).
\end{aligned}$$

This term is small for the same reason as above. Thus we may choose ϵ to go to zero slowly with h - for definiteness let us take $\epsilon = |\log h|^{-1}$.

The current:
In order to calculate the current we write

$$\mathrm{tr}[J_p(\vec{\phi})\tilde{\gamma}] = 2\Re\mathrm{tr}[\vec{\phi}(-ih\nabla + \mu\vec{A})\tilde{\gamma}],$$

so we only need to consider

$$\begin{aligned}
&\mathrm{tr}[\vec{\phi}(-ih\nabla + \mu\vec{A})\tilde{\gamma}] \\
= \;& \epsilon \int \tilde{M}(u)\mathrm{tr}[\vec{\phi}(-ih\nabla + \mu\vec{A})\tilde{\Pi}(u)]\, du \\
= \;& \epsilon \int \tilde{M}(u)\mathrm{tr}[\vec{\phi}(-ih\nabla g_r(\cdot - u))Pg_r(\cdot - u)]\, du \\
& +\epsilon \int \tilde{M}(u)\mathrm{tr}[\vec{\phi}g_r(\cdot - u)(-ih\nabla + \mu\vec{A})Pg_r(\cdot - u)]\, du
\end{aligned}$$

Since $\Pi_j^{(2)} f \Pi_k^{(2)}$ is small when $j \neq k$, $f \in C_0^\infty$, we get that the highest order contribution comes from a part of the second term, namely:

$$\begin{aligned}
& \epsilon \int \tilde{M}(u)\mathrm{tr}[g_r(\cdot - u)\vec{\phi}\begin{pmatrix} (a+a^*)/2 \\ (a^* - a)/(2i) \end{pmatrix} Pg_r(\cdot - u)]\, du \\
\approx \;& \epsilon \int \tilde{M}(u)\mathrm{tr}[g_r^2(\cdot - u)\left\{\vec{\phi}\begin{pmatrix} \mu h \\ i\mu h \end{pmatrix}\Pi_0^{(2)} + \vec{\phi}\begin{pmatrix} \mu h \\ -i\mu h \end{pmatrix}\Pi_1^{(2)}\right\}]\, du.
\end{aligned}$$

If we remember that $\mu h = 1$ and choose $\phi_2 = 0$ we can calculate the trace as:

$$\begin{aligned}
& \epsilon \int \tilde{M}(u) g_r^2(x-u)\phi_1(x)\left(\Pi_0^{(2)}(x,x) + \Pi_1^{(2)}(x,x)\right)\, dxdu \\
= \;& \frac{\epsilon\mu}{2\pi h}\int \tilde{M}(u) g_r^2(x-u)\phi_1(x)\, dxdu \\
= \;& \frac{\epsilon\mu}{2\pi h}\int_{|u|\leq 1}\int r^{-2}g^2((x-u)/r)\phi_1(x)\, dxdu \\
\approx \;& \frac{\epsilon\mu}{2\pi h}\int \phi_1(x)\, dx.
\end{aligned}$$

If we remember that this term has to be multiplied by h^{-1} it is easy to see that we have reached our aim. □

Lemma 2.2. *Let $\phi \in C_0^\infty(\mathbb{R}^2)$, then*

$$\|[\Pi_j^{(2)}, \phi]\|_{\mathcal{B}(L^2)} \leq C_j\sqrt{h/\mu}\|\nabla\phi\|_\infty,$$

where the norm of the operator on the left is the operator norm as a bounded operator in L^2.

Proof. We use Schur's Lemma i.e. the following bound on the norm of an integral kernel:

$$\|K(x,y)\|_{\mathcal{B}(L^2)} \leq \max(\sup_x \int |K(x,y)|\, dy, \sup_y \int |K(x,y)|\, dx).$$

The integral kernel $K(x,y)$ of $[\Pi_j^{(2)},\phi]$ is

$$K(x,y)=\Pi_j^{(2)}(x,y)(\phi(y)-\phi(x))=\Pi_j^{(2)}(x,y)\int_0^1(y-x)\cdot\nabla\phi(x+t(y-x))\,dt.$$

So we estimate:

$$\begin{aligned}\int|K(x,y)|\,dy &\le \|\nabla\phi\|_\infty\int|\Pi_j^{(2)}(x,y)||x-y|\,dy\\ &= \|\nabla\phi\|_\infty\sqrt{h/\mu}\int|\Pi_j^{(2)}(x,y)|\sqrt{\mu/h}|x-y|\,dy.\end{aligned}$$

Now we use the fact that $|\Pi_j^{(2)}(x,y)|=f(\sqrt{\mu/h}(x-y))$, where f has exponential decay, to bound the last integral uniformly in x. It is easy to see that the above estimate works equally well for $\sup_y\int|K(x,y)|\,dx$. □

3. Why $\vec{j}_{MTF}\approx\vec{j}$

The first positive indication that $\vec{j}_{MTF}\approx\vec{j}$ comes from the following calculation:

Let us look at $E((1+t)\vec{B},V_Z)$ and differentiate at $t=0$ (this corresponds to putting $\vec{a}=\vec{A}$ in the current operator). Now,

$$\begin{aligned}H((1+t)\vec{B},V_Z) &= (1+t)\left(\sum_{j=1}^{Z}(\frac{-i}{\sqrt{1+t}}\nabla_j+\vec{A}(\sqrt{1+t}x_j))^2+\vec{B}(x_j)\cdot\vec{\sigma_j}\right)\\ &\quad+\sum_{j=1}^{Z}V_Z(x_j)+\sum_{1\le j<k\le Z}\frac{1}{|x_j-x_k|}.\end{aligned}$$

By changing variables to $y_j=\sqrt{1+t}x_j$, we get that $H((1+t)\vec{B},V_Z)$ is unitarily equivalent to the operator:

$$\begin{aligned}\tilde{H}(\vec{B},V_Z) &= (1+t)\left(\sum_{j=1}^{Z}(-i\nabla_j+\vec{A}(x_j))^2+\vec{B}(x_j)\cdot\vec{\sigma_j}\right)\\ &\quad+\sqrt{1+t}\left(\sum_{j=1}^{Z}V_Z(x_j)+\sum_{1\le j<k\le Z}\frac{1}{|x_j-x_k|}\right).\end{aligned}$$

So, we get (if the derivative with respect to t exists):

$$\begin{aligned}\frac{d}{dt}|_{t=0}E((1+t)\vec{B},V_Z) &= \langle\Psi_0|\sum_{j=1}^{Z}(-i\nabla_j+\vec{A}(x_j))^2+\vec{B}(x_j)\cdot\vec{\sigma_j}|\Psi_0\rangle\\ &\quad+\frac{1}{2}\langle\Psi_0|\sum_{j=1}^{Z}V_Z(x_j)+\sum_{1\le j<k\le Z}\frac{1}{|x_j-x_k|}|\Psi_0\rangle\\ &= E_{KIN}(\vec{B},V_Z)+\frac{1}{2}E_{POT}(\vec{B},V_Z),\end{aligned}\tag{1}$$

where Ψ_0 denotes a ground state wave function, and E_{KIN} (resp E_{POT}) denotes the ground state kinetic (resp potential) energy[4].

Remark 3.1. Notice that this is an identity for normal, finite-size atoms. There are no limits involved.

Remark 3.2. This identity has a striking similarity with the *virial theorem* for atoms without magnetic fields. In fact, the identity can be understood as a *virial theorem for atoms in constant magnetic fields.* Upon taking $\vec{B} = \vec{0}$, we get the usual identity

$$0 = E_{KIN}(\vec{0}, V_Z) + \frac{1}{2} E_{POT}(\vec{0}, V_Z).$$

As noticed in the remark above, our identity is similar to the so-called virial theorem in quantum mechanics. Now, the virial theorem, can be proved by calculating a certain commutator. Doing this in our case will help us get a useful identity for other test function $\vec{a}$ than the special choice $\vec{a} = \vec{A}$ above:

3.1. 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

$$(U_l \psi)(x_1, \ldots, x_N) = l^{-3Z/2} \psi(l^{-1}x_1, \ldots, l^{-1}x_Z),$$

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

$$U_l^{-1} H(\vec{B}, V_Z) U_l = Z l^{-1} H_Z(h, \mu)$$

and

$$U_l^{-1} J_Z(\vec{B}, Bl\vec{a}(x/l)) U_l = Z l^{-1} \hat{J}_Z(h, \mu, \mu\vec{a}),$$

where

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

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

Here $\vec{p} = -i\nabla$, $h = l^{-1/2}Z^{-1/2}$ and $\mu = Bl^{3/2}Z^{-1/2}$. 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 $H_Z(h, \mu)$, which exists by assumption.

[4] To my knowledge this identity has not previously appeared in the litterature. Any references on the subject would be appreciated.

3.2. 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

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

using the commutator formula from Section 4 below. Thereby we will find, using that the matrix element of a commutator with H vanishes in any eigenstate of H, that

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

where

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

Remark 3.3. If we take $\tilde{a}(x) = -1/2(x_1, x_2, x_3)$ in the above formula, we get (1).

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

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

Theorem 3.4.

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

as $Z\to\infty$. Here ρ_β is the unique minimizer in scaled MTF-theory.

In order to calculate the other two contributions to the current some more work is needed, but from here the ideas are the same as those used in [LSY94].

Theorem 3.5. *Suppose there exists $C < \infty$ such that $\mu h \le C$, then as $h \to 0$ we get*

$$\begin{aligned}
&\langle\Psi_{scaled}|\tilde{J}_{Z,KIN}(h,\mu,\tilde{a})|\Psi_{scaled}\rangle \\
&= -\frac{3}{2}Z\int(\partial_{x_1}a_2 - \partial_{x_2}a_1)\hat{P}_3(|v_{eff}|_-)\,dx \\
&\quad -Z\int(\partial_{x_1}a_2 - \partial_{x_2}a_1)v_{eff}\rho_\beta\,dx + o(Z),
\end{aligned}$$

and

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

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

Using the results above we finally get:

Theorem 3.6. *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 $\mu h \leq C$, then as $h \to 0$ (or equivalently $Z \to \infty$)*

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

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

The term $\langle\Psi_{scaled}|\tilde{J}_{Z,INT}(h,\mu,\tilde{a})|\Psi_{scaled}\rangle$ 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. 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.
Concerning $J_{Z,KIN}$: 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. It is, however, this term which forces us to limit ourselves to the case $\mu h \leq C$ (or $B \leq CZ^{4/3}$), for a further discussion of this see [Fou00b]. It will be the aim of new work to get around this difficulty.

4. Commutator

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 $\vec{B} = \text{curl}\vec{A}$ will not necessarily be constant in space. We will be working in a one particle situation instead of the many-particle problems discussed in the major part of this article.

Let us 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

$$\mathbb{B} = \begin{pmatrix} 0 & B_3 & -B_2 \\ -B_3 & 0 & B_1 \\ B_2 & -B_1 & 0 \end{pmatrix} = \{\partial_{x_j}A_k - \partial_{x_k}A_j\}_{j,k}.$$

The range of the matrix $\mathbb{B}$ is exactly the vectors orthogonal to $\vec{B}$.

Remark 4.1. Notice that if $\vec{B} = (1,0,0)$ and $\tilde{a} = (-a_2, a_1, 0)$, then $\mathbb{B}\tilde{a} = (a_1, a_2, 0)$.

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 4.2. *Let us write $\vec{a} = \mathbb{B}\tilde{a}$, then the following formula is true:*

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

Proof. The proof of Lemma 4.2 is essentially just a calculation. □

Corollary 4.3. *Let ϕ be an eigenfunction for H, i.e. $H\phi = \lambda\phi$, then*

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

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