

On the semiclassical asymptotics of the current and magnetisation of a non-interacting electron gas at zero temperature in a strong constant magnetic field.

S. Fournais*

Department of Mathematical Sciences and MaPhySto[†]
University of Aarhus
Denmark

Abstract

We calculate the asymptotic form of the quantum current/magnetisation of a non-interacting electron gas at zero temperature. The calculation uses coherent states and a novel commutator identity for the current operator.

Contents

1	Introduction	2
1.1	Semiclassics for the energy	4
1.2	Difficulties	6
1.3	Organisation of the paper	7
1.4	Notation and preliminaries	7
2	Commutator identity	8

*Partially supported by the European Union, grant FMRX-960001.

[†]Centre for Mathematical Physics and Stochastics, funded by a grant from the Danish National Research Foundation.

3	Known results	10
4	Gauge invariance of the current	11
5	Lower bound	12
6	Calculation of the current	18
A	A density matrix with a strong current	20

1 Introduction

In recent years a lot of mathematical research has been focused on understanding quantum mechanics in magnetic fields. The semiclassical results obtained so far in this area have concentrated on the *energy* (i.e. the sum of the negative eigenvalues) and the *density*. Nevertheless, in the presence of a magnetic field, the *current* (and the magnetisation) is as natural a quantity as the density, but it has not received the same attention in the mathematical community. There are two possible reasons for this: The current vanishes for a Schrödinger operator without magnetic field, i.e. current is truly a property of problems with magnetic fields. Secondly, the current of a *classical* electron gas at equilibrium vanishes, and therefore, as was proved in [Fou98], in a standard semiclassical limit the leading (Weyl-like) term for the current is zero. There exists, however, another semiclassical limit, introduced by Lieb, Solovej and Yngvason in [LSY94], in which the magnetic field strength μ is allowed to vary as the semiclassical parameter \hbar tends to zero. The new semiclassical limit was introduced in order to study ground state properties of large atoms in magnetic fields as strong as those which exist on the surface of a neutron star. The purpose of this paper is to study the current in this semiclassical limit, applications to the calculation of the current/magnetisation of large atoms in strong magnetic fields will be given in a later paper.

When attacking semiclassical problems in strong magnetic fields there are two different approaches possible: One can use the very precise machinery developed by Ivrii and others (see [Ivr98] and [Sob94]). This will give very good remainder estimates and can be applied quite directly to the current. The drawback of the method is that it is technically involved and requires a certain degree of smoothness of the potentials. An alternative approach is

the variational approach used by Lieb, Solovej and Yngvason in the paper [LSY94] to calculate the energy and the density. This method uses coherent states to approximate the true ground state and (magnetic) Lieb-Thirring inequalities to bound the error terms. Here we will apply this latter technique to calculate the current. As will be explained below some new ideas are necessary in order to do so since the current operator is a priori too big to fit in the scheme. We get around this difficulty by applying a novel commutator formula for the current. This method unfortunately only works for magnetic fields which are not too strong. In a later paper [Fou99] we will apply Ivrii's microlocal techniques to the current and thereby improve the error estimates and enlarge the range of allowed magnetic field strengths. Notice, however, that it is necessary to use the commutator formula in order to calculate the current - an *approximate* ground state does not necessarily have the right current. This is illustrated in Appendix A where we construct a trial density matrix that gives the correct semiclassical energy but fails to give the right current.

In this paper we study the current and magnetisation of an electron gas in a strong constant magnetic field. Suppose the dynamics of an electron is governed by the Pauli-operator

$$\mathbf{P} = \mathbf{P}(\mu\vec{A}, V) = (-ih\nabla + \mu\vec{A})^2 + V(x) + h\mu\vec{\sigma} \cdot \vec{B},$$

acting in $L^2(\mathbb{R}^3; \mathbb{C}^2)$. Here V is a real potential, $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli spin matrices:

$$\begin{aligned}\sigma_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \sigma_2 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\ \sigma_3 &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},\end{aligned}$$

and $\vec{B} = \nabla \times \vec{A}$. The operator \mathbf{P} contains two parameters $h, \mu \in \mathbb{R}_+$, where h is a semi-classical parameter, which we will let tend to zero, and μ is parameter measuring the strength of the magnetic field. We will let $\mu \rightarrow +\infty$ as $h \rightarrow 0$ in such a way that the product μh remains bounded below, i.e. $\mu h \geq c > 0$.

Let ψ be any state, then the *current in the state* ψ is the distribution \vec{j}_ψ

given by:

$$\int \vec{j}_\psi \cdot \vec{a} = \langle \psi | \mathbf{J}(\mu\vec{a}) | \psi \rangle,$$

where $\mathbf{J}(\mu\vec{a})$ is the operator:

$$\mathbf{J}(\mu\vec{a}) = \mu\vec{a}(-ih\nabla + \mu\vec{A}) + (-ih\nabla + \mu\vec{A})\mu\vec{a} + h\mu\vec{\sigma}\vec{b},$$

with $\vec{b} = \text{rot}\vec{a}$. We will study the *total current of a non-interacting electron gas at zero temperature* i.e. we sum the current of all eigenfunctions below zero (we set the chemical potential equal to zero). Thus the definition of the current (as a distribution) is:

$$\int \vec{j} \cdot \vec{a} dx = \text{tr}[\mathbf{J}(\mu\vec{a})1_{(-\infty,0]}(\mathbf{P})].$$

The current is given as the rotation of the magnetisation: $\vec{j} = \text{rot}\vec{M}$, thus results for the current translate directly into results for the magnetisation.

1.1 Semiclassics for the energy

The energy of the electron gas is given by:

$$E(\vec{A}, V) = \text{tr}[\mathbf{P}(\mu\vec{A}, V)1_{(-\infty,0]}(\mathbf{P}(\mu\vec{A}, V))].$$

Notice, that this is clearly a negative quantity. The semiclassical asymptotics of the energy has been calculated by [LSY94] (constant magnetic field) and [ES97] (non constant fields), and it was found, under very general conditions on V, \vec{A} , that $E(\vec{A}, V) \approx \frac{\mu}{h^2} E_{scl}(\vec{A}, V)$, where

$$E_{scl}(\vec{A}, V) = -\frac{2}{3\pi} \int \sum_{n=0}^{\infty} d_n |\vec{B}| [2n\mu h |\vec{B}| + V(x)]_-^{3/2} dx,$$

with $d_0 = \frac{1}{2\pi}$ and $d_n = \frac{1}{\pi}$ for $n \geq 1$. Here and in what follows we use the notation

$$[x]_- = \begin{cases} -x & x \leq 0 \\ 0 & x > 0 \end{cases}$$

Now, formally¹ $\vec{j} = \frac{\delta E}{\delta \vec{A}}$, so we would expect that

$$\begin{aligned} \frac{h^2}{\mu} \int \vec{j} \cdot \vec{a} \, dx &\approx \frac{d}{ds} \Big|_{s=0} E_{scl}(\vec{A} + s\vec{a}, V) \\ &= \frac{-2}{3\pi} \sum_{n=0}^{\infty} d_n \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) \\ &\quad \times \left([2nh\mu + V(x)]_-^{3/2} - 3nh\mu [2nh\mu + V(x)]_-^{1/2} \right) dx, \end{aligned}$$

as h tends to zero. This is indeed the result of the paper:

Theorem 1.1. *Suppose $\vec{A} = \frac{1}{2}(-x_2, x_1, 0)$, that $\vec{a} = (a_1, a_2, 0) \in C_0^\infty$, and that $V, \tilde{a} \cdot \nabla V \in L^{3/2} \cap L^{5/2}$, where $\tilde{a} = (-a_2, a_1, 0)$. Suppose furthermore that $\mu h \rightarrow \beta \in (0, +\infty)$ as $h \rightarrow 0$. Then*

$$\begin{aligned} \lim_{h \rightarrow 0} \frac{h^2}{\mu} \int \vec{j} \cdot \vec{a} \, dx &= \frac{-2}{3\pi} \sum_{\nu=0}^{\infty} d_\nu \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) \\ &\quad \times \left([2\nu\beta + V(x)]_-^{3/2} - 3\nu\beta [2\nu\beta + V(x)]_-^{1/2} \right) dx. \end{aligned}$$

Theorem 1.1 only deals with the current perpendicular to the magnetic field. It turns out that the current parallel to the field is more difficult to analyse. We have the following result:

Theorem 1.2. *Let the assumptions be as in Theorem 1.1 except that $\vec{a} \in C_0^\infty$ is arbitrary (i.e. a_3 is not necessarily vanishing) and suppose V satisfies the following additional symmetry constraint: $V(x_1, x_2, -x_3) = V(x_1, x_2, x_3)$. Then*

$$\begin{aligned} \lim_{h \rightarrow 0} \frac{h^2}{\mu} \int \vec{j} \cdot \vec{a} \, dx &= \frac{-2}{3\pi} \sum_{\nu=0}^{\infty} d_\nu \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) \\ &\quad \times \left([2\nu\beta + V(x)]_-^{3/2} - 3\nu\beta [2\nu\beta + V(x)]_-^{1/2} \right) dx. \end{aligned}$$

¹It is easy to prove that

$$\text{tr}[\mathbf{J}(\mu\vec{a})1_{(-\infty, 0]}(\mathbf{P})] = \frac{d}{dt} \Big|_{t=0} E(\vec{A} + t\vec{a}, V),$$

if the derivative on the right hand exists.

1.2 Difficulties

Let us recall how the density is calculated [LS77]:

The density ρ is defined as

$$\int \rho \phi dx = \text{tr}[\phi 1_{(-\infty, 0]}(\mathbf{P}(\mu \vec{A}, V))],$$

for all $\phi \in C_0^\infty(\mathbb{R})$. Formally, ρ is the variational derivative of the energy with respect to V i.e. $\rho \stackrel{\text{formally}}{=} \frac{\delta E}{\delta V}$. To calculate the asymptotics of the density we use the following variational principle:

$$E(\vec{A}, V) = \inf_{0 \leq \gamma \leq 1} \text{tr}[\gamma \mathbf{P}(\mu \vec{A}, V)].$$

Let $H(s) = \mathbf{P}(\mu \vec{A}, V + s\phi)$ and let $E(s)$ be the corresponding energy. Then, by using $1_{(-\infty, 0]}(\mathbf{P}(\mu \vec{A}, V))$ in the variational principle for $E(s)$, we obtain:

$$E(s) - E(0) \leq s \int \rho \phi dx.$$

If we now divide by $s \neq 0$ on both sides of the inequality, multiply by h^2/μ , and let h and s tend successively to zero, then we get:

$$\int \rho \phi dx \rightarrow \int \frac{\delta E_{scl}}{\delta V} \phi dx.$$

Unfortunately, this technique does not work for the current: If we define

$$\tilde{H}(s) = \mathbf{P}(\mu \vec{A}, V) + s \mathbf{J}(\mu \vec{a}),$$

and let $\tilde{E}(s)$ be the corresponding energy, then we get

$$\begin{aligned} \tilde{E}(s) &\leq \text{tr}[1_{(-\infty, 0]}(\mathbf{P}(\mu(\vec{A} + s\vec{a}), V)) \tilde{H}(s)] \\ &= E(\vec{A} + s\vec{a}, V) - s^2 \mu^2 \text{tr}[\vec{a}^2 1_{(-\infty, 0]}(\mathbf{P}(\mu(\vec{A} + s\vec{a}), V))]. \end{aligned}$$

The first term on the right hand side is known to be of order $\frac{\mu}{h^2}$, but the second term is of order $\mu^2 \frac{\mu}{h^2}$! Thus, this term - which is quadratic in s and therefore without interest for us - spoils the asymptotic picture.

The morale of this calculation is, that the operator \mathbf{J} is too big - adding just a bit of it, changes the energy dramatically. The way out of this problem is to realize that $\langle \phi | \mathbf{J} | \phi \rangle$ is 'small' for all ϕ which are eigenfunctions of $\mathbf{P}(\mu \vec{A}, V)$.

1.3 Organisation of the paper

In Section 2 we prove a commutator formula for \mathbf{J} . This formula expresses \mathbf{J} as a commutator with \mathbf{P} plus an operator which is a factor μ smaller than \mathbf{J} . Since the commutator does not contribute to the trace, we hereby reduce the problem of calculating the current considerably. Unfortunately, this commutator formula only gives information about the current orthogonal to the magnetic field - this is the reason why the parallel current is more difficult.

In Section 4 we prove that the current is *gauge invariant* i.e. that $\vec{j} \cdot \vec{a}$ only depends on the magnetic field $\vec{b} = \text{rot} \vec{a}$ generated by \vec{a} .

Then, in Sections 5 and 6 we use the 'variational principle' - i.e. the method used above to calculate the density - to calculate the orthogonal current. Using symmetry, gauge invariance and the result on the orthogonal current, we can prove Theorem 1.2.

Finally, in Appendix A, we give some arguments to support the necessity of using our commutator formula: We construct a density matrix which has asymptotically (as $\hbar \rightarrow 0$) the same energy and density as the ground state, but does not have the right current.

1.4 Notation and preliminaries

The results in Section 3 and the calculations in Sections 5 and 6 are only for a constant magnetic field and there we fix the choice of the vector potential as $\vec{A}(x) = \frac{1}{2}(-x_2, x_1, 0)$. The commutator formula in Section 2 is valid for general, everywhere nonvanishing magnetic fields, so in that section \vec{A} denotes an arbitrary vector potential.

We will denote the magnetic momentum operator as $p_{\vec{A}} = (-i\hbar\nabla + \mu\vec{A})$. Furthermore, we will denote the closed ball of radius r centered around the point x by $B(x, r)$.

All through the paper we will apply the standard convention that c or C denote arbitrary constants.

Finally a few words on the Pauli operator in a constant magnetic field:

With our choice of \vec{A} , the magnetic field is parallel to the 3rd unit vector \vec{e}_3 and therefore

$$\mathbf{P} = \begin{pmatrix} p_{\vec{A}}^2 + \mu\hbar + V(x) & 0 \\ 0 & p_{\vec{A}}^2 - \mu\hbar + V(x) \end{pmatrix},$$

and thus

$$\begin{aligned} \text{tr}[\mathbf{J}(\mu\vec{a})1_{(-\infty,0]}(\mathbf{P})] &= \mu\text{tr}[(\vec{a} \cdot p_{\vec{A}} + p_{\vec{A}} \cdot \vec{a} + hb_3)1_{(-\infty,0]}(p_{\vec{A}}^2 + \mu h + V(x))] \\ &\quad + \mu\text{tr}[(\vec{a} \cdot p_{\vec{A}} + p_{\vec{A}} \cdot \vec{a} - hb_3)1_{(-\infty,0]}(p_{\vec{A}}^2 - \mu h + V(x))]. \end{aligned}$$

We therefore can (and will) calculate the current as the sum of the two terms on the right hand side.

2 Commutator identity

Let us assume $|\vec{B}(x)| \neq 0$ for all x , where $\vec{B} = \nabla \times \vec{A}$. 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*

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

Before we give the proof of Lemma 2.2 we state an easy consequence:

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

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

Proof. $\langle\phi; [H, J_p(\tilde{a})]\phi\rangle = 0$ for all eigenfunctions ϕ . □

Now we prove Lemma 2.2.

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

$$\begin{aligned} [H, p_{\tilde{A}}] &= [p_{\tilde{A}}^2, p_{\tilde{A}}] + [V, p_{\tilde{A}}] \\ &= ih\nabla V - ih\mu \begin{pmatrix} (p_{\tilde{A}}; \mathbb{B}e_1) + (\mathbb{B}e_1, p_{\tilde{A}}) \\ (p_{\tilde{A}}; \mathbb{B}e_2) + (\mathbb{B}e_2, p_{\tilde{A}}) \\ (p_{\tilde{A}}; \mathbb{B}e_3) + (\mathbb{B}e_3, p_{\tilde{A}}) \end{pmatrix}, \end{aligned}$$

$$\begin{aligned} [H, f] &= [p_{\tilde{A}}^2, f] = \sum_j p_{\tilde{A},j}[p_{\tilde{A},j}, f] + [p_{\tilde{A},j}, f]p_{\tilde{A},j} \\ &= -ih \sum_j (p_{\tilde{A},j}\partial_{x_j}f + \partial_{x_j}fp_{\tilde{A},j}) \\ &= -ih(p_{\tilde{A}} \cdot \nabla f + \nabla f \cdot p_{\tilde{A}}). \end{aligned}$$

Based on these two equalities we get:

$$\begin{aligned} &[H, J_p(\tilde{a})] \\ &= \tilde{a} \cdot [H, p_{\tilde{A}}] + [H, p_{\tilde{A}}] \cdot \tilde{a} + p_{\tilde{A}} \cdot [H, \tilde{a}] + [H, \tilde{a}] \cdot p_{\tilde{A}} \\ &= 2ih\tilde{a} \cdot \nabla V \\ &\quad - ih\mu \left\{ \tilde{a} \cdot \begin{pmatrix} (p_{\tilde{A}}; \mathbb{B}e_1) + (\mathbb{B}e_1, p_{\tilde{A}}) \\ (p_{\tilde{A}}; \mathbb{B}e_2) + (\mathbb{B}e_2, p_{\tilde{A}}) \\ (p_{\tilde{A}}; \mathbb{B}e_3) + (\mathbb{B}e_3, p_{\tilde{A}}) \end{pmatrix} + \begin{pmatrix} (p_{\tilde{A}}; \mathbb{B}e_1) + (\mathbb{B}e_1, p_{\tilde{A}}) \\ (p_{\tilde{A}}; \mathbb{B}e_2) + (\mathbb{B}e_2, p_{\tilde{A}}) \\ (p_{\tilde{A}}; \mathbb{B}e_3) + (\mathbb{B}e_3, p_{\tilde{A}}) \end{pmatrix} \cdot \tilde{a} \right\} \\ &\quad - ih \left\{ \begin{pmatrix} p_{\tilde{A}} \cdot \nabla \tilde{a}_1 + \nabla \tilde{a}_1 \cdot p_{\tilde{A}} \\ p_{\tilde{A}} \cdot \nabla \tilde{a}_2 + \nabla \tilde{a}_2 \cdot p_{\tilde{A}} \\ p_{\tilde{A}} \cdot \nabla \tilde{a}_3 + \nabla \tilde{a}_3 \cdot p_{\tilde{A}} \end{pmatrix} \cdot p_{\tilde{A}} + p_{\tilde{A}} \cdot \begin{pmatrix} p_{\tilde{A}} \cdot \nabla \tilde{a}_1 + \nabla \tilde{a}_1 \cdot p_{\tilde{A}} \\ p_{\tilde{A}} \cdot \nabla \tilde{a}_2 + \nabla \tilde{a}_2 \cdot p_{\tilde{A}} \\ p_{\tilde{A}} \cdot \nabla \tilde{a}_3 + \nabla \tilde{a}_3 \cdot p_{\tilde{A}} \end{pmatrix} \right\}. \end{aligned}$$

Now

$$\begin{aligned}
& \sum \tilde{a}_j \{ (p_{\bar{A}}; \mathbb{B}e_j) + (\mathbb{B}e_j; p_{\bar{A}}) \} + \sum \{ (p_{\bar{A}}; \mathbb{B}e_j) + (\mathbb{B}e_j; p_{\bar{A}}) \} \tilde{a}_j \\
&= \sum_{j,k} \left\{ \tilde{a}_j (p_{\bar{A},k} \mathbb{B}_{k,j} + \mathbb{B}_{k,j} p_{\bar{A},k}) + (p_{\bar{A},k} \mathbb{B}_{k,j} + \mathbb{B}_{k,j} p_{\bar{A},k}) \tilde{a}_j \right\} \\
&= 2 \sum_{j,k} \left\{ \tilde{a}_j \mathbb{B}_{k,j} p_{\bar{A},k} + p_{\bar{A},k} \mathbb{B}_{k,j} \tilde{a}_j \right\} + \sum_{j,k} \left\{ \tilde{a}_j [p_{\bar{A},k}, \mathbb{B}_{k,j}] + [\mathbb{B}_{k,j}, p_{\bar{A},k}] \tilde{a}_j \right\} \\
&= 2(\mathbb{B}\tilde{a}, p_{\bar{A}}) + (p_{\bar{A}}, \mathbb{B}\tilde{a}) \\
&= 2J_p(\vec{a}).
\end{aligned}$$

Finally,

$$\begin{aligned}
& \begin{pmatrix} p_{\bar{A}} \cdot \nabla \tilde{a}_1 + \nabla \tilde{a}_1 \cdot p_{\bar{A}} \\ p_{\bar{A}} \cdot \nabla \tilde{a}_2 + \nabla \tilde{a}_2 \cdot p_{\bar{A}} \\ p_{\bar{A}} \cdot \nabla \tilde{a}_3 + \nabla \tilde{a}_3 \cdot p_{\bar{A}} \end{pmatrix} \cdot p_{\bar{A}} + p_{\bar{A}} \cdot \begin{pmatrix} p_{\bar{A}} \cdot \nabla \tilde{a}_1 + \nabla \tilde{a}_1 \cdot p_{\bar{A}} \\ p_{\bar{A}} \cdot \nabla \tilde{a}_2 + \nabla \tilde{a}_2 \cdot p_{\bar{A}} \\ p_{\bar{A}} \cdot \nabla \tilde{a}_3 + \nabla \tilde{a}_3 \cdot p_{\bar{A}} \end{pmatrix} \\
&= \sum_j \left\{ (p_{\bar{A}} \cdot \nabla \tilde{a}_j + \nabla \tilde{a}_j \cdot p_{\bar{A}}) p_{\bar{A},j} + p_{\bar{A},j} (p_{\bar{A}} \cdot \nabla \tilde{a}_j + \nabla \tilde{a}_j \cdot p_{\bar{A}}) \right\} \\
&= \sum_{j,k} \left\{ (p_{\bar{A},k} (\partial_k \tilde{a}_j) + (\partial_k \tilde{a}_j) p_{\bar{A},k}) p_{\bar{A},j} + p_{\bar{A},j} (p_{\bar{A},k} (\partial_k \tilde{a}_j) + (\partial_k \tilde{a}_j) p_{\bar{A},k}) \right\} \\
&= 2 \sum_{j,k} \left\{ p_{\bar{A},k} (\partial_k \tilde{a}_j) p_{\bar{A},j} + p_{\bar{A},j} (\partial_k \tilde{a}_j) p_{\bar{A},k} \right\} \\
&\quad + \sum_{j,k} \left\{ [\partial_k \tilde{a}_j, p_{\bar{A},k}] p_{\bar{A},j} - p_{\bar{A},j} [\partial_k \tilde{a}_j, p_{\bar{A},k}] \right\} \\
&= 2(p_{\bar{A}}; (D\tilde{a} + (D\tilde{a})^t) p_{\bar{A}}) - i\hbar \sum_{j,k} [p_{\bar{A},j}, \partial_k^2 \tilde{a}_j] \\
&= 2(p_{\bar{A}}; (D\tilde{a} + (D\tilde{a})^t) p_{\bar{A}}) - \hbar^2 \sum_{j,k} \partial_j \partial_k^2 \tilde{a}_j.
\end{aligned}$$

□

3 Known results

In this section we will recall some results on semiclassics of the energy and density in a constant magnetic field. These are all taken from [LSY94].

First we have a magnetic Lieb-Thirring inequality for constant magnetic field:

Theorem 3.1. *Let $|V|_- \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$ and let $e_j(\mu, V)$ denote the negative eigenvalues of the operator $p_{\vec{A}}^2 - \mu h + V(x)$. Then*

$$\sum_j |e_j(\mu, V)| \leq L_1 \mu h^{-2} \int |V(x)|_-^{3/2} dx + L_2 h^{-3} \int |V(x)|_-^{5/2} dx,$$

where the constants L_1, L_2 are independent of h, μ and V .

The result on the semiclassics of the energy in a constant magnetic field is:

Theorem 3.2. *Suppose $|V|_- \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$ and let $E(\vec{A}, V)$ and $E_{scl}(\vec{A}, V)$ be as given in Section 1. Then*

$$\lim_{h \rightarrow 0} \left(\frac{E(\vec{A}, V)}{\frac{\mu}{h^2} E_{scl}(\vec{A}, V)} \right) = 1,$$

uniformly in the magnetic field strength μ .

By the variational principle, we get as in Section 1.2:

Corollary 3.3. *Let us keep the assumptions from Theorem 3.2. Suppose $\phi \in L^{5/2}(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$, then*

$$\frac{h^2}{\mu} \text{tr}[\phi 1_{(-\infty, 0]}(\mathbf{P}(\mu \vec{A}, V))] = \frac{1}{\pi} \int \sum_{n=0}^{\infty} d_n [2n\mu h + V(x)]_-^{1/2} \phi(x) dx + o(1),$$

as $h \rightarrow 0$.

4 Gauge invariance of the current

In this section we will prove that the current $\int \vec{j} \cdot \vec{a}$, as a function of \vec{a} , only depends on the magnetic field $\vec{b} = \nabla \times \vec{a}$ generated by \vec{a} , i.e. that if $\vec{a} = \tilde{a} + \nabla \phi$ then $\int \vec{j} \cdot \vec{a} = \int \vec{j} \cdot \tilde{a}$:

Lemma 4.1. *Suppose V is relatively bounded with respect to $-h^2 \Delta$ and that $\text{Spec}(\mathbf{P}(h, \mu, V))$ below zero is discrete. Then $\forall \phi \in C_0^\infty(\mathbb{R}^3)$ we have $\int \vec{j} \cdot \nabla \phi = 0$.*

Proof. The proof follows from the commutator formula below:

$$[\mathbf{P}, \phi] = ih\mathbf{J}(\nabla \phi).$$

□

5 Lower bound

Let $M = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & 0 \end{pmatrix} \in C_0^\infty(\mathbb{R}^3)$ and let $b_3(x) = \frac{M_{11}(x)+M_{22}(x)}{2}$.

In this section we prove a semi-classical lower bound for the energy of the operator

$$H(t) = p_{\bar{A}} \cdot S_t(x) p_{\bar{A}} - \mu h(1 + t b_3(x)) + V(x),$$

where $S_t(x) = 1 + tM(x)$.

We will need the following easily proved localisation formula:

Lemma 5.1. *Let $g \in C^\infty(\mathbb{R}^3; \mathbb{R})$, and let $S(x)$ be any symmetric, real matrix, then*

$$\begin{aligned} 2\langle fg | p_{\bar{A}} \cdot S(x) p_{\bar{A}} | gf \rangle &= \langle f | g^2 p_{\bar{A}} \cdot S(x) p_{\bar{A}} | f \rangle + \langle f | p_{\bar{A}} \cdot S(x) p_{\bar{A}} g^2 | f \rangle \\ &\quad - 2h^2 \langle f | \nabla g \cdot S(x) \nabla g | f \rangle, \end{aligned}$$

for all $f \in L^2$.

We will also need to diagonalise the 'kinetic energy part' of $H(t)$ - for constant matrices $S(t)$, this is the content of the next lemma:

Lemma 5.2. *Let $S_t = I + tM$, where M is a constant matrix, and t is small. Let the matrix N_t solve the equation $e^{2tN_t} = I + tM$, and define a unitary operator U_t on L^2 by:*

$$(U_t f)(x) = \Lambda_t^{1/2} f(e^{tN_t} x),$$

$\Lambda_t = |\det e^{tN_t}|$. Then

$$U_t p_{\bar{A}} \cdot S_t p_{\bar{A}} U_t^{-1} = (-ih\nabla + \mu \tilde{A}_t)^2,$$

where $\tilde{A}_t(x) = e^{tN_t} \vec{A}(e^{tN_t} x)$.

Remark 5.3. If $M = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & 0 \end{pmatrix}$, then $|\text{rot } \tilde{A}_t| = 1 + \frac{1}{2}t(M_{11} +$

$M_{22}) + t^2 c + O(t^3)$, where c is a negative constant (depending on M). Thus, we see from the above, that for $t \neq 0$:

$$\inf \text{Spec} \left(p_{\bar{A}} \cdot S_t p_{\bar{A}} - \mu h \left(1 + \frac{1}{2} t (M_{11} + M_{22}) \right) \right) \rightarrow -\infty,$$

as $\mu h \rightarrow \infty$. This is the reason why the lower bound below does not work in that case.

Theorem 5.4. Suppose that $[V]_- \in L^{3/2} \cap L^{5/2}$ and that

$$M(x) = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & 0 \end{pmatrix} \in C_0^\infty.$$

Let $E(t) = \text{tr}[H(t)1_{(-\infty, 0]}(H(t))]$, and suppose, that $\mu h \rightarrow \beta$ as $h \rightarrow 0$. Then we have the following lower bound on $E(t)$:

$$\liminf_{h \rightarrow 0} \frac{h^2}{\mu} E(t) \geq \frac{-1}{3\pi^2} \sum_{\nu} \int \frac{b_{u,t}}{\Lambda_{u,t}} [(2\nu + 1)\beta b_{u,t} - \beta(1 + tb_3(u)) + V(u)]_-^{3/2} du,$$

where $b_{u,t} = |\text{rot}_x \sqrt{1 + tM(u)} \vec{A}(\sqrt{1 + tM(u)}x)|$ and $\Lambda_{u,t} = |\det \sqrt{1 + tM(u)}|$.

Remark 5.5. Notice, that due to the 2nd order discrepancy between $b_{u,t}$ and $\mu(1 + tb_3(u))$ (see Remark 5.3), we really need the matrix $M(x)$ to have compact support, since this assures the convergence of the integral in the lower bound for $\nu = 0$.

Proof. It is clear, that we get a lower energy by replacing $V(x)$ by $-[V(x)]_-$, so we will assume $V(x) = -[V(x)]_-$ in the proof.

Coherent states:

If \vec{B} is a (constant) vector, then the projection onto the ν th Landau level of $(-ih\nabla + \mu\frac{1}{2}\vec{B} \times x)^2$ has integral kernel [LSY94, p.95]:

$$\Pi_{\nu}^{(2)}(x_{\perp}, y_{\perp}) = \frac{\mu b}{2\pi h} \exp\{i(x_{\perp} \times y_{\perp}) \frac{\mu \vec{B}}{2h} - |x_{\perp} - y_{\perp}|^2 \frac{\mu b}{4h}\} L_{\nu}(|x_{\perp} - y_{\perp}|^2 \frac{\mu b}{2h}),$$

where we have written $x \in \mathbb{R}^3$ as $(x_{\perp}, x_{\parallel})$, with $x_{\perp} \perp \vec{B}$ and $x_{\parallel} \parallel \vec{B}$. Furthermore, we have written $b = |\vec{B}|$ and L_{ν} are Laguerre polynomials normalised by $L_{\nu}(0) = 1$. Let us now write

$$\Pi_{\nu,p}(x, y) = \Pi_{\nu}^{(2)}(x_{\perp}, y_{\perp}) e^{ip(x_{\parallel} - y_{\parallel})},$$

with $p \in \mathbb{R}$, then

$$(-ih\nabla + \mu\frac{1}{2}\vec{B} \times x)^2 \Pi_{\nu,p}(x, y) = \epsilon_{\nu,p}(h, b) \Pi_{\nu,p}(x, y),$$

with $\epsilon_{\nu,p}(h, b) = (2\nu + 1)h\mu b + h^2p^2$, and

$$\Pi_{\nu,p}(x, x) = \frac{\mu b}{2\pi h}.$$

Let us finally introduce a localisation function $g \in C_0^\infty(\mathbb{R}^3)$, $\int g^2 = 1$ and write $g_r(x) = r^{-3/2}g(x/r)$, where $r = h^{1-\alpha}$, $\alpha < 1$. Then, we write

$$Q(\nu, u, p, t) = g_r(\cdot - u)U_{t,u}^{-1}\Pi_{\nu,p,u,t}U_{t,u}g_r(\cdot - u),$$

where $U_{t,u}$ is the unitary operator described in Lemma 5.2, with $N_t = N_{t,u}$ satisfying $e^{2tN_{t,u}} = I + tM(u)$, and where $\Pi_{\nu,p,u,t} = \Pi_{\nu,p}$ with $\vec{B} = \vec{B}_{t,u}$ being the magnetic field generated by $e^{tN_{t,u}}\vec{A}(e^{tN_{t,u}}x)$. Below, we will in general insert an extra index u on the quantities, where this is needed, as exemplified here by $N_{t,u}$ and $\vec{B}_{t,u}$.

Useful identities:

We find:

$$\begin{aligned} & \text{tr}[p_{\vec{A}} \cdot S(u)p_{\vec{A}}Q(\nu, u, p, t)] \\ &= \text{tr}[p_{\vec{A}} \cdot S(u)p_{\vec{A}}U_{t,u}^{-1}g_r(e^{2tN_{t,u}} \cdot - u)\Pi_{\nu,p,u,t}g_r(e^{2tN_{t,u}} \cdot - u)U_{t,u}] \\ &= \text{tr}[(-ih\nabla + \mu\vec{A}_{t,u})^2g_r(e^{2tN_{t,u}} \cdot - u)\Pi_{\nu,p,u,t}g_r(e^{2tN_{t,u}} \cdot - u)] \\ &= \frac{\mu b_{t,u}}{2\pi h\Lambda_{t,u}} \left(\epsilon_{p,\nu}(h, b_{t,u}) + h^2 \int (\nabla g_r((e^{2tN_{t,u}}x - u))^2 dx) \right). \end{aligned} \quad (5.1)$$

Here we used the localisation formula in the last equality.

For a normalised function $f \in L^2$ we get:

$$\begin{aligned} & \langle f | p_{\vec{A}} \cdot S(x)p_{\vec{A}} | f \rangle \quad (5.2) \\ & \geq \int \langle f | g_r(\cdot - u)p_{\vec{A}} \cdot S(x)p_{\vec{A}}g_r(\cdot - u) | f \rangle du - h^2C \int (\nabla g_r)^2 \\ & = \int \langle f | g_r(\cdot - u)p_{\vec{A}} \cdot S(u)p_{\vec{A}}g_r(\cdot - u) | f \rangle du \\ & \quad + \int \langle f | g_r(\cdot - u)p_{\vec{A}} \cdot (S(x) - S(u))p_{\vec{A}}g_r(\cdot - u) | f \rangle du - h^2C \int (\nabla g_r)^2. \end{aligned}$$

The second term can be estimated as:

$$\begin{aligned} & \left| \int \langle f | g_r(\cdot - u)p_{\vec{A}} \cdot (S(x) - S(u))p_{\vec{A}}g_r(\cdot - u) | f \rangle du \right| \quad (5.3) \\ & \leq \int F_r(u) \langle f | g_r(\cdot - u)p_{\vec{A}} \cdot S(u)p_{\vec{A}}g_r(\cdot - u) | f \rangle du, \end{aligned}$$

where $F_r(u) = 2 \sup_{x \in B(u,r)} |S(x) - S(u)|$. Thus, the first two terms in (5.2) can be estimated as:

$$\begin{aligned} & \int \langle f | g_r(\cdot - u) p_{\bar{A}} \cdot S(x) p_{\bar{A}} g_r(\cdot - u) | f \rangle du \\ & + \int \langle f | g_r(\cdot - u) p_{\bar{A}} \cdot (S(x) - S(u)) p_{\bar{A}} g_r(\cdot - u) | f \rangle du \\ & \geq \sum_{\nu} \iint \frac{1 - F_r(u)}{2\pi} \epsilon_{p,\nu}(h, b_{t,u}) \langle f | Q(\nu, u, p, t) | f \rangle dp du. \end{aligned}$$

For the potential we get:

$$\begin{aligned} \langle f | V * g_r^2 | f \rangle &= \int V(u) \langle f | g_r^2(\cdot - u) | f \rangle du \\ &= \sum_{\nu} \iint V(u) \frac{1}{2\pi} \langle f | Q(\nu, u, p, t) | f \rangle dp du. \end{aligned} \tag{5.4}$$

Lower bound:

Now we are ready to prove the lower bound on the energy. We have to bound the sum $\sum_{j=1}^N \langle f_j | H(t) | f_j \rangle$ from below, with a bound independent of N . Let us take a (small) $\delta > 0$ and write

$$H(t) = \delta(p_{\bar{A}}^2 - \mu h) + (1 - \delta)(p_{\bar{A}}^2 - \mu h) + t(p_{\bar{A}} \cdot M p_{\bar{A}} - \mu h b_3) + V(x).$$

Let us furthermore take an $\epsilon > 0$ and choose R such that

$$\int_{|x| \geq R} |V(x)|^{3/2} dx < \epsilon \quad \text{and} \quad \int_{|x| \geq R} |V(x)|^{5/2} dx < \epsilon.$$

Since $M(x) \in C_0^\infty$ we will assume that $M(x) = 0$ for $|x| \geq R$. Choose finally, a partition of unity θ_1^2, θ_2^2 of positive real functions, satisfying: $\theta_1(x) = 0$ for $|x| \geq 2R$ and $\theta_2(x) = 0$ for $|x| \leq R$.

Then

$$\begin{aligned}
& \sum_{j=1}^N \langle f_j | H(t) | f_j \rangle \\
= & \sum_{j=1}^N \langle f_j | \theta_1 H(t) \theta_1 | f_j \rangle + \sum_{j=1}^N \langle f_j | \theta_2 H(t) \theta_2 | f_j \rangle \\
& - h^2 \sum_{j=1}^N \langle f_j | (\nabla \theta_1)^2 + (\nabla \theta_2)^2 | f_j \rangle \\
= & (1 - \delta) \sum_{j=1}^N \langle f_j | \theta_1 \left(p_{\bar{A}} \cdot \left(I + \frac{t}{1 - \delta} M(x) \right) p_{\bar{A}} \right. \\
& \quad \left. - \mu h \left(1 + \frac{t}{1 - \delta} b_3 * g_r^2 \right) + \frac{V(x)}{1 - \delta} * g_r^2 \right) \theta_1 | f_j \rangle \\
& + \sum_{j=1}^N \langle f_j | \theta_1 \left(\delta (p_{\bar{A}}^2 - \mu h) + (V - V * g_r^2) \right. \\
& \quad \left. - \mu h t (b_3 - b_3 * g_r^2) - h^2 (\nabla \theta_1)^2 - h^2 (\nabla \theta_2)^2 \right) \theta_1 | f_j \rangle \\
& + \sum_{j=1}^N \langle f_j | \theta_2 \left(p_{\bar{A}}^2 - \mu h + V(x) - h^2 (\nabla \theta_1)^2 - h^2 (\nabla \theta_2)^2 \right) \theta_2 | f_j \rangle. \quad (5.5)
\end{aligned}$$

The first term can be bounded below by

$$\begin{aligned}
& \frac{1 - \delta}{2\pi} \sum_{\nu} \iint \left\{ (1 - F_r(u)) \epsilon_{p,\nu} \left(h, b_{u, \frac{t}{1-\delta}} \right) - \mu h \left(1 + \frac{t}{1 - \delta} b_3(u) \right) + \frac{V(u)}{1 - \delta} \right\} \\
& \times \sum_{j=1}^N \langle f_j | \theta_1 Q(\nu, u, p, \frac{t}{1 - \delta}) \theta_1 | f_j \rangle dp du.
\end{aligned}$$

Since

$$0 \leq \sum_{j=1}^N \langle f_j | \theta_1 Q(\nu, u, p, \frac{t}{1 - \delta}) \theta_1 | f_j \rangle \leq \frac{\mu b_{u, \frac{t}{1-\delta}}}{2\pi h \Lambda_{\frac{t}{1-\delta}, u}},$$

and $\langle f_j | \theta_1 Q(\nu, u, p, \frac{t}{1-\delta}) \theta_1 | f_j \rangle = 0$ if $|u| \geq 3R + r$, we get a lower bound by replacing $\sum_{j=1}^N \langle f_j | \theta_1 Q(\nu, u, p, \frac{t}{1-\delta}) \theta_1 | f_j \rangle$ by a function $M(\nu, u, p, \frac{t}{1-\delta})$, which

is the characteristic function of the set

$$\left\{ (\nu, u, p) \mid (1 - F_r(u))\epsilon_{p,\nu}(h, b_{u, \frac{t}{1-\delta}}) - \mu h \left(1 + \frac{t}{1-\delta} b_3(u)\right) + \frac{V(u)}{1-\delta} \leq 0 \right. \\ \left. \text{and } |u| \leq 3R + r \right\},$$

times $-\frac{\mu b_{u, \frac{t}{1-\delta}}}{2\pi h \Lambda_{\frac{t}{1-\delta}, u}}$. Thus, the lower bound becomes

$$-\frac{1-\delta}{2\pi} \sum_{\nu} \iint_{\{|u| \leq 3R+r\}} \frac{\mu b_{u, \frac{t}{1-\delta}}}{2\pi h \Lambda_{\frac{t}{1-\delta}, u}} \times \\ \left[(1 - F_r(u))\epsilon_{p,\nu}(h, b_{u, \frac{t}{1-\delta}}) - \mu h \left(1 + \frac{t}{1-\delta} b_3(u)\right) + \frac{V(u)}{1-\delta} \right]_{-} dp du.$$

We do the p integration explicitly and get:

$$-(1-\delta) \sum_{\nu} \int_{\{|u| \leq 3R+r\}} \frac{1 - F_r(u)}{2\pi} \frac{4\mu b_{u, \frac{t}{1-\delta}}}{6\pi h^2 \Lambda_{\frac{t}{1-\delta}, u}} \\ \times \left[(2\nu + 1)h\mu b_{u, \frac{t}{1-\delta}} + \frac{1}{1 - F_r(u)} \left(-\mu h \left(1 + \frac{t}{1-\delta} b_3(u)\right) + \frac{V(u)}{1-\delta} \right) \right]_{-}^{3/2} du.$$

The last two terms in (5.5) are error terms, and will be bounded below using the magnetic Lieb-Thirring inequality. Since $r = h^{1-\alpha}$ and $\mu h \leq C$, we have for small h that

$$\int |(V(x) - V * g_r^2(x)) - \mu h (b_3(x) - b_3 * g_r^2(x)) - h^2 (\nabla \theta_1)^2 - h^2 (\theta_2)^2|^q dx < \epsilon,$$

for $q = 3/2$ and $q = 5/2$. Therefore, we get by application of the magnetic Lieb-Thirring inequality that the first error term in (5.5) can be bounded below by

$$-C\epsilon h^{-3} (\delta^{-1/2} + \delta^{-3/2}).$$

We can use the Lieb-Thirring inequality directly to bound the second error term from below by

$$-C\epsilon h^{-3},$$

where we used the definition of θ_2 . \square

6 Calculation of the current

In this section we will finally find the asymptotics of the current:

By applying the commutator identity from Section 2, we get

$$\begin{aligned} -\mathrm{tr}[\mathbf{J}(\mu\tilde{a})1_{(-\infty,0]}(\mathbf{P})] &= \mathrm{tr}[(p_{\bar{A}} \cdot M(x)p_{\bar{A}} + \mu h\sigma_3 b_3)1_{(-\infty,0]}(\mathbf{P})] \\ &\quad + \mathrm{tr}[\tilde{a} \cdot \nabla V 1_{(-\infty,0]}(\mathbf{P})], \end{aligned} \quad (6.1)$$

where $M(x) = -(D\tilde{a}(x) + (D\tilde{a}(x))^t)$.

The asymptotics of the second term in (6.1) is easy to calculate using the results on the density from [LSY94].

Lemma 6.1. *When $[V]_-, \tilde{a} \cdot \nabla V \in L^{3/2} \cap L^{5/2}$, then*

$$\begin{aligned} &\left| \mathrm{tr}[(\tilde{a} \cdot \nabla V)1_{(-\infty,0]}(\mathbf{P})] - \frac{-2\mu}{3\pi h^2} \sum_{\nu=0}^{\infty} d_{\nu} \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) [2\nu\mu h + V(x)]_-^{3/2} dx \right| \\ &= o(h^{-3} + \mu h^{-2}). \end{aligned}$$

For the first term in (6.1) we need the result from Section 5. Let us write the term as

$$\begin{aligned} &\mathrm{tr}[(p_{\bar{A}} \cdot M(x)p_{\bar{A}} - \mu h b_3)1_{(-\infty,0]}(p_{\bar{A}}^2 - \mu h + V(x))] \\ &\quad + \mathrm{tr}[(p_{\bar{A}} \cdot M(x)p_{\bar{A}} + \mu h b_3)1_{(-\infty,0]}(p_{\bar{A}}^2 + \mu h + V(x))], \end{aligned} \quad (6.2)$$

and analyse each term separately.

Lemma 6.2. *Suppose $[V]_- \in L^{3/2} \cap L^{5/2}$ and $\tilde{a} = (-a_2, a_1, 0) \in C_0^{\infty}(\mathbb{R}^3)$. Write $M(x) = -(D\tilde{a}(x) + (D\tilde{a}(x))^t)$. Suppose furthermore, that $\mu h \rightarrow \beta \in (0, +\infty)$ as $h \rightarrow 0$. Then*

$$\begin{aligned} &\lim_{h \rightarrow 0} \frac{h^2}{\mu} \mathrm{tr}[(p_{\bar{A}} \cdot M(x)p_{\bar{A}} - \mu h b_3)1_{(-\infty,0]}(p_{\bar{A}}^2 - \mu h + V(x))] = \\ &\quad \sum_{\nu=0}^{\infty} \frac{2\nu\beta}{2\pi} \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) [2\nu\mu h + V(x)]_-^{1/2} dx. \end{aligned}$$

Proof. The proof is easy, using the variational principle for the energy and the lower bound from Section 5: We write

$$H(t) = p_{\bar{A}}^2 - \mu h + V(x) + t(p_{\bar{A}} \cdot M(x)p_{\bar{A}} - \mu h b_3),$$

and $E(t) = \text{tr}[H(t)1_{(-\infty,0]}(H(t))] = \inf_{0 \leq \gamma \leq 1} \text{tr}[\gamma H(t)]$. Then the lower bound combined with the variational principle gives:

$$\lim_{h \rightarrow 0} \frac{h^2}{\mu} \text{tr}[(p_{\vec{A}} \cdot M(x)p_{\vec{A}} - \mu h b_3)1_{(-\infty,0]}(p_{\vec{A}}^2 - \mu h + V(x))] = \frac{d}{dt} \Big|_{t=0} \sum_{\nu} \int \frac{-b_{u,t}}{3\pi^2 \Lambda_{u,t}} [(2\nu + 1)\beta b_{u,t} - \beta(1 + t b_3(u)) + V(u)]_-^{3/2} du.$$

Now we obtain the result, if we remember that $b_{u,t} = (1 + t b_3(u) + O(t^2))$, and that $\frac{b_{u,t}}{\Lambda_{u,t}} = 1 + O(t^2)$. \square

Now, since μh is bounded, it is easy to use the same methods to treat the spin-up part. The result is similar:

Lemma 6.3. *Suppose $[V]_- \in L^{3/2} \cap L^{5/2}$ and $\tilde{a} = (-a_2, a_1, 0) \in C_0^\infty(\mathbb{R}^3)$. Suppose furthermore, that $\mu h \rightarrow \beta \in (0, +\infty)$ as $h \rightarrow 0$. Then*

$$\lim_{h \rightarrow 0} \frac{h^2}{\mu} \text{tr}[(p_{\vec{A}} \cdot M(x)p_{\vec{A}} + \mu h b_3)1_{(-\infty,0]}(p_{\vec{A}}^2 + \mu h + V(x))] = \sum_{\nu=0}^{\infty} \frac{2(\nu + 1)\beta}{2\pi} \int (\partial_{x_1} a_2 - \partial_{x_2} a_1) [2(\nu + 1)\mu h + V(x)]_-^{1/2} dx.$$

If we put the three lemmas together we obtain Theorem 1.1.

Finally, we prove Theorem 1.2:

Proof. Using Theorem 1.1 we may assume $\vec{a} = (0, 0, a_3)$, with $a_3 \in C_0^\infty$. Let U be the unitary operator on $L^2(\mathbb{R}^3, \mathbb{C}^2)$ defined by

$$Uf(x_1, x_2, x_3) = f(x_1, x_2, -x_3),$$

and write a_3 as $a_3 = a_{3,even} + a_{3,odd}$ where $a_{3,even}$ ($a_{3,odd}$) is even (odd) under the reflection $x_3 \mapsto -x_3$. Now, since V is invariant under conjugation by U we get:

$$\text{tr}[\mathbf{J}(\mu \vec{a})1_{(-\infty,0]}(\mathbf{P})] = \text{tr}[U\mathbf{J}(\mu \vec{a})U1_{(-\infty,0]}(\mathbf{P})] = \text{tr}[\mathbf{J}(\mu(0, 0, a_{3,odd}))1_{(-\infty,0]}(\mathbf{P})].$$

We can easily find a function $\tilde{a} = (\tilde{a}_1, \tilde{a}_2, 0) \in C_0^\infty$ such that $\text{rot} \tilde{a} = \text{rot}(0, 0, a_{3,odd})$. We thus finish the proof by appealing to Theorem 1.1 and the gauge invariance of the current. \square

A A density matrix with a strong current

We want to prove that it is necessary to use something like our commutator argument 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.

We will work with $\mu h = 1$ i.e $\mu = h^{-1}$ and will only look at one spin component i.e.

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

Lemma A.1. *There exists a potential $V(x) \in C_0^\infty(\mathbb{R}^3)$ and a test function $\vec{\phi} = (\phi_1, \phi_2, 0) \in C_0^\infty(\mathbb{R}^3)$ together with a density matrix i.e. an operator γ satisfying $0 \leq \gamma \leq 1$ such that*

$$\text{tr}[H\gamma] = E_{scl} + o\left(\frac{\mu}{h^2}\right),$$

and

$$\frac{h^2}{\mu} |\text{tr}[J(\mu\phi)\gamma]| \rightarrow \infty,$$

as $h \rightarrow 0$.

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 trial density matrix γ will be constructed as a perturbation of the density matrix used in [LSY94]. 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 smaller². 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. Let us choose $V \in C_0^\infty(\mathbb{R}^3)$, which satisfies $[V(x)]_- = 10$ for all $x \in B(0, 2)$. We will choose a test vector $\vec{\phi} = (\phi_1, \phi_2, 0)$, which is supported in $B(0, 1)$.

²This can be seen from the commutator formula

The density matrix γ' constructed in [LSY94] is

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

where $M(\nu, u, p)$ is the characteristic function of the set (in $(\mathbb{N}_+ \cup \{0\}) \times \mathbb{R}_u^3 \times \mathbb{R}_p$)

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

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

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

In this last expression g_r is a localisation function $g_r(x) = r^{-3/2} g(x/r)$, $0 \leq g \in C_0^\infty(\mathbb{R}^3)$, $\int g^2 = 1$ and $r = h^{1-\alpha}$ for some $0 < \alpha < 1$. Furthermore, $\Pi_\nu^{(2)}(x_\perp, y_\perp)$ is the (two-dimensional) integral kernel of the projection to the ν -th Landau level:

$$\Pi_\nu^{(2)}(x_\perp, y_\perp) = \frac{\mu}{2\pi h} \exp\{i(x_\perp \times y_\perp) \frac{\mu \vec{B}}{2h} - |x_\perp - y_\perp|^2 \frac{\mu}{4h}\} L_\nu(|x_\perp - y_\perp|^2 \frac{\mu}{2h}),$$

where we have written $x \in \mathbb{R}^3$ as (x_\perp, x_\parallel) , with $x_\perp \perp \vec{B}$ and $x_\parallel \parallel \vec{B}$. Furthermore, L_ν are Laguerre polynomials normalised by $L_\nu(0) = 1$.

Let now \tilde{M} be the characteristic function of $B(0, 1)_u \times [-h^{-1}, h^{-1}]_p$, and write

$$\tilde{\gamma} = \epsilon \iint \tilde{M}(u, p) \tilde{\Pi}(u, p) \, dudp,$$

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

$$\tilde{\Pi}(u, p)(x, y) = g_r(x - u) P(x_\perp, y_\perp) e^{ip(x_3 - y_3)} g_r(y - u).$$

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 $\delta \rightarrow 0$ as $h \rightarrow 0$. We will not do this, since it will not affect order of magnitude estimates and only obscure notation.

We need to calculate

$$\mathrm{tr}[H\gamma] = E_{scl} + \mathrm{tr}[H\tilde{\gamma}],$$

and

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

Notice, that since γ gives the right *density* to highest order, we do not need to calculate the spin current i.e. $\mathrm{tr}[\mu h b_3 \gamma]$, since we know this to be of order $\frac{\mu}{h^2}$ once we have proved that γ gives the right energy. Furthermore, we may assume that γ' does *not* satisfy the requirements of the lemma - if it does we do not have to construct anything.

The energy:

$$\mathrm{tr}[H\tilde{\gamma}] = \epsilon \iint \tilde{M}(u, p) \mathrm{tr}[H\tilde{\Pi}(u, p)] \, dudp.$$

we use the AMS-localisation formula:

$$2gp_A^2g - (p_A^2g^2 + g^2p_A^2) = [[g, p_A^2], g].$$

Let us first look at the potential energy:

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

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

$$\begin{aligned} & \mathrm{tr}[(p_A^2 - \mu h)\tilde{\Pi}(u, p)] \\ &= \frac{1}{2} \mathrm{tr} \left((p_A^2 g_r^2(\cdot - u) + g_r^2(\cdot - u) p_A^2 - 2\mu h)P + 2[[g_r(\cdot - u), p_A^2], g_r(\cdot - u)]P \right) \\ &= \frac{1}{2} \mathrm{tr} \left(4\mu h g_r^2(\cdot - u)P + 2h^2 (\nabla g_r(\cdot - u))^2 P \right). \end{aligned}$$

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

$$\begin{aligned} & \mathrm{tr}[\vec{\phi}(-ih\nabla + \mu\vec{A})\tilde{\gamma}] \\ &= \epsilon \iint \tilde{M}(u, p) \mathrm{tr}[\vec{\phi}(-ih\nabla + \mu\vec{A})\tilde{\Pi}(u, p)] \, dudp \\ &= \epsilon \iint \tilde{M}(u, p) \mathrm{tr}[\vec{\phi}(-ih\nabla g_r(\cdot - u))P g_r(\cdot - u)] \, dudp \\ & \quad + \epsilon \iint \tilde{M}(u, p) \mathrm{tr}[\vec{\phi}g_r(\cdot - u)(-ih\nabla + \mu\vec{A})P g_r(\cdot - u)] \, dudp \end{aligned}$$

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:

$$\begin{aligned} & \epsilon \iint \tilde{M}(u, p) \mathrm{tr}[g_r(\cdot - u) \vec{\phi} \begin{pmatrix} (a + a^*)/2 \\ (a^* - a)/(2i) \\ 0 \end{pmatrix} P g_r(\cdot - u)] \, dudp \\ & \approx \epsilon \iint \tilde{M}(u, p) \mathrm{tr}[g_r^2(\cdot - u) \left\{ \vec{\phi} \begin{pmatrix} \mu h \\ i\mu h \\ 0 \end{pmatrix} \Pi_0^{(2)} + \vec{\phi} \begin{pmatrix} \mu h \\ -i\mu h \\ 0 \end{pmatrix} \Pi_1^{(2)} \right\}] \, dudp. \end{aligned}$$

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

$$\begin{aligned} & \epsilon \iint \tilde{M}(u, p) g_r^2(x - u) \phi_1(x) \left(\Pi_0^{(2)}(x_\perp, x_\perp) + \Pi_1^{(2)}(x_\perp, x_\perp) \right) \, dx dudp \\ &= \frac{\epsilon\mu}{\pi h} \iiint \tilde{M}(u, p) g_r^2(x - u) \phi_1(x) \, dx dudp \\ &= \frac{\epsilon\mu}{\pi h} \int_{-h^{-1}}^{h^{-1}} dp \int_{|u| \leq 1} \int r^{-3} g^2((x - u)/r) \phi_1(x) \, dx du \\ &\approx \frac{\epsilon\mu}{\pi h^2} \int \phi_1(x) \, dx. \end{aligned}$$

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

Lemma A.2. *Let $\phi \in C_0^\infty(\mathbb{R}^3)$, 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:

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

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 $\sup_y \int |K(x, y)| dx$. \square

ACKNOWLEDGEMENTS

The author wishes to thank the Schrödinger Institute in Vienna for hospitality during the fall term 1999, especially Thomas and Maria Hoffmann-Ostenhof. Furthermore, the author acknowledges many useful discussions with Thomas Østergaard Sørensen and Jan Philip Solovej.

References

- [ES97] L. Erdős and J.P. Solovej, *Semiclassical Eigenvalue Estimates for the Pauli Operator with Strong non-homogeneous magnetic fields. II. Leading order asymptotic estimates*, Commun. Math. Phys. **188** (1997), 599–656.

- [Fou98] S. Fournais, *Semiclassics of the Quantum Current*, Comm. in P.D.E **23** (1998), no. 3-4, 601–628.
- [Fou99] S. Fournais, *Semiclassics of the quantum current in a strong constant magnetic field*, University of Aarhus Preprint (1999), no. 9.
- [Ivr98] V. Ivrii, *Microlocal Analysis and Semiclassical Spectral Asymptotics*, Springer Verlag, 1998.
- [LS77] E.H. Lieb and B. Simon, *The Thomas-Fermi Theory of Atoms, Molecules and Solids*, Adv. Math. (1977), no. 23, 22–116.
- [LSY94] E. Lieb, J.P. Solovej, and J. Yngvason, *Asymptotics of heavy atoms in high magnetic fields: II. Semiclassical regions.*, Commun. Math. Phys. (1994), no. 161, 77–124.
- [Sob94] A.V. Sobolev, *The quasiclassical asymptotics of local Riesz means for the Schrödinger operator in a strong homogeneous magnetic field*, Duke Math Journal **74** (1994), no. 2, 319–429.