Local trace asymptotics in the self-generated magnetic field

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1 Global theory

1.1 Statement of the problem

Let us consider the following operator (quantum Hamiltonian) in $\mathbb{R}^d$ with $d = 3$

$$H = H_{A,V} = \left((hD - A) \cdot \sigma\right)^2 - V(x)$$

(1.1)

where $A, V$ are real-valued functions and $V \in L^2 \cap L^4$, $A \in H^1$. Than this operator is self-adjoint. We are interested in $\text{Tr}^{-} H_{A,V}$ (the sum of all negative eigenvalues of this operator). Let

$$E^* = \inf_{A \in H^1_0(B(0,1))} E(A),$$

(1.2)

$$E(A) := \left(\text{Tr}^{-} H_{A,V} + \kappa^{-1} h^{-2} \int |\partial A|^2 \, dx\right)$$

(1.3)

with $\partial A = (\partial_i A_j)$ a matrix. Semiclassical asymptotics for such objects were studied first in [EFS2] as a first step to consider asymptotics of the ground state energy for atoms and molecules in the self-generated magnetic fields.
which was achieved in [EFS3] where Scott correction term was recovered.

Similarly, this paper is the first step to the recovering sharper asymptotics of the ground state energy for atoms and molecules in the self-generated magnetic fields, hopefully up to and including Dirac and Schwinger corrections. To do this we improve theorem 1.1 of [EFS2] (see theorems 2.5, 2.7, 4.1 and 4.2 below).

The estimate from above is delivered by $A = 0$ and Weyl formula with an error $O(h^{-1})$ as $V \in \mathcal{C}^{2,1}$

\begin{equation}
E^* \leq \text{Weyl}_1 + O(h^{-1});
\end{equation}

where

\begin{equation}
\text{Weyl}(\tau) = \frac{1}{3\pi^2} h^{-3} \int (V + \tau)^{\frac{3}{2}} dx,
\end{equation}

\begin{equation}
\text{Weyl}_1 = \int_{-\infty}^{0} \tau d_{\tau} \text{Weyl}(\tau) = \frac{2}{15\pi^2} \int V^{\frac{3}{2}} dx.
\end{equation}

Also for estimates $o(h^{-2})$ we need to include into $\text{Weyl}_1$ the corresponding boundary term. The purpose of this paper is to provide an estimate from below

\begin{equation}
E^* \geq \text{Weyl}_1 - O(h^{-1});
\end{equation}

We will use also $\text{Weyl}(x, \tau)$ and $\text{Weyl}_1(x)$ defined the same way albeit without integration with respect to $x$.

In this version (v3) we fix several significant errors, include asymptotics with $o(h^{-1})$ remainder and provide a bit more details.

### 1.2 Preliminary

Let us estimate from below. First we need the following really simple theorem (cf. 3.1 [EFS1])

\footnote{Which means that the second derivatives of $V$ are continuous with the continuity modulus $O(\log |x - y|^{-1})$, see section 4.5 of [I2]). If there is a boundary it does not pose any problem as it is in the classically forbidden region.}

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Theorem 1.1. Let $V \in \mathcal{L}^{\frac{5}{2}} \cap \mathcal{L}^4$. Then

\begin{equation}
E^* \geq -Ch^{-3}
\end{equation}

and either

\begin{equation}
\frac{1}{\kappa h^2} \int |\partial A|^2 \, dx \leq Ch^{-3}.
\end{equation}

or $E(A) \geq ch^{-3}$.

**Proof.** Using the Magnetic Lieb-Thirring inequality (5) of [LLS])

\begin{equation}
\int \text{tr} \ e_1(x, x, \tau) \, dx \geq -Ch^{-3} \int V_+^\frac{5}{4} \, dx - Ch^2 \int \left( h^{-2} \int |\partial A|^2 \, dx \right)^\frac{3}{4} \left( h^{-8} \int V_+^4 \, dx \right)^\frac{1}{4}
\end{equation}

we conclude that for any $\delta > 0$

\begin{equation}
E(A) \geq -Ch^{-3} - C\delta^3 h^{-3} + (\kappa^{-1} - \delta^{-1})h^{-1} \int |\partial A|^2 \, dx
\end{equation}

which implies both statements of the theorem. \qed

Theorem 1.2. Let $V_+ \in \mathcal{L}^{\frac{5}{2}} \cap \mathcal{L}^4$, $\kappa \leq ch^{-1}$ and

\begin{equation}
V \leq -K^{-1}(1 + |x|^\delta) + K.
\end{equation}

Then there exists a minimizer $A$.

**Proof.** Consider a minimizing sequence $A_j$. Without any loss of the generality one can assume that $A_j \to A_\infty$ weakly in $\mathcal{H}^1$ and in $\mathcal{L}^6$ and strongly in $\mathcal{L}^p_{\text{loc}}$ with any $p < 6$. Then $A_\infty$ is a minimizer.

Really, due to (1.10) non-positive spectra of $H_{A_j, V}$ are discrete and the number of non-positive eigenvalues is bounded by $N_h$. Without any loss of the generality one can assume that $\lambda_{j,k}$ have limits (we go to the subsequence if needed) which are either $< 0$ or $= 0$. Here $\lambda_{j,k}$ are ordered eigenvalues of $H_{A_j, V}$.

We claim that those limits are also eigenvalues and if $\lambda_{j,k}, \ldots, \lambda_{j,k+r-1}$ have the same limit $\bar{\lambda} \leq 0$, it is eigenvalue of at least multiplicity $r$. Indeed,
let \( u_{j,k} \) be corresponding eigenfunctions, orthonormal in \( L^2 \). Then in virtue of \( A_j \) being bounded in \( L^\infty \) and \( V \in L^4 \) we can estimate

\[
\|Du_{j,k}\| \leq K \|u_{j,k}\|^{1-\sigma} \cdot \|u_{j,k}\|^\sigma \leq K \|Du_{j,k}\|^{1-\sigma} \cdot \|u_{j,k}\|^\sigma
\]

with \( \sigma > 0 \) which implies \( \|Du_{j,k}\| \leq K \). Also assumption (1.12) implies that \( \|(1 + |x|)^{\sigma/2}u_{j,k}\| \) are bounded and therefore without any loss of the generality one can assume that \( u_{j,k} \) converge strongly.

Then

\[
\lim_{j \to \infty} \Tr^{-} H_{A_j,V} \geq \Tr^{-} H_{A_{\infty},V}, \quad \lim \inf \int |\partial A_j|^2 \, dx \geq \int |\partial A_{\infty}|^2 \, dx
\]

and therefore \( E(A_{\infty}) \leq E^* \) (and then it is a minimizer and there are equalities and in particular there no other eigenvalues of \( H_{A_{\infty},V} \)).

**Remark 1.3.** We don’t know if the minimizer is unique. Also we do not impose here any restrictions on \( K \) (which may depend on \( h \)) in (1.12) or \( \kappa > 0 \). From now on until further notice let \( A \) be a minimizer.

**Proposition 1.4.** Let \( A \) be a minimizer. Then

\[
(1.13) \quad \frac{2}{\kappa h^2} \Delta A_j(x) = \Phi_j := -\sum_k (\sigma_j \sigma_k (hD_k - A_k)x + \sigma_k \sigma_j (hD_k - A_k)y) e(x, y, \tau)|_{y=x}
\]

where \( A = (A_1, A_2, A_3) \), \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \) and \( e(x, y, \tau) \) is the Schwartz kernel of the spectral projector of \( H_{A,V} \).

**Proof.** Consider variation \( \delta A \) of \( A \) and variation of \( \Tr^{-}(H) \). Note that the spectral projector of \( H \) is

\[
(1.14) \quad \theta(\tau - H) = \frac{1}{2\pi i} \int_{-\infty}^{\tau} \text{Res}_\mathbb{R} (\tau - H)^{-1}
\]

and therefore

\[
\delta \Tr \theta(\tau - H) = \frac{1}{2\pi i} \int_{-\infty}^{\tau} \text{Res}_\mathbb{R} \Tr (\tau - H)^{-1}(\delta H)(\tau - H)^{-1} = \\
\frac{1}{2\pi i} \int_{-\infty}^{\tau} \text{Res}_\mathbb{R} \Tr (\delta H)(\tau - H)^{-2} = -\partial_\tau \frac{1}{2\pi i} \int_{-\infty}^{\tau} \text{Res}_\mathbb{R} \Tr (\delta H)(\tau - H)^{-1} = \\
- \partial_\tau \Tr (\delta H) \theta(\tau - H).
\]
Plugging it into

\begin{equation}
\text{Tr}^{-}(H) = \int_{-\infty}^{0} \tau d\tau \text{ Tr} \theta(\tau - H) = - \int_{-\infty}^{0} \text{Tr} \theta(\tau - H) d\tau
\end{equation}

and integrating with respect to \( \tau \) we arrive after simple calculations to

\begin{equation}
\delta \text{Tr}^{-}(H) = \text{Tr}(\delta H)\theta(\tau - H) = - \int \Phi(x)\delta A(x) \, dx
\end{equation}

where \( \Phi(x) \) is the right-hand expression of (1.13). Therefore

\begin{equation}
\delta E(A) = \int (-\Phi(x) - \frac{2}{\kappa h^2}\Delta A(x))\delta A(x) \, dx
\end{equation}

which implies (1.13).

\begin{proposition}
If for \( \kappa = \kappa^* \)

\begin{equation}
E^* \geq \text{Weyl}_1 - CM
\end{equation}

with \( M \geq Ch^{-1} \) then for \( \kappa \leq \kappa^*(1 - \epsilon_0) \)

\begin{equation}
\frac{1}{\kappa h^2} \int |\partial A|^2 \, dx \leq C_1 M.
\end{equation}

Proof. Proof is obvious based also on the upper estimate \( E^* \leq \text{Weyl}_1 + Ch^{-1} \).
\end{proposition}

### 1.3 Estimates. I

**Proposition 1.6.** Let (1.19) be fulfilled and let

\begin{equation}
\varsigma = \kappa Mh^\frac{5}{2} \leq c
\end{equation}

Then as \( \tau \leq c \)

(i) Operator norm in \( L^2 \) of \((hD)^k \theta(\tau - H)\) does not exceed \( C \) for \( k = 0, 1, 2 \);

(ii) Operator norm in \( L^2 \) of \((hD)^k ((hD - A) \cdot \sigma) \theta(\tau - H)\) does not exceed \( C \) for \( k = 0, 1 \).
Proof. (i) Let \( u = \theta (\tau - H)f \). Then \( \| u \| \leq \| f \| \) and as

\[
\| A \|_6 \leq C \| \partial A \| \leq C (\kappa M)^{1 \over 2} \theta h
\]

we conclude that

\[
\| hD u \| \leq \| (hD - A) u \| + \| A u \| \leq \| (hD - A) u \| + C \| A \| \| u \|_3 \leq \]

\[
\| (hD - A) u \| + C (\kappa M)^{1 \over 2} h \| u \|^{3/4} \| u \|_6^{1/4} \leq \]

\[
\| (hD - A) u \| + C^{1 \over 2} \| u \|^{3/4} \| hD u \|^{1/4} \leq \]

\[
\| (hD - A) u \| + {1 \over 2} \| hD u \| + C \| u \|
\]

so due to (1.20)

\[
\| hD u \| \leq 2 \| (hD - A) u \| + C \| u \|
\]

On the other hand, for \( B = \nabla \times A \) and \( \tau \leq c \)

\[
\| (hD - A) u \|^2 \leq C \| u \|^2 + (h|B|u, u) \leq C \| u \|^2 + h \| B \| \| u \|_4^2 \leq \]

\[
C \| u \|^2 + C(\kappa M)^{1 \over 2} h^2 \| u \| \cdot \| u \|_6 \leq C \| u \|^2 + C(\kappa M)^{1 \over 2} h \| u \| \| hD u \|
\]

and due to (1.22) we conclude that

\[
\| hD u \| + \| (hD - A) u \| \leq C \| u \|. \tag{1.23}
\]

So, for \( j = 0, 1 \) statement (i) is proven. Further, as \( h^2D^2 = (hD - A)^2 + A(hD - A) + AhD - h[D, A] \) we in the same way as before (and using (1.23)) conclude that

\[
\| h^2D^2 u \| \leq C \| u \|^2 + {1 \over 4} \| hD(hD - A) u \| + {1 \over 4} \| h^2D^2 u \|
\]

and therefore

\[
\| h^2D^2 u \| \leq C \| u \|^2 + C \| AhD u \|
\]

and repeating the same arguments we get \( \| h^2D^2 u \| \leq C \| u \| \); so for \( j = 2 \) statement (i) is proven.

(ii) Statement (ii) is proven in the same way. \( \square \)
Corollary 1.7. Let (1.19) and (1.20) be fulfilled. Then as \( \tau \leq c \)

\[
(1.24) \quad e(x, x, \tau) \leq Ch^{-3}, \quad \left| ((hD - A) \cdot \sigma) e(x, y, \tau) \right|_{x=y} \leq Ch^{-3}.
\]

Proof. Due to proposition 1.6 operator norms from \( L^2 \) to \( C \) of both \( \theta(\tau - H) \) and \( ((hD - A) \cdot \sigma) \theta(\tau - H) \) do not exceed \( C \) and the same is true for an adjoint operator which imply both claims. \( \square \)

Corollary 1.8. Let (1.19) and (1.20) be fulfilled and \( A \) be a minimizer. Then for arbitrarily small exponent \( \delta > 0 \)

\[
(1.25) \quad \| \partial A \|_{C^{1-\delta}} \leq C\kappa h^{-1},
\]

\[
(1.26) \quad \| \partial A \|_{\infty} \leq h^{-\frac{\delta}{2}}
\]

where \( C^\theta \) is the scale of Hölder spaces and \( \delta > 0 \) is arbitrarily small.

Proof. Really, due to (1.13) for a minimizer \( \| \Delta A \|_{\infty} \leq C\kappa h^{-1} \). Also we know that \( \| \partial A \| \leq C(\kappa Mh^2)^{\frac{1}{2}} \leq Ch^{\frac{1}{2}} \) due to (1.20). Then (1.25) holds due to the standard properties of the elliptic equations\(^2\).

Therefore if at some point \( y \) we have \( |\partial A(y)| \geq \mu \), it is true in its \( \epsilon (\mu \kappa^{-1})^{1-\delta} \)-vicinity (provided \( \mu \leq \kappa h^{-1} \)) and then

\[
\| \partial A \|^{2} \geq \mu^{2}(\mu h \kappa^{-1})^{3(1-\delta)}
\]

and we conclude that

\[
\mu^{2}(\mu h \kappa^{-1})^{3(1-\delta)} \leq C\kappa h^{2} M \iff \mu^{5-3\delta} \leq C\kappa^{4-3\delta} h^{-1+3\delta} M
\]

and one can see easily that (1.26) holds due to (1.20) and \( h^{-1} \leq M \leq h^{-3} \).

On the other hand, if \( \mu \geq \kappa h^{-1} \) then we need to take \( \epsilon \)-vicinity and then \( \mu^{2} \leq C\kappa M h^{2} \leq Ch^{\frac{1}{2}} \) where we used (1.20) again. Then (1.26) is proven. \( \square \)

Remark 1.9. (i) It is not clear if it is possible to generalize this theory to arbitrary \( d \geq 2 \) with magnetic field energy is given by

\[
(1.27) \quad \frac{1}{\kappa h^{d-1}} \int \left( |\partial A|^{2} - |\nabla \cdot A|^{2} \right) dx
\]

Surely one should use generalized Pauli matrices \( \sigma_{j} \) in the definition of the operator. Especially problematic are \( d \geq 5 \).

\( ^{2} \) Actually we can slightly improve this statement.

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Therefore while arguments of section 2 below remain valid for $d \neq 3$, so far they remain conditional (if a minimizer exists and satisfies some crude estimates).

2 Microlocal analysis unleashed

2.1 Sharp estimates

Now we can unleash the full power of microlocal analysis but we need to extend it to our framework. It follows by induction from (1.25)–(1.26) and the arguments we used to derive these estimates that

\begin{equation}
\| \partial A \|_{C^{\theta-\delta}} \leq C_{\kappa} h^{-1-\delta},
\end{equation}

so $A$ is “smooth” in $\varepsilon = h$ scale while for rough microlocal analysis as in [BI] and section 2.3 of [I2] one needs $\varepsilon = C h \log h$ at least. We consider in this section arbitrary $d \geq 2$; see however remark 1.9.

Note that

\begin{equation}
\text{For a commutator of a pseudo-differential operator with a smooth symbol and } C^{\theta+1} \text{ function } A \text{ a usual commutator formula holds modulo } O(h^{\theta+1}\|\partial A\|_{C^{\theta}}) \text{ for any non-integer } \theta > 0.
\end{equation}

Proposition 2.1. Assume that

\begin{equation}
\mu := \| \partial A \|_{C^{\infty, B(x,1)}} \leq C_0,
\end{equation}

and in in $B(x,1)$

\begin{equation}
|V| \geq \varepsilon_0.
\end{equation}

Then for $|\alpha| \leq 2, |\beta| \leq 2, \theta > 1$

\begin{equation}
\left| F_{t \to h^{-1} \tau} \chi_T(t)((hD_x)^\alpha (hD_y)^\beta U(x, y, t)) \right|_{x = y} \leq C h^{1-d+s} T^{-s} + C h^{-d+\theta} T^2 \|\partial A\|_{C^{\theta}}
\end{equation}

where $\chi \in C^{\infty}([-1, -\frac{1}{2}] \cup [\frac{1}{2}, 1]), \chi_T(t) = \chi(t/T), Ch \leq T \leq \varepsilon, |\tau| \leq \varepsilon$ and $U(x, y, t)$ is the Schwartz kernel of $e^{ih^{-1}tA}$. 


Proof. Consider first \( T \approx 1 \). First, using standard propagation arguments as in [BI] and section 2.3 of [I2] one can prove the finite propagation speed with respect to \( x \), namely that

\begin{align}
|F_{t \to h^{-1}x}(hD_x)^\alpha(hD_y)^\beta U| \leq Ch^s \quad \text{as } |x - y| \geq C_0 T, \; \tau \leq c_0
\end{align}

with an arbitrarily large exponent \( s \). Further, using (2.6) we prove the finite propagation speed with respect to \( \xi \):

\begin{align}
|F_{t \to h^{-1}x}(hD_x)^\alpha(hD_y)^\beta \varphi_1(hD_x)\varphi_2(hD_y)U| \leq Ch^s + Ch^\theta \| \partial A \|_{C^\theta}
\end{align}

as \( \varphi_1, \varphi_2 \in C^\infty_0 \), \( \text{dist}(\text{supp} \varphi_1, \text{supp} \varphi_2) \geq C_0 T, \; \tau \leq c_0 \)

where the last term in the right-hand expression is due to the non-smoothness of \( A \).

Furthermore, using (2.6) and (2.7) we prove that as (2.4) is fulfilled there is a propagation:

\begin{align}
|F_{t \to h^{-1}x}(hD_x)^\alpha(hD_y)^\beta U| \leq Ch^s + Ch^\theta \| \partial A \|_{C^\theta}
\end{align}

as \( |x - y| \leq \epsilon_0 T, \; |\tau| \leq \epsilon, \; T \leq \epsilon \)

which implies (2.5) under additional assumption \( T \approx 1 \); here the last term in the right-hand expression is inherited from (2.7).

Finally, for \( Ch \leq T \leq \epsilon \) we use rescaling \( t \mapsto t/T, \; x \mapsto x/T, \; h \mapsto h/T \) and we use “homogenized” \( C^\theta \) norms. Detailed proof for will be published later.

Corollary 2.2. In the framework of proposition 2.1 as \(|\alpha| \leq 2, \; |\beta| \leq 2 \)

\begin{align}
|F_{t \to h^{-1}x}[\bar{\chi}_T(t)((hD_x)^\alpha(hD_y)^\beta U(x,y,t))]|_{x=y} \leq Ch^{1-d} + CT^2h^{-d+\theta}\| \partial A \|_{C^\theta}
\end{align}

where \( \bar{\chi} \in C^\infty([-1, 1]) \) and

\begin{align}
|[(hD_x - A(x)) \cdot \sigma]^\alpha((hD_y - A(y)) \cdot \sigma)^\beta e(x,y,t)|_{x=y} - \text{Weyl}_{\alpha,\beta}(x)| \leq Ch^{1-d} + Ch^{-d+\frac{1}{2}(\theta+1)}\| \partial A \|_{C^\theta}^{\frac{1}{2}}
\end{align}

\text{Weyl}_{\alpha,\beta}(x)
where

\[ \text{Weyl}_{\alpha,\beta}(x) = \text{const} \ h^{-d} \int_{\{H(x,\xi) \leq \tau\}} ((\xi - A(x)) \cdot \sigma)^{\alpha + \beta} \ d\xi \]  

is the corresponding Weyl expression and

\[ H(x,\xi) = (\xi - A(x) \cdot \sigma)^{2} - V(x); \]

in particular Weyl is 0 as \(|\alpha| + |\beta| = 1\).

**Proof.** Obviously summation of (2.5) over \( C_0 h \leq |t| \leq T \) and a trivial estimate by \( Ch^{1-d} \) of the contribution of the interval \(|t| \leq C_0 h\) implies (2.9).

Then the standard Tauberian arguments and (2.9) imply that (2.10) would be correct if we used Tauberian expression with \( T = T^* \) instead of \( \text{Weyl} \) where we pick up

\[ T^* = \epsilon \min\left(1, h^{-\frac{1}{2}(\theta-1)}\|\partial A\|_{\psi, \theta}^{-\frac{1}{2}}\right). \]

Meanwhile the Tauberian formula and (2.5) imply that the contribution of an interval \( \{t : |t| \asymp T\} \) with \( h \leq T \leq T^* \) to the Tauberian expression does not exceed the right-hand expression of (2.5) divided by \( T \), i.e.

\[ Ch^{1-d+s} T^{-s-1} + CT h^{-d+\theta} \|\partial A\|_{\psi, \theta}; \]

summation over \( T_* := h^{1-\delta} \leq T \leq T^* \) results in the right-hand expression of (2.10).

So, we need to calculate only the contribution of \( \{t : |t| \leq T_*\} \) but one can see easily that modulo indicated error it coincides with \( \text{Weyl}_{\alpha,\beta} \). \( \square \)

**Corollary 2.3.** (i) If assumption (2.3) is replaced by

\[ \mu := \|\partial A\|_{\infty} \leq Ch^{-1+\sigma} \]

with \( \sigma > 0 \) then

\[ |\left[ ((hD_x - A(x)) \cdot \sigma)^{\alpha} (hD_y - A(y)) \cdot \sigma)^{\beta} e(x,y,t) \right]|_{x=y} =
\]

\[ \text{Weyl}_{\alpha,\beta}(x) \leq C \bar{\mu} h^{-d} + C \bar{\mu}^{-\frac{1}{2}} h^{-d+\frac{1}{2}(\theta+1)} \|\partial A\|_{\psi, \theta}^{\frac{1}{2}} \]

and

\[ T^* = \epsilon \min\left(\bar{\mu}^{-1}, \bar{\mu} h^{-\frac{1}{2}(\theta-1)}\|\partial A\|_{\psi, \theta}^{-\frac{1}{2}}\right) \]

with \( \bar{\mu} = \max\left(\mu, 1\right) \).
(ii) As \( d \geq 3 \) one can skip assumption (2.4).

**Proof.** As \( d \geq 3 \) (ii) is proven by the standard rescaling technique: \( x \mapsto x\ell, \ h \mapsto h\ell^{-\frac{1}{2}}, \ A \mapsto A\ell^{-\frac{1}{2}} \) with \( \ell = \max(\epsilon |V|, h^{\frac{3}{2}}) \) (see [I1] and chapter 5 of [I2].

As \( \mu \geq 1 \) (i) is proven by the standard rescaling technique \( x \mapsto \mu x, \ h \mapsto h\mu. \)

**Proposition 2.4.** Let \( \kappa \leq c \), (2.14) be fulfilled, and let \( A \) be a minimizer. As \( d = 2 \) let (2.4) be also fulfilled. Then as \( \theta \in (1, 2) \)

\[
(2.17) \quad \|\partial A\|_{\theta^{-1}} + h^{\theta-1}\|\partial A\|_{\theta} \leq C\kappa + C\|\partial A\|' 
\]

with

\[
(2.18) \quad \|\partial A\|' := \sup_y \|\partial A\|_{L^2(B(y, 1))}. 
\]

**Proof.** Consider expression for \( \Delta A \). According to (1.13) and (2.15) we get then for any \( \theta \in (1, 2) \)

\[
(2.19) \quad \|\Delta A\| + h\partial \Delta A \leq C\kappa(\bar{\mu} + \mu^{-\frac{1}{2}} h^{\frac{1}{2}(\theta-1)}\|\partial A\|_{\theta}^{\frac{1}{2}})
\]

which implies that for any \( \theta' \in (1, 2) \)

\[
h^{\theta'-1}\|\partial A\|_{\theta'} \leq C\kappa(\bar{\mu} + \mu^{-\frac{1}{2}} h^{\frac{1}{2}(\theta-1)}\|\partial A\|_{\theta}^{\frac{1}{2}}) + C\mu,
\]

and picking up \( \theta' = \theta \) we conclude that

\[
(2.20) \quad h^{\theta-1}\|\partial A\|_{\theta} \leq C(\kappa \bar{\mu} + \kappa^2 \mu^{-1}) + C\mu.
\]

As \( \kappa \leq c \) the right-hand expression does not exceed \( C(\kappa + \mu) \); then the right-hand expression in (2.19) also does not exceed \( C(\kappa + \mu) \); then \( \|\partial A\|_{\theta^{-1}} \leq C(\kappa + \mu) \) and then \( \mu \leq C\kappa + C\|\partial A\|' \), which implies (2.17). \( \square \)

Having this strong estimate to \( A \) allows us to prove

**Theorem 2.5.** Let \( \kappa \leq c \), (2.14) be fulfilled, and let \( d = 3 \). Then

\[
(2.21) \quad E^* = \text{Weyl}_1 + O(h^{-1})
\]
and a minimizer $A$ satisfies

\begin{equation}
\|\partial A\| \leq C \kappa^{\frac{1}{2}} h^{\frac{1}{2}}
\end{equation}

and

\begin{equation}
\|\partial A\|_{\varphi^{\theta}-1} + h^{\theta-1} \|\partial A\|_{\varphi^{\theta}} \leq C \kappa^{\frac{1}{2}} h^{\frac{1}{2}} + C \kappa.
\end{equation}

**Proof.** In virtue of (2.9) and (2.17) the Tauberian error with $T \asymp 1$ when calculating $\text{Tr} H_{a,V}^-$ does not exceed

\begin{equation}
\bar{C} \mu^2 h^{2-d} + C(\kappa + \|\partial A\|) h^{2-d}.
\end{equation}

We claim that

\begin{equation}
\text{Weyl error when calculating } \text{Tr} H_{a,V}^- \text{ also does not exceed (2.24).}
\end{equation}

Then

\begin{equation}
E^*(A) \geq \text{Weyl}_1 - C \mu^2 h^{2-d} - C(\kappa + \|\partial A\|') h^{2-d} + \kappa^{-1} h^{1-d} \|\partial A\|^2 \geq \\
\text{Weyl}_1 - Ch^{2-d} + \frac{1}{2\kappa} h^{1-d} \|\partial A\|^2
\end{equation}

because $\bar{\mu} \leq C \|\partial A\| + 1$ due to (2.17). This implies an estimate of $E^*$ from below and combining with the estimate $E^* \leq E^*(0) = \text{Weyl}_1 + Ch^{2-d}$ from above we arrive to (2.21) and (2.22) and then (2.23) due to (2.17).

To prove (2.25) let us plug $A_\epsilon$ instead of $A$ into $e_1(x, x, 0)$. Then in virtue of rough microlocal analysis contribution of $\{t : T_* \leq |t| \leq \epsilon\}$ with $T_* = h^{1-\delta}$ would be negligible and contribution of $\{t : |t| \leq T_*\}$ would be $\text{Weyl}_1 + O(h^{2-d})$.

Let us calculate an error which we made plugging $A_\epsilon$ instead of $A$ into $e_1(x, x, 0)$. Obviously it does not exceed $Ch^{-d} \|A - A_\epsilon\|_\infty$ and since $\|A - A_\epsilon\|_\infty \leq C \epsilon^{\theta+1} \|\partial A\|_{\varphi^{\theta}}$ this error does not exceed $Ch^{\theta+1-d-4\delta} \|\partial A\|_{\varphi^{\theta}}$ which is marginally worse than what we are looking for. However it is good enough to recover a weaker version of (2.21) and (2.22) with an extra factor $h^{-\delta_1}$ in their right-hand expressions. Then (2.17) implies a bit weaker version of (2.23) and in particular that its left-hand expression does not exceed $C$.

Knowing this let us consider the two term approximation. With the above knowledge one can prove easily that the error in two term approximation does not exceed $Ch^{3-d-\delta'}$ with $\delta' = 100\delta$. 

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Then the second term in the Tauberian expression is

\[
\int ((H_{A,V} - H_{A_\varepsilon,V})e^{\Delta}(x,y,0)) \big|_{y=x} dx.
\]

where subscript \(A_\varepsilon\) means that we plugged \(A_\varepsilon\) instead of \(A\) and superscript \(\Delta\) means that we consider Tauberian expression with \(T = T^* = \varepsilon\). But then the contribution of \(\{ t : T_* \leq |t| \leq T^* \} \) is also negligible and modulo \(Ch^{\theta+2-d-4\delta}\|\partial A\|_{C^\theta}\) we get a Weyl expression. However

\[
(H_{A,V} - H_{A_\varepsilon,V}) = -2(\xi - A_\varepsilon) \cdot (A - A_\varepsilon) + |A - A_\varepsilon|^2
\]

and the first term kills Weyl expression as integrand is odd with respect to \((\xi - A_\varepsilon)\) while the second as one can see easily makes it smaller than \(Ch^{\theta-d-\delta}\). Therefore (2.25) has been proven.

\[\square\]

**Remark 2.6.** (i) For \(d = 2\) we cannot skip (2.4) at the stage we did it for \(d \geq 3\). However results of the next section allow us to cure this problem using partition-and-rescaling technique.

(ii) Actually we have an estimate

\[
|\partial A(x) - \partial A(y)| \leq C\kappa|x - y|(|\log |x - y|| + 1) + C\mu.
\]

Combining with (2.22) we conclude that

\[
\|\partial A\|_\infty \leq C\kappa^{(d+1)/(d+2)}|\log h|^{d/(d+2)}h^{1/(d+2)}
\]

### 2.2 Classical dynamics and sharper estimates

Now we want to improve remainder estimate \(O(h^{2-d})\) to \(o(h^{2-d})\). Sure, we need to impose condition to the classical dynamical system and as \(|\partial A| = O(h^\sigma)\) with \(\sigma > 0\) due to (2.30) it should be dynamical system associated with Hamiltonian flow generated by \(H_{0,V}\):

\[
H_{0,V}
\]

(2.31) The set of periodic points of the dynamical system associated with Hamiltonian flow generated by \(H_{0,V}\) has measure 0 on the energy level 0.
Recall that on \( \{(x, \xi) : H_{0,V}(x, \xi) = \tau \} \) a natural density \( d\mu_\tau = dx d\xi : dH|_{H=\tau} \) is defined.

The problem is we do not have quantum propagation theory for \( H_{A,V} \) as \( A \) is not a “rough” function. However it is rather regular function, almost \( C^2 \), and \( (A - A_\xi) \) is rather small: \( |A - A_\xi| \leq \eta = Ch^{2-3\delta} \) and \( |\partial (A - A_\xi)| \leq Ch^{1-3\delta} \) and therefore we can apply a method of successive approximations with the unperturbed operator \( H_{A_\xi,V} \) as long as \( \eta T/h \leq h^\sigma \) i.e. as \( T \leq h^{1-4\delta} \). Here we however have no use for such large \( T \) and consider \( T = O(h^\delta) \).

Consider

\[
F_{t \rightarrow h^{-1}\tau}(t) \chi_T(t) U(x, y, t),
\]

and consider terms of successive approximations. Then if we forget about microhyperbolicity arguments the first term will be \( O(h^{-d})T \), the second \( O(h^{-1-d}\eta T^2) = O(h^{1-d-\delta'}) \) and the error \( O(h^{-2-d}\eta T^3) = O(h^{2-d-3\delta'}) \).

Therefore as our goal is \( O(h^{1-d}) \) we need to consider the first two terms only. The first term is the same expression (2.32) with \( U \) replaced by \( U_\epsilon \).

Consider the second term, it corresponds to

\[
(2.33) \quad U'_\epsilon = \left[ i\hbar^{-1} \int_0^T e^{i(t-t')h^{-1}H_{A_\xi,V}}(H_{A,V} - H_{A_\xi,V}) e^{it'\hbar^{-1}H_{A_\xi,V}} dt' \right]
\]

and then

\[
(2.34) \quad \text{Tr} (e^{ih^{-1}tA_\xi}\psi) = ih^{-1} \text{Tr} \left( (H_{A,V} - H_{A_\xi,V}) e^{ih^{-1}tH_{A_\xi,V}} \psi_t \right)
\]

with

\[
\psi_t = \int_0^T e^{ih^{-1}tH_{A_\xi,V}}\psi e^{-ih^{-1}tH_{A_\xi,V}} dt'.
\]

Here \([S](x, y)\) denotes the Schwartz kernel of operator \( S \). We claim that

\[
(2.35) \quad |F_{t \rightarrow h^{-1}\tau}(t) \text{Tr} U'_\epsilon \psi| \leq C\eta T^2 h^{-d}.
\]

Here in comparison with the trivial estimate we gained factor \( h \). The proof of (2.35) can be done easily by the standard rough microlocal analysis arguments and we will provide a detailed proof later.

Therefore we arrive to the estimate

\[
(2.36) \quad |F_{t \rightarrow h^{-1}\tau}(t) \text{Tr} \left( (e^{it'\hbar^{-1}H_{A_\xi,V}} - e^{it\hbar^{-1}H_{A_\xi,V}}) \psi \right) | \leq Ch^{1-d}.
\]

On the other hand traditional methods imply that as \( d \geq 3 \)

\[
(2.37) \quad |F_{t \rightarrow h^{-1}\tau}(t) \text{Tr} (e^{it\hbar^{-1}H_{A_\xi,V}} \psi) | \leq Ch^{1-d} T \mu(\nabla_{T,\phi}) + C_{T,\phi} h^{1-d-\delta}
\]
where $\Pi_T$ is the set of points on energy level 0, periodic with periods not exceeding $T$, $\Pi_{T,\rho}$ is its $\rho$-vicinity, $\rho > 0$ is arbitrarily small.

**Theorem 2.7.** Let $\kappa \leq c$, (2.14) be fulfilled, and let $d = 3$. Furthermore, let condition (2.31) be fulfilled (i.e. $\mu_0(\Pi_{\infty}) = 0$). Then

\[(2.38) \quad E^* = \text{Weyl}_1^* + o(h^{-1})\]

where

\[(2.39) \quad \text{Weyl}_1^* = \text{Weyl}_1 + \kappa h^{-1} \int V_{\frac{1}{2}} \Delta V \, dx\]

calculated in the standard way for $H_0, V$ and a minimizer $A$ satisfies similarly improved versions of (2.22) and (2.23).

**Remark 2.8.** (i) Under stronger assumptions to the Hamiltonian flow one can recover better estimates like $O(h^{2-d} |\log h|^{-2})$ or even $O(h^{2+\delta-d})$ (like in subsubsection 4.4.4.3 of [I2]).

(ii) We leave to the reader to calculate the numerical constants $\kappa_*$ here and in (3.4), $\kappa = \kappa_1 - \frac{2}{3} \kappa_2$.

**3 Local theory**

**3.1 Localization**

The results of the previous section have two shortcomings: first, they impose the excessive requirement to $\kappa$; second, they are not local. However curing the second shortcoming we make the way to addressing the first one as well using the partition and rescaling technique.

We localize the first term in $E(A)$ by using the same localization as in [EFS1]: namely we take $\text{Tr}^- (\psi H \psi)$ where $\psi \in C_0^\infty (B(0, \frac{1}{2}))$, $0 \leq \psi \leq 1$ and some other conditions will be imposed to it later. Note that

\[(3.1) \quad \text{Tr}^- (\psi H \psi) \geq \int e_1(x, x, 0) \psi^2(x) \, dx.\]

Really, operator $H = H\theta(-H) + H(1 - \theta(-H))$ where $\theta(\tau - H)$ is a spectral projector of $H$ and therefore in the operator sense $H \geq H^- := HE(0)$ and
\( \psi H \psi \geq \psi H^- \psi \) and therefore all negative eigenvalues of \( \psi H \psi \) are greater than or equal to eigenvalues of the negative operator \( \psi H^- \psi \) and then

\[
\text{Tr}^-(\psi H \psi) \geq \text{Tr} \psi H^- \psi = \text{Tr} \int_{-\infty}^{0} \tau d\tau E(\tau)\psi^2
\]

which is exactly the right-hand expression of (3.1).

**Remark 3.1.** (i) The right-hand expression of (3.1) is an another way to localize operator trace. Each approach has its own advantages. In particular, no need to localize \( A \) (see (ii)) and the fact that proposition 1.5 obviously remains true (due to corollary 2.3) are advantages of \( \text{Tr}^- (\psi H \psi) \)-localization.

(ii) As \( \text{Tr}^- (\psi H \psi) \) does not depend on \( A \) outside of \( B(0, \frac{3}{4}) \) we may assume that \( A = 0 \) outside of \( B(0, 1) \). Really, we can always subtract a constant from \( A \) without affecting traces and also cut-off \( A \) outside of \( B(0, 1) \) in a way such that \( A' = A \) in \( B(0, \frac{3}{4}) \) and \( \| \partial A' \| \leq c \| \partial A \|_{B(0, 1)} \); the price is to multiply \( \kappa \) by \( c^{-1} \) – as long as principal parts of asymptotics coincide.

(iii) Additivity rather than sub-additivity (4.2) and the trivial estimate from the above are advantages of \( \text{Tr} \psi H^- \psi \)-localization. It may happen that the latter definition is more useful in applications to theory of heavy atoms and molecules and we will need to recover our results under it.

Let us estimate from the above:

**Proposition 3.2.** Let \( \ell(x) \) be a scaling function\(^3\) and \( \psi \) be a function such that \( |\partial^\alpha \psi| \leq c \psi \ell^{-2|\alpha|} \) for all \( \alpha : |\alpha| \leq 2 \) and \( |\psi| \leq \ell^{3/4} \).

Then, as \( A = 0 \),

\[
(3.2) \quad \text{Tr}^- (\psi H \psi) = \int \text{Weyl}_1(x) \psi^2(x) \, dx + O(h^{-1})
\]

and under assumption (2.31)

\[
(3.3) \quad \text{Tr}^- (\psi H \psi) = \int \text{Weyl}_1^*(x) \psi^2(x) \, dx + o(h^{-1})
\]

with

\[
(3.4) \quad \text{Weyl}_1^*(x) = \text{Weyl}_1(x) + \kappa_1 h^{-1} V_1^2 \Delta V + \kappa_2 h^{-1} V_2^2 |\nabla V|^2
\]

calculated in the standard way for \( H_0, V \).

\(^3\) I.e. \( \ell \geq 0 \) and \( |\partial \ell| \leq \frac{1}{2} \).

\(^4\) Such compactly supported functions obviously exist.
Proof. Let us consider $\tilde{H} = \psi H \psi$ as a Hamiltonian and let $\tilde{e}(x, y, \tau)$ be the Schwartz kernel of its spectral projector. Then

\begin{equation}
\text{Tr}^{-}(\psi H \psi) = \int \tilde{e}_1(x, x, 0) \, dx = \sum_j \int \tilde{e}_1(x, x, 0) \psi_j^2 \, dx
\end{equation}

where $\psi_j^2$ form a partition of unity in $\mathbb{R}^3$ and we need to calculate the right hand expression.

(i) Consider first an $\epsilon \ell$-admissible partition of unity in $B(0, 1)$. Let us consider $\gamma$-scale in such element where $\gamma = \max(\epsilon \ell^2, h)$ and we will use 1 scale in $\xi$. Then after rescaling $x \mapsto x/\gamma$ semiclassical parameter rescales $h \mapsto h_{\text{new}} = h/\gamma$ and the contribution of each $\gamma$-element to a semiclassical remainder does not exceed $C \rho(h/\gamma)^{-1}$ with $\rho \leq \ell^4$ having the same magnitude over element as $\gamma \geq 2h$. Then contribution of $\ell$ element to a semiclassical error does not exceed $C \rho(h/\gamma)^{-1} \times \ell^3 \gamma^{-3} \propto Ch^{-1} \rho \ell^{-4} \leq Ch^{-1} \ell^5$.

As $\ell^2 \asymp h$ the same arguments work with $\ell$ replaced by $h^{\frac{1}{2}}$ and $\gamma = h$ and effective semiclassical parameter $\epsilon \ell^2$.

Therefore the total contribution of all partition elements in $B(0, 1)$ to a semiclassical error does not exceed $Ch^{-1}$.

(ii) However we need to consider contribution of the rest of $\mathbb{R}^3$. Here we use $\gamma = \frac{1}{2} |x|$, 1-scale with respect to $\xi$ and take $\rho = h \gamma^{-2}$; then contribution of $\gamma$-element to a semiclassical error does not exceed $C \rho(h/\gamma)^{-1} \leq C \gamma^{-1}$ and summation over partition results in $C$. Thus (3.2) is proven.

(iii) Note that contribution of zone $\|\{x : \ell \leq \eta\}$ to the remainder does not exceed $C \ell^2 h^{-1}$; applying in zone $\|\{x : \ell \geq \eta\}$ sharp asymptotics under assumption (2.31) we prove (3.3). \hfill $\square$

Corollary 3.3. In the framework of proposition 3.2(i), (ii)

\begin{equation}
E^*_\psi := \inf_A E_\psi(A) \leq \text{Weyl}_1 + Ch^{-1}
\end{equation}

and

\begin{equation}
E^*_\psi \leq \text{Weyl}_1^* + Ch^{-1}
\end{equation}

respectively with

\begin{equation}
E_\psi(A) := \text{Tr}^{-}(\psi H \psi) + \frac{1}{\kappa h^2} \int |\partial A|^2 \, dx.
\end{equation}

Really, we just pick $A = 0$. 

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\subsection{3.2 Estimate from below}

Now let us estimate $E_\psi(A)$ from below. We already know that

\begin{equation}
E_\psi(A) \geq \int e_1(x, x, 0) \psi^2 \, dx + \frac{1}{\kappa h^2} \int_{B(0,1)} |\partial A|^2 \, dx.
\end{equation}

However we need an equation for an optimizer and it would be easier for us to deal with even lesser expression involving $\tau$-regularization. Let us rewrite the first term in the form

\[
\int_{-\infty}^{0} \tilde{\varphi}(\tau/L) \, d_r e(x, x, \tau) + \int_{-\infty}^{0} (1 - \tilde{\varphi}(\tau/L)) \, d_r e(x, x, \tau) \geq \\
\int_{-\infty}^{L} \left( \tilde{\varphi}(\tau/L)(\tau - L) \, d_r e(x, x, \tau) + (1 - \tilde{\varphi}(\tau/L)) \, d_r e(x, x, \tau) \right)
\]

where $\tilde{\varphi} \in C^\infty_0([-1, 1])$ equals 1 in $[-\frac{1}{2}, \frac{1}{2}]$ and let us estimate from below

\begin{equation}
E_\psi'(A) = \int \int_{-\infty}^{0} \tilde{\varphi}(\tau/L)\tau \, d_r e(x, x, \tau) + \\
(1 - \tilde{\varphi}(\tau/L))\tau \, d_r e(x, x, \tau) \psi(x) \, dx + \\
\frac{1}{\kappa h^2} \int_{B(0,1)} |\partial A|^2 (\varphi(x) + K^{-1}) \, dx.
\end{equation}

**Proposition 3.4.** Let $A$ be a minimizer of $E_\psi'(A)$. Then

\begin{equation}
\frac{2}{\kappa h^2} \Delta A_j(x) = \Phi_j := \\
\sigma_j \sigma_k (hD_k - A_k)_x + \sigma_k \sigma_j (hD_k - A_k)_y \times \\
\int_{-\infty}^{L} \left[ \tilde{\varphi}(\tau/L)(\tau - L) \, \text{Res}_\mathbb{R}(\tau - H)^{-1} \psi(\tau - H)^{-1} + \\
(1 - \tilde{\varphi}(\tau/L))\tau (\tau - L) \, \text{Res}_\mathbb{R}(\tau - H)^{-1} \psi(\tau - H)^{-1} \right] (x, y) \, d\tau \bigg|_{y=x}
\end{equation}

where again $[S](x, y)$ is the Schwartz kernel of $S$.

**Proof.** Follows immediately from the proof of proposition 1.4. \hfill \Box
Proposition 3.5. Let (1.19) and (1.20) be fulfilled. Then as $\tau \leq c$

(i) Operator norm in $L^2$ of $(hD)^k(\tau - H)^{-1}$ does not exceed $C|\text{Im } \tau|^{-1}$ for $k = 0, 1, 2$;

(ii) Operator norm in $L^2$ of $(hD)^2((hD - A) \cdot \sigma)(\tau - H)^{-1}$ does not exceed $C|\text{Im } \tau|^{-1}$ for $k = 0, 1, 2$.

Proof. Proof follows the same scheme as the proof of proposition 1.6.

Proposition 3.6. Let (1.19) and (1.20) be fulfilled. Then $|\Phi(x)| \leq Ch^{-3}$.

Proof. Let us estimate

\begin{equation}
(3.12) \quad |\int \tau \varphi(\tau/L) \text{Res}_\mathbb{R} \left[ T(\tau - H)^{-1} \psi(\tau - H)^{-1} \right](x, y) d\tau|
\end{equation}

where $L \leq c$ and $\varphi \in C^\infty([1, 1])$ and a similar expression with a factor $(\tau - L)$ instead of $\tau$; here either $T = I$, or $T = (hD_k - A_k)x$ or $T = (hD_k - A_k)y$.

Proposition 3.5 implies that the Schwartz kernel of the integrand does not exceed $Ch^{-3}|\text{Im } \tau|^{-2}$ and therefore expression (3.12) does not exceed $CL^2 \times h^{-3}L^{-2} = Ch^{-3}$.

Then what comes out in $\Phi$ from the term with the factor $\tilde{\varphi}(\tau/h)$ does not exceed $Ch^{-3}$.

Representing $(1 - \tilde{\varphi}(\tau/h))$ as a sum of $\varphi(\tau/L)$ with $L = 2^n h$ with $n = 0, \ldots, [\log h] + c$ we estimate the output of each term by $Ch^{-3}$ and thus the whole sum by $Ch^{-3}|\log h|$.

To get rid of the logarithmic factor we rewrite $(\tau - H)^{-1}\psi(\tau - H)^{-1}$ as $-\partial(\tau - H)^{-1}\psi + (\tau - H)^{-2}[h, \psi](\tau - H)^{-1}$; if we plug only the second part we recover a factor $h/L$ where $h$ comes from the commutator and $1/L$ from the increased singularity; an extra operator factor in the commutator is not essential. Then summation over partition results in $Ch^{-3}$.

Plugging only the first part we do not use the above decomposition but an equality $\text{Res}_\mathbb{R}(\tau - H)^{-1} d\tau = d, \theta(\tau - H)$. \hfill \Box

Corollary 3.7. Let (1.19) and (1.20) be fulfilled and $A$ be a minimizer. Then (1.25) and (1.26) hold.

Proof. Proof follows the proof of corollary 1.8. \hfill \Box

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Now we can recover both proposition 2.4 and finally theorems 2.5 and 2.7:

**Theorem 3.8.** Let (1.19) and \( \kappa \leq c \) be fulfilled. Then

(i) The following estimate holds:

\[
E^*_\psi = \int \text{Weyl}_1(x)\psi^2(x)\,dx = O(h^{-1})
\]

and a minimizer \( A \) satisfies (2.22) and (2.23);

(ii) Furthermore, let assumption (2.31) be fulfilled (i.e. \( \mu_0(\Pi_\infty) = 0 \)). Then

\[
E^*_\psi - \int \text{Weyl}^*_1(x)\psi^2(x)\,dx = o(h^{-1})
\]

and a minimizer \( A \) satisfies similarly improved versions of (2.22) and (2.23).

4 Rescaling

4.1 Case \( \kappa \leq 1 \)

We already have an upper estimate: corollary 3.3. Let us prove a lower estimate. Consider an error

\[
\left( \int \text{Weyl}_1(x)\psi^2\,dx - E_\psi(A) \right)_+.
\]

Obviously \( \text{Tr}^- \) is sub-additive

\[
\text{Tr}^-\left( \sum_j \psi_jH\psi_j \right) \geq \sum_j \text{Tr}^-\left( \psi_jH\psi_j \right)
\]

and therefore so is \( E_\psi(A) \). Then we need to consider each partition element and use a lower estimate for it. While considering partition we use so called ISM identity

\[
\sum_j \psi_j^2 = 1 \implies H = \sum_j \left( \psi_jH\psi_j + \frac{1}{2}[[H, \psi_j], \psi_j] \right).
\]
In virtue of theorem 1.1, from the very beginning we need to consider
\begin{equation}
M = \kappa^{\beta} h^{-\frac{1}{2} - \alpha}
\end{equation}
with \( \alpha = \frac{3}{2} \), \( \beta = 0 \) and \( \kappa \leq c \). But we need to satisfy precondition (1.20) which is then
\begin{equation}
\kappa^{\beta+1} h^{-\alpha} \leq c.
\end{equation}
If (4.5) is fulfilled with \( \alpha = 0 \) we conclude that the final error is indeed \( O(h^{-1}) \) or even \( o(h^{-1}) \) without any precondition.

Let precondition (4.5) fail. Let us use \( \gamma \)-admissible partition of unity \( \psi \) with \( \psi \) satisfying after rescaling assumptions of proposition 3.2.

Note that rescaling \( x \mapsto x/\gamma \) results in \( h \mapsto h_{\text{new}} = h/\gamma \) and after rescaling in the new coordinates \( \|\partial A\|^2 \) acquires factor \( \gamma^d - 2 \) and thus factor \( \kappa^{-1} h^{1-d} \) becomes \( \kappa^{-1} h_{\text{new}}^{1-d} = \kappa^{-1}_{\text{new}} h_{\text{new}}^{1-d} \) with \( \kappa \mapsto \kappa_{\text{new}} = \kappa \gamma \).

Then after rescaling precondition (4.5) is satisfied provided before rescaling \( \kappa^{\beta+1} h^{-\alpha} \gamma^{\alpha+\beta+1} \leq c \). Let us pick up \( \gamma = \kappa^{-(\beta+1)/((\alpha+\beta+1))} h^\alpha/((\alpha+\beta+1)) \). Obviously if before rescaling condition (4.5) failed, then \( h \ll \gamma \leq 1 \).

But then expression (4.1) with \( \psi \) replaced by \( \psi_j \) does not exceed \( C(h/\gamma)^{2-d} \) and the total expression (4.1) does not exceed \( C h^{-1} \gamma^{-2} = C \kappa^{\beta} h^{-\frac{3}{2} - \alpha'} \) with
\begin{align*}
\beta' &= 2(\beta + 1)/((\alpha + \beta + 1)), \quad \alpha' = -\frac{1}{2} + 2\alpha/(\alpha + \beta + 1);
\end{align*}

So, actually we can pick up \( M \) with \( \alpha, \beta \) replaced by \( \alpha', \beta' \) and we have a precondition (4.5) with these new \( \alpha', \beta' \) and we do not need an old precondition. Repeating the rescaling procedure again we derive a proper estimate with again weaker precondition etc.

One can see easily that \( \alpha' + \beta' + 1 = \frac{5}{2} \) and therefore on each step \( \alpha + \beta + 1 = \frac{5}{2} \) and we have recurrent relation for \( \alpha' \): \( \alpha' = -\frac{1}{2} + \frac{4}{5} \alpha \); and therefore we have sequence for \( \alpha \) which decays and then becomes negative. Precondition (4.5) has been removed completely and estimate \( M = O(h^{-1}) \) has been established. After this under assumption (2.31) we can prove even sharper asymptotics. Thus we arrive to

**Theorem 4.1.** Let \( d = 3 \), \( V \in C^{2,1} \), \( \kappa \leq c \) and let \( \psi \) satisfy assumption of proposition 3.2. Then

(i) Asymptotics (3.13) holds;
(ii) Further, if assumption (2.31) is fulfilled then asymptotics (3.13) holds;

(iii) If (3.13) or (3.14) holds for $E_{\psi}(A)$ (we need only an estimate from below) then $\|\partial A\| = O(\kappa h^{\frac{1}{2}})$ or $\|\partial A\| = o(\kappa h^{\frac{1}{2}})$ respectively.

4.2 Case $1 \leq \kappa \leq h^{-1}$

We can consider even the case $1 \leq \kappa \leq h^{-1}$. The simple rescaling-and-partition arguments with $\gamma = \kappa^{-1}$ lead to the following

(4.6) As $1 \leq \kappa \leq h^{-1}$ remainder estimate $O(\kappa^2 h^{-1})$ holds and for a minimizer $\|\partial A\|^2 \leq C\kappa^3 h$.

However we would like to improve it and, in particular prove that as $\kappa$ is moderately large remainder estimate is $O(h^{-1})$ and even $o(h^{-1})$ under non-periodicity assumption.

**Theorem 4.2.** Let $d = 3$, $V \in C^{2,1}$, and let $\psi$ satisfy assumptions of proposition 3.2. Then

(i) As

\begin{equation}
\kappa \leq \kappa^* := \epsilon h^{-\frac{1}{2}} \left| \log h \right|^{-\frac{1}{2}}
\end{equation}

asymptotics (3.13) holds;

(ii) Furthermore as $\kappa = o(\kappa^*)$ and assumption (2.31) is fulfilled then asymptotics (3.14) holds;

(iii) As $1 \leq \kappa \leq ch^{-1}$ the following estimate holds:

\begin{equation}
|E_{\psi}^* - \int Weyl_2(x)\psi^2 \, dx| \leq Ch^{-3}(\kappa h)^{\frac{9}{2}} \log\kappa h^2
\end{equation}

Proof. (i) From (2.20) we conclude as $\kappa \geq c$ that $h^{1-\theta}|\partial A|_{\kappa^*} \leq C\kappa(\kappa + \bar{\mu})$. Then using arguments of subsection 2.2 one can prove easily that for $\kappa \leq h^{\sigma-\frac{1}{2}}$

$$|F_{t \rightarrow h^{-1} \tau}(t)(hD_x)^\alpha(hD_x)^\beta(U(x, y, t) - U_\epsilon(x, y, t) - U_\epsilon'(x, y, t))| \leq Ch^{1-d}$$

where we use the same 2-term approximation, $T = \epsilon\bar{\mu}^{-1}$. Let us take then $x = y$, multiply by $\epsilon^{-d}\psi(\epsilon^2(y - z))$ and integrate over $y$. Using rough
microlocal analysis one can prove easily that from both $U_\varepsilon(x,y,t)$ and $U'_\varepsilon$ we get $O(h^{1-d})$ and in the end of the day we arrive to the estimate $|\Delta A_\varepsilon| \leq C\kappa\bar{\mu}$ which implies

\begin{equation}
(4.9) \quad |\partial^2 A_\varepsilon| \leq C\kappa\bar{\mu}|\log h| + C\mu
\end{equation}

where obviously one can skip the last term. Here we used property of the Laplace equation. For our purpose it is much better than $|\partial^2 A_\varepsilon| \leq C\kappa^2|h| + C\mu$ which one could derive easily.

Again using arguments of subsection 2.2 one can prove easily that

\begin{equation}
(4.10) \quad |\Tr(\psi H_{A,V}^\varepsilon) - \Tr(\psi H_{A,v}^-)| \leq C\bar{\mu}^2 h^{2-d}
\end{equation}

and therefore

\begin{equation}
(4.11) \quad |\Tr(\psi H_{A,v}^-) - \int \text{Weyl}_1(x)\psi^2(x)\,dx| \leq C\bar{\mu}^2 h^{2-d}
\end{equation}

and finally for an optimizer

\begin{equation}
(4.12) \quad \|\partial A\|^2 \leq C\kappa\bar{\mu}^2 h.
\end{equation}

Here $\mu$ and $\bar{\mu}$ were calculated for $A$, but it does not really matter as due to $|\partial^2 A| \leq C\kappa^2 h^{-\delta}$ we conclude that $|\partial A - \partial A_\varepsilon| \leq C\kappa^2 h^{-\delta\varepsilon} \leq C$ due to restriction to $\kappa$.

Then, as $d = 3$

\begin{equation}
(4.13) \quad \mu^2(\mu/\kappa\bar{\mu}|\log h|)^3 \leq \kappa\bar{\mu}^2 h
\end{equation}

and if $\mu \geq 1$ we have $\bar{\mu} = \mu$ and (4.13) becomes $\kappa^{-3}|\log h|^{-3} \leq C\kappa h$ which impossible under (4.7).

So, $\mu \leq 1$ and (4.13) implies (3.13) and (4.12), (4.13) imply that for an optimizer $\|\partial A\| \leq C(\kappa h)^{1/2}$ and $\mu \leq C\kappa^4 h|\log h|^d$. So (i) is proven.

(ii) Proof of (ii) follows then in virtue of arguments of subsection 2.2.

(iii) If $\kappa_h^* \leq \kappa \leq h^{-1}$ we apply partition-and-rescaling. So, $h \mapsto h' = h/\gamma$ and $\kappa \mapsto \kappa' = \kappa\gamma$ and to get into (4.7) we need $\gamma = \epsilon\kappa^{-1/2}h^{-1/2}\log(\kappa h)|^{-1}$ leading to the remainder estimate $Ch^{-1}\gamma^{-2}$ which proves (ii).

\begin{remark}
Remark 4.3. In versions 1 and 2 (v1 and v2) we lost a logarithmic factor in (4.7) and (4.8) (it was $h^{-1/2}$ and $h^{-1}\kappa^3$).
\end{remark}
Bibliography

[BI] M. Bronstein, M., V. Ivrii: Sharp Spectral Asymptotics for Operators with Irregular Coefficients. Pushing the Limits. Comm. Partial Differential Equations, 28, 1&2:99–123 (2003).

[EFS1] L. Erdős, S. Fournais, J.P. Solovej: Stability and semiclassics in self-generated fields. arXiv:1105.0506

[EFS2] L. Erdős, S. Fournais, J.P. Solovej: Second order semiclassics with self-generated magnetic fields. arXiv:1105.0512

[EFS3] L. Erdős, S. Fournais, J.P. Solovej: Scott correction for large atoms and molecules in a self-generated magnetic field. arXiv:1105.0521

[ES] L. Erdős, J.P. Solovej: Ground state energy of large atoms in a self-generated magnetic field. Commun. Math. Phys., 294 No. 1, 229-249 (2010) arXiv:0903.1816

[I1] V. Ivrii: Sharp spectral asymptotics for operators with irregular coefficients. Pushing the limits. II. Comm. Part. Diff. Equats., 28 (1&2):125–156, (2003).

[I2] V. Ivrii: Microlocal Analysis and Sharp Spectral Asymptotics, in progress: available online at http://www.math.toronto.edu/ivrii/futurebook.pdf

[IS] V. Ivrii, V. and I. M. Sigal: Asymptotics of the ground state energies of large Coulomb systems. Ann. of Math., 138:243–335 (1993).

[LLS] E. H. Lieb, M. Loss and J. P. Solovej: Stability of Matter in Magnetic Fields, Phys. Rev. Lett., 75, 985–989 (1995) arXiv:cond-mat/9506047