Magnetic calculus and semiclassical trace formulas

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Abstract

The aim of this paper is to show how the magnetic calculus developed in Mantoiu and Purice (2004 J. Math. Phys. 45 1394–417), Iftimie \textit{et al} (2007 Publ. RIMS 43 585–624), Iftimie \textit{et al} (Commun. Partial Differ. Equ. to appear), Mantoiu \textit{et al} (2007 J. Funct. Anal. 250 42–67) and Lein \textit{et al} (arXiv:0901.3704) permits us to give new information on the nature of the coefficients of the expansion of the trace of a function of the magnetic Schrödinger operator whose existence was established in (Helffer and Robert 1990 Asymptotic Anal. 3 91–103).

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1. Introduction

Let us consider the magnetic Schrödinger operator on \(\mathbb{R}^d\) defined by

\[
P^A(\hbar) = \sum_{j=1}^{d} \left( \hbar D_{x_j} - A_j(x) \right)^2 + V(x),
\]

where \(D_{x_j} := -i\partial_{x_j}\) and we assume

Hypothesis 1.1.

\(\bullet\) \(\hbar \in \mathcal{I} \subset ]0, +\infty[, \) with \(\mathcal{I}\) a bounded set having 0 as accumulation point,

\(\bullet\) \(A = (A_1, \ldots, A_d)\) with \(A_j \in C^\infty(\mathbb{R}^d)\),

\(\bullet\) \(V \in C^\infty, V \geq -C.\)

It is known that the operator associated with \(P^A(\hbar)\) on \(C_0^\infty(\mathbb{R}^d)\) admits a unique self-adjoint extension on \(L^2(\mathbb{R}^d)\), which can be defined as the Friedrichs extension. We denote this extension by \(\tilde{P}^A(\hbar)\). For any function \(g \in C_0^\infty(\mathbb{R})\), we can define by the abstract functional calculus \(g(\tilde{P}^A(\hbar))\).
We will also make the following assumption concerning the potential function $V$:

**Hypothesis 1.2.**

\[ \Sigma_V := \lim \inf_{|x| \to \infty} V(x) > \inf V. \]

It is known in this case by Persson’s theorem (see for example [1]) that the spectrum is discrete in $]-\infty, \Sigma_V[$. More precisely, there exist non-empty for $t \not= 0$ without changing the asymptotic behavior of $V$, where $H_{\text{eff}}$, Helffer–Robert’s class and in the magnetic pseudodifferential calculus of [16, 17, 21, 22].

Thus if we have two vector potentials $A$ and $\tilde{A}$, such that $dA = d\tilde{A} = B$, we know that there exists $\phi \in C^\infty(\mathbb{R}^d)$ such that $A = \tilde{A} + \phi$, and the conjugation by the multiplication operator by $\exp i\phi$ gives a unitary equivalence between $\tilde{G}(h)$ and $G(h)$. Hence $\text{Tr} g(\tilde{G}(h))$ and its expansion should depend only on $B$. We would like to investigate how it depends effectively on $B$.

Our main theorem is the following.

**Theorem 1.3.** Under the previous assumptions on $A$ and $V$ and with $H_h = \tilde{G}(h)$, there exists a sequence of distributions $T_j^B \in \mathcal{D}'(\mathbb{R})$ ($j \in \mathbb{N}$) such that for any $g \in C_0^\infty(\mathbb{R})$ with $\text{supp} \subset \subset ]-\infty, \infty[ \setminus N$, and for any $N \in \mathbb{N}$, there exist $C_N$ and $h_N$, such that

\[ (2\pi \hbar)^d \text{Tr} g(H_h) - \sum_{0 \leq k \leq N} \hbar^k T_j^B (g) \leq C_N \hbar^{N+1}, \forall h \in [0, h_N] \cap \mathbb{N}. \]

More precisely there exist $k_j \in \mathbb{N}$ and universal polynomials $P_j(u_{\alpha}, v_{\beta,j,k})$ depending on a finite number of variables, indexed by $\alpha \in \mathbb{N}^{2d}$ and $\beta \in \mathbb{N}^d$, such that the distributions

\[ T_j^B (g) = \sum_{0 \leq k \leq k_j} \int g^{(k)}(F(x, \xi)) P_j(\alpha_{x,k}^{\alpha,\beta}, \beta B_{jk}(x)) \, dx \, d\xi, \]

where $F(x, \xi) = \xi^2 + V(x)$, satisfy (1.2). Finally, $T_j^B = 0$ for $j$ odd.

This theorem was obtained under stronger assumptions in [6], but the main difference with the statement above was that the expression of $T_j^B (g)$ was given in terms of a vector potential $A$ such that $dA = B$. Challenging calculations followed in order to recover a gauge-invariant expression for the first three terms:

\[ T_0^B (g) := \int \mathbb{S} \, dx \, d\xi g(F(x, \xi)), \quad T_1^B (g) := 0, \]

\[ T_2^B (g) := -\frac{1}{12} \int \mathbb{S} \, dx \, d\xi g''(F(x, \xi))[(\Delta V)(x) + \|B(x)\|^2]. \]

The approach of [6] did not permit us to recover the same kind of result for any term of the expansion. In contrast, we will show that, when it can be applied the magnetic calculus permits us to give this expression naturally. To state the results at the intersection of the domains of validity of the two calculi is actually unnecessary. Following essential arguments presented in [8] in the case without a magnetic potential, we will show how we can use the Agmon exponential decay estimates in order to modify the behavior of $V$ and $A$ at infinity, without changing the asymptotic behavior of $\text{Tr} g(\tilde{G}(h))$, in order to enter simultaneously in Helffer–Robert’s class and in the magnetic pseudodifferential calculus of [16, 17, 21, 22].
The paper is organized as follows. In section 2, we review the now standard \( \hbar \)-pseudodifferential Weyl calculus and the attached functional calculus. Section 3 is devoted to the presentation of the gauge-invariant magnetic calculus \[16, 17, 21, 22\]. In the last section will give the proof of the main theorem.

We will constantly use the notations \( X \equiv \mathbb{R}^d \), \( \mathcal{Z} := \mathcal{X} \times \mathcal{X} \), with \( \mathcal{X} \) the dual of \( \mathcal{X} \). The points of \( \mathbb{Z} \) will be denoted as \( X = (x, \xi) \). Recall that \( \mathbb{Z} \) has a canonical symplectic form \( \sigma((x, \xi), (y, \eta)) := \xi(y) - \eta(x) = \sum_{1 \leq j \leq d} (\xi_j y_j - \eta_j x_j) \). We denote by \( \mathcal{C}^\infty_1(\mathcal{Y}) \) the space of \( C^\infty \)-functions on the vector space \( \mathcal{Y} \) having at most polynomial growth at infinity together with all their derivatives. We denote by \( \mathcal{C}^\infty_0(\mathcal{Y}) \) the subspace of functions having a unique polynomial upper bound for all their derivatives.

2. The \( \hbar \)-pseudodifferential Weyl calculus and trace formulas

Following \[15, 16\] with any Schwartz test function \( \phi \in \mathcal{S}(\mathcal{Z}) \) we associate a bounded linear operator \( \Omega_{\mathcal{B}}(\phi) \) on the Hilbert space \( \mathcal{H} := L^2(\mathcal{X}) \):

\[
[\Omega_{\mathcal{B}}(\phi)u](x) := (2\pi \hbar)^{-d} \int_{\mathcal{X}} \int_{\mathcal{X}} dy \, \eta \, e^{i(x-y)\phi} \left( \frac{x + y}{2} \right) u(y), \quad \forall u \in \mathcal{S}(\mathcal{X}),
\]

for some constant \( \hbar > 0 \). It is easy to prove that \( \Omega_{\mathcal{B}}(\phi) \in \mathcal{B}(\mathcal{H}) \) and

\[
\|\Omega_{\mathcal{B}}(\phi)\|_{\mathcal{B}(\mathcal{H})} \leq \int_{\mathcal{X}} dx \|\tilde{\mathcal{F}}^{-1}(\phi)(x, \cdot)\|_{\infty}
\]

where \( \tilde{\mathcal{F}}^{-1} \) denotes the inverse Fourier transform with respect to the second variable. Moreover it is not hard to prove, by using Schur’s lemma, that \( \Omega_{\mathcal{B}} : \mathcal{S}(\mathcal{Z}) \rightarrow \mathcal{B}(\mathcal{H}) \) extends to an isomorphism of topological vector spaces \( \Omega_{\mathcal{B}} : \mathcal{S}'(\mathcal{Z}) \rightarrow \mathcal{B}(\mathcal{S}(\mathcal{X}); \mathcal{S}'(\mathcal{X})) \). We can transport the operator multiplication from \( \mathcal{B}(\mathcal{H}) \) back to a non-commutative product on \( \mathcal{S}(\mathcal{Z}) \) \[3\]

\[
\Omega_{\mathcal{B}}(\phi) \Omega_{\mathcal{B}}(\psi) = \Omega_{\mathcal{B}}(\phi \ast_{\mathcal{B}} \psi), \quad \forall (\phi, \psi) \in [\mathcal{S}(\mathcal{Z})]^2.
\]

Explicitly we have

\[
(\phi \ast_{\mathcal{B}} \psi)(X) := (\pi \hbar)^{-d} \int_{\mathcal{Z}} dY \int_{\mathcal{Z}} dZ \exp[-(2i/\hbar)\sigma(Y, Z)] \phi(X-Y) \psi(X-Z).
\]

One can prove that

\[
\mathcal{M}(\mathcal{Z}) := \{ \Phi \in \mathcal{S}'(\mathcal{Z}) \mid \Phi \ast_{\mathcal{B}} \phi \in \mathcal{S}(\mathcal{Z}), \phi \ast_{\mathcal{B}} \Phi \in \mathcal{S}(\mathcal{Z}), \forall \phi \in \mathcal{S}(\mathcal{Z}) \},
\]

that is obviously an algebra for the \( \ast_{\mathcal{B}} \)-multiplication and even a *-algebra for the anti-involution given by complex conjugation of distributions.

The limit \( \hbar \rightarrow 0 \), that has a rather singular behavior, should correspond in some sense to the classical algebra of observables that is a commutative algebra. A precise meaning of this limit can be given in the context of strict deformation quantization (see \[19\]), but is out of our aims in this paper. In contrast, the asymptotics \( \hbar \rightarrow 0 \), known as the semi-classical asymptotics, and considered in the frame of asymptotic series in \( \hbar \), is an important problem and we concentrate on some of its aspects when magnetic fields are present.

The Moyal algebra contains many interesting subalgebras, among them the usual Hörmander symbols

\[
S^m_1(\mathcal{X}) := \left\{ F \in C^\infty(\mathcal{Z}) \mid \sup_{(x, \xi) \in \mathbb{Z}} |(\xi)^{-m+|\alpha|}| \left( \partial_x^\alpha \partial_{\xi}^\alpha F \right)(x, \xi) | < \infty \right\}.
\]
A symbol $F \in S^m_1(\mathcal{X})$ of strictly positive order $m > 0$ satisfying

$$\exists \xi > 0, \exists R > 0 \text{ such that } C(\xi)^m \leq |F(x, \xi)|, \quad \forall (x, \xi) \in \mathbb{E} \text{ with } |x| \geq R$$

is called elliptic and has the property that it has a positive constant $a \geq 0$ such that for any $\mathfrak{g} \in \mathbb{E} \setminus \mathbb{R} \cup (\infty, -a)$ the distribution $\mathfrak{g} F$ has an inverse $(\mathfrak{g} F)^{-1}$ with respect to the $\mathfrak{g}_h$-product and this inverse belongs to the class $S^{-m}_1(\mathcal{X})$. In other words, the operator $\mathcal{D}_0(F)$ has a self-adjoint extension with a resolvent that has a symbol of the Hörmander class $S^{-m}_1(\mathcal{X})$.

An important problem is how to relate this pseudodifferential calculus (defined by the Moyal product $\mathfrak{g}_h$) with the usual functional calculus for self-adjoint operators, when these operators are of the form $\mathcal{D}_0(F)$ with $F \in S^m_1(\mathcal{X})$ elliptic ($m > 0$).

In dealing with semi-classical problems, the parameter $\hbar$ is no longer constant and it is important to consider asymptotic series in $\hbar$. An essential fact is that the Moyal product $\mathfrak{g}_h$ has a 'suitable' behavior with respect to such asymptotic series. More precisely, let us consider the space $S^{(s,m)}_1(\mathcal{X})$ of $h$-symbols of the form $F : \mathbb{I} \times \mathbb{E} \to \mathbb{C}$ such that

$$F(h) \in C^\infty(\mathbb{E}), \quad \forall h \in \mathbb{I}, \quad \sup_{x \in \mathbb{E}} h^{-\frac{1}{2}} |z(x)| \leq C N$$

We refer to [5, 23] for a systematic discussion and for more general $h$-symbols. In the frame of these symbol classes, the Moyal product $\mathfrak{g}_h$ has the following property (see [5, 23]):

$$\forall (F, G) \in S^{(s,m)}_1(\mathcal{X}) \times S^{(s,m)}_1(\mathcal{X}), \quad F \mathfrak{g}_h G \in S^{(s+\frac{1}{2},m)}_1(\mathcal{X})$$

and

$$F \mathfrak{g}_h G - F \mathfrak{g}_h \cdot G \in S^{(s+\frac{1}{2},m+\frac{1}{2})}_1(\mathcal{X})$$

We usually work with elements $F \in S^{(s,m)}_1(\mathcal{X})$ having an asymptotic expansion of the form

$$F(h, x, \xi) \sim \hbar^s \sum_{k \in \mathbb{N}} h^k F_k(x, \xi), \quad \text{with } F_k \in S^{m-k}_1(\mathcal{X}), \quad (2.2)$$

using the asymptotic series of Hörmander. The symbol $\hbar^s F_0 \in S^{(s,m)}_1(\mathcal{X})$ is then called the principal symbol of $F$.

What is important here is to find a class of functions (actually essentially $C_0^\infty$) such that $g(F)$ is a nice pseudodifferential operator with simple rules of computation for the principal symbol. We begin with the general Dynkin–Helffer–Sjöstrand formula (see [2, 11, 12])

$$g(P) = -\pi^{-1} \lim_{e \to 0} \int_{|\mu| \geq e} \frac{d\hat{g}}{d\xi}(\lambda, \mu) (\lambda + i\mu - P)^{-1} d\lambda d\mu, \quad (2.3)$$

which is true for any self-adjoint operator $P$ and any $g$ in $C_0^\infty(\mathbb{R})$.

Here the function $(\lambda, \mu) \mapsto \hat{g}(\lambda, \mu)$ is a compactly supported, almost analytic extension of $g$ to $\mathbb{C}$. This means that $\hat{g} = g$ on $\mathbb{R}$ and that for any $N \in \mathbb{N}$ there exists a constant $C_N$ such that $|\hat{g}(\lambda, \mu)| \leq C_N |\mu|^N$.

The main result due to Helffer–Robert (see also [2] and references therein) is that, for $P = \mathcal{D}_0(F)$ a self-adjoint operator with an $h$-symbol $F$ real and semibounded from below and having an asymptotic expansion as above $(2.2)$ with $s = 0$ and $g$ in $C_0^\infty(\mathbb{R})$, the operator $g(P)$ is an $h$-pseudodifferential operator of the form $\mathcal{D}_0(\hat{g}_h(F))$, whose Weyl symbol $\hat{g}_h(F)(h, \xi, x)$ admits a formal asymptotic expansion in $h$:

$$\hat{g}_h(F)(h, \xi, x) \sim \hbar^k g_k(F)(x, \xi), \quad (2.4)$$

with

$$g_0(F) = g(F_0), \quad g_1(F) = F_1 \cdot g^0(F_0), \quad g_k(F) = \sum_{i=1}^{2k-1} d_{k,i} g^{(i)}(F_0), \quad \forall k \geq 2. \quad (2.5)$$

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where $d_{k,l}$ are the universal polynomial functions of the symbols $\partial_x^\alpha \partial_\xi^\beta F_\ell$, with $|\alpha| + |\beta| + \ell \leq k$. For $k = 2$, one has

$$d_{2,1} = F_2, \quad d_{2,2} = p_{2,2} + (1/2) F_1^2, \quad d_{2,3} = p_{2,3} \quad (2.6)$$

with

$$p_{2,2}(x, \xi) = \frac{1}{8} \sum_{j,k} \left( \frac{2 \partial_x^2 F_0 \partial_\xi^2 F_0 - \partial^2 F_0 \partial_x^2 F_0 - \partial_x F_0 \partial_\xi F_0}{\partial x_j \partial x_k \partial_\xi_j \partial_\xi_k} \right) \quad (2.7)$$

$$p_{2,3}(x, \xi) = \frac{1}{24} \sum_{j,k} \left( 2 \partial_x^2 \partial_\xi^2 F_0 \partial_x F_0 \partial_\xi F_0 - \partial^2 F_0 \partial_x F_0 \partial_\xi F_0 \partial_\xi F_0 
- \partial_x F_0 \partial_x F_0 \partial_\xi F_0 \partial_\xi F_0 \right). \quad (2.8)$$

The main point in the proof is that one can construct for $\Re z \not= 0$ a parametrix (= approximate inverse) for $(P - z)$ with a nice control as $\Re z$ tends to 0. The constants controlling the estimates on the symbols explode as $\Re z \to 0$ but the choice of the almost analytic extension of $f$ absorbs any negative power of $|\Re z|$.

As a consequence, one gets that for $\hbar$ small enough, if for some interval $I$ and some $\epsilon_0 > 0$,

$$F_0^{-1}(I + [-\epsilon_0, \epsilon_0]) \text{ is compact}, \quad (2.9)$$
then the spectrum of $\mathcal{D} p_\hbar(F_0)$ is discrete in $I$. In particular, one gets that, if $F_0(x, \xi) \to +\infty$ as $|x| + |\xi| \to +\infty$, then the spectrum of $\mathcal{D} p_\hbar(F_0)$ is discrete ($\mathcal{D} p_\hbar(F_0)$ has compact resolvent). In fact one gets more precisely the following theorem (due to Helffer–Robert).

**Theorem 2.1.** Let $P = \mathcal{D} p_\hbar(F)$ be a self-adjoint operator with an $\hbar$-symbol $F$ real and semibounded from below, having an asymptotic expansion of the form (2.2) and also satisfying (2.9) with $I = [E_1, E_2]$; then, for any $g$ in $C^\infty_0([E_1, E_2])$, we have the following expansion in powers of $\hbar$:

$$\text{Tr}[g(\mathcal{D} p_\hbar(F))] \sim (2\pi \hbar)^{-d} \sum_{j \geq 0} \hbar^j T_j(g), \quad (2.10)$$

where $g \mapsto T_j(g)$ are distributions in $\mathcal{D}'([E_1, E_2])$.

In particular we have, when $F_1 = F_2 = 0$,

$$T_0(g) = \iint g(F_0(x, \xi)) \, dx \, d\xi,$$

$$T_1(g) = 0,$$

$$T_2(g) = -\frac{1}{24} \iint \left( \frac{\partial^2 F_0}{\partial x_j \partial x_k} \frac{\partial^2 F_0}{\partial x_j \partial x_k} - \frac{\partial^2 F_0}{\partial x_j \partial x_k} \frac{\partial^2 F_0}{\partial x_j \partial x_k} \right) \, dx \, d\xi. \quad (2.11)$$

This theorem is obtained by integration of the symbol of $g(\mathcal{D} p_\hbar(F))$ given in (2.4), because we have the needed regularity so that the trace of a trace-class operator $\mathcal{D} p_\hbar(\tilde{g}_\hbar(F))$ is given by the integral of the symbol $\tilde{g}_\hbar(F)$ over $\Sigma$. According to the definition of the Weyl quantization, the distribution kernel is given by the oscillatory integral:

$$K(x, y; \hbar) = (2\pi \hbar)^{-d} \int_{\mathcal{X}} \exp \left( i \frac{\hbar}{2} (x - y) \cdot \xi \right) \tilde{g}_\hbar(F) \left( \hbar, \xi, \frac{x + y}{2} \right) \, d\xi, \quad (2.12)$$

and the trace of $\mathcal{D} p_\hbar(\tilde{g}_\hbar(F))$ is the integral over $\mathcal{X}$ of the restriction to the diagonal of the distribution kernel: $K(x, x) = (2\pi \hbar)^{-d} \int_{\mathcal{X}} \tilde{g}_\hbar(F)(\hbar, \xi, x) \, d\xi$. 

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Of course, one could think of using the theorem with $g$ the characteristic function of an interval, in order to get, for example, the behavior of the counting function attached to this interval. This is of course not directly possible and this will be only obtained through Tauberian theorems \cite{13, 15, 18} and at the price of additional errors. Let us however remark that, if the function $g$ is not regular, then the length of the expansion depends on the regularity of $g$. So it will not be surprising that, by looking at the Riesz means: $g_{s,E}(t) := \max \left\{ 0, (E - t)^s \right\}$ for some $s \geq 0$ and $E \in (E_1, E_2)$, we will get a better expansion when $s$ is large.

Under some assumptions on $A$ and $V$, including the condition $\text{div } A = 0$, one can show that $P^A(h)$ is an $h$-pseudodifferential operator whose total Weyl-symbol $F(x, \xi) = (\xi - A)^2 + V$ is in some class of \cite{6}. More precisely, we have to assume that for any $\alpha \in \mathbb{N}^d$, we have
\begin{equation}
|\partial_x^\alpha V(x)| \leq C_{\alpha}(V(x) + C + 1),
\end{equation}
and, for $j = 1, \ldots, d$, the following non-gauge covariant conditions:
\begin{equation}
|\partial_x^\alpha A_j(x)| \leq C_{\alpha}(V(x) + C + 1)^{1/2}.
\end{equation}

3. The $h$-magnetic quantization

3.1. Results for fixed $h$

We consider a magnetic field described by a bounded smooth closed 2-form $B$ on $\mathcal{X} \equiv \mathbb{R}^d$ and the associated modified symplectic form on $\mathbb{Z}$,
\[ \sigma^B(x, y) := \eta(z) - \zeta(y) + B_z(y, z), \]
that may be used to define the classical Hamiltonian system in the given magnetic field. For the quantum description we also consider the Hilbert space $\mathcal{H} = L^2(\mathcal{X})$, we choose a smooth vector potential $A$, i.e. a 1-form satisfying the equality $B = dA$ and we define the following gauge covariant representation, for all $\phi \in \mathcal{S}(\mathbb{Z})$ and all $u \in \mathcal{S}(\mathcal{X})$:
\[ [\mathcal{O}_p^\phi(\phi)u](x) := (2\pi h)^{-d} \int_{\mathcal{X}} \int_{\mathbb{Z}} dy \, d\eta \, e^{2i\eta(x-y)} e^{i \int_{y} A \phi \left( \frac{x+y}{2}, \eta \right)} u(y), \]
where $\int_{[x, y]} A$ denotes the integration of the 1-form $A$ along the oriented segment $[x, y]$. This gauge-covariant ‘magnetic quantization’ allows us to define a ‘magnetic’ Moyal product $\phi^B_h$:
\begin{equation}
(\phi^B_h \psi)(X) := (\pi h)^{-2d} \int_{\mathcal{X}} \int_{\mathbb{Z}} dy \, dZ \exp \left[ - (2i/h) \sigma^B(X, Z) \right] \phi(X - Y) \psi(X - Z)
\end{equation}
\begin{equation}
= (\pi h)^{-2d} \int_{\mathcal{X}} \int_{\mathbb{Z}} dy \, dZ \, e^{-(2i/h)\sigma(Y, Z)} \, e^{-(i/h)\theta^B(x, y, z)} \phi(X - Y) \psi(X - Z)
\end{equation}
\begin{equation}
= (\pi h)^{-2d} \int_{\mathcal{X}} \int_{\mathbb{Z}} dy \, dZ \, e^{-(2i/h)\sigma(X-Y,X-Z)} \, e^{-(i/h)\theta^B(x, y, z)} \phi(Y) \psi(Z).
\end{equation}

$\theta^B(x, y, z) := \int_{(x-y-z, x+y-z, x-y+z)} B$, $\theta^B(x, y, z) := \int_{(x+y+z, x+y-z, x-y+z)} B$. Here $(x - y - z, x + y - z, x - y + z)$ denotes the triangle defined by the three points $x - y - z$, $x + y - z$ and $x - y + z$, with the usual trigonometric orientation and the integrals of $B$ denote the integrals of the 2-form on the given oriented triangle. Associated with this product we can define a ‘magnetic’ Moyal algebra for the magnetic field $B$:
\[ \mathcal{M}^B(\mathbb{Z}) := \left\{ \Phi \in \mathcal{S}(\mathbb{Z}) \mid \Phi^B_h \psi \in \mathcal{S}(\mathbb{Z}), \quad \phi^B_h \Phi \in \mathcal{S}(\mathbb{Z}), \quad \forall \phi \in \mathcal{S}(\mathbb{Z}) \right\}. \]

This ‘magnetic’ Moyal calculus preserves a large number of the nice features of the usual Moyal calculus and we recall some of them that are useful for our analysis of semiclassical trace formulas.
Proposition 3.1 (Propositions 3.5 and 3.10 in [22]). For any magnetic field $B$ with components of class $C_{00}^\infty(X)$, one can find a vector potential $A$ with components also of class $C_{00}^\infty(X)$ and then the application $\Omega^A_p : S(\mathcal{E}) \rightarrow \mathbb{B}(L^2(\mathcal{X}))$ extends to an isomorphism of vector spaces $\Omega^A_p : S(\mathcal{E}) \rightarrow \mathbb{B}(S(\mathcal{X}); S'(\mathcal{X}))$. The above isomorphism has a restriction $\Omega^A_p : L^2(\mathcal{E}) \rightarrow \mathbb{B}_2(L^2(\mathcal{X}))$ that is unitary (here $\mathbb{B}_2(L^2(\mathcal{X}))$ is the algebra of Hilbert–Schmidt operators on $L^2(\mathcal{X}))$.

Proposition 3.2 (Proposition 4.23 in [21] and lemma 1.2 in [16]). For any magnetic field $B$ with components of class $C_{00}^\infty(X)$, we have the following inclusions:

$$C_{pol}^\infty(\mathcal{E}) \subset \mathcal{M}^B(\mathcal{E}); \quad S_1^m(\mathcal{X}) \subset \mathcal{M}^B(\mathcal{E}).$$

Proposition 3.3 (Theorem 2.11 in [20]). For any magnetic field $B$ with components of class $BC^\infty(X)$ the ‘magnetic’ Moyal product defines a continuous map $S^m_1(\mathcal{X}) \times S^m_1(\mathcal{X}) \ni (F, G) \mapsto F^\#^B G \in S^{m_1+m_2}_1(\mathcal{X}),$

and for any $N \in \mathbb{N}$ there is a canonical expansion

$$F^\#^B G = \sum_{j=0}^{N-1} H_j + R_N,$$

where $H_j \in S^{m_1+m_2-j}_1(\mathcal{X}), \quad R_N \in S^{m_1+m_2-N}_1(\mathcal{X})$

in which $H_0 = F \cdot G$.

Proposition 3.4 (Theorem 3.1 in [16]). For any magnetic field $B$ with components of class $BC^\infty(X)$ we have that for any associated vector potential $A$,

$$\Omega^A_p [S^m_1(\mathcal{X})] \subset \mathbb{B}(L^2(\mathcal{X}))$$

and there exist two positive constants $c, p$ depending only on the dimension $d$ of $\mathcal{X}$ such that

$$\|\Omega^A_p (F)\|_{\mathbb{B}(L^2(\mathcal{X}))} \leq c \sup_{|a| \leq p} \left( \sup_{|\xi| \leq p} \left| (\partial_x^a \partial_{\xi}^a F)(x, \xi) \right| \right).$$

Proposition 3.5 (Theorems 4.1 and 4.3 in [16] and proposition 6.31 in [17]). Suppose the magnetic field $B$ is of class $BC^\infty(X)$; then

- if $F \in S^m_1(\mathcal{X})$ is a real function, $\Omega^A_p (F)$ is a bounded self-adjoint operator on $L^2(\mathcal{X})$ for any vector potential $A$ of $B$; the resolvent of $\Omega^A_p (F)$ has a ‘magnetic’ symbol of class $S^m_1(\mathcal{X})$;
- if $F \in S^m_1(\mathcal{X})$ is a real elliptic symbol with $m > 0$, then $\Omega^A_p (F)$ has a self-adjoint extension in $L^2(\mathcal{X})$ for any vector potential $A$ of $B$ and the resolvent has a ‘magnetic’ symbol of class $S^m_1(\mathcal{X})$; if we choose $A$ with components of class $C_{00}^\infty(X)$, then $\Omega^A_p (F)$ is essentially self-adjoint on $S(\mathcal{X})$ and its self-adjoint extension has as domain the ‘magnetic’ Sobolev space:

$$\mathcal{H}_{m}^A(\mathcal{X}) := \{ u \in L^2(\mathcal{X}) | \Omega^A_p (p_m) u \in L^2(\mathcal{X}), \text{ where } p_m(x, \xi) := (\xi)^m \};$$

- if $F \in S^m_1(\mathcal{X})$, with $m \in \mathbb{R}$, satisfies $\Re F(x, \xi) \geq C|\xi|^m$ for $|\xi| \geq R$, with some strictly positive constants $C$ and $R$, then for any $r \in \mathbb{R}$ there exist two positive constants $C_0$ and $C_1$ such that for any $u \in \mathcal{H}_{m}^A(\mathcal{X})$ we have

$$\Re (u, \Omega^A_p (F) u)_{L^2(\mathcal{X})} \geq C_0 \| u \|^2_{\mathcal{H}_{m}^A(\mathcal{X})} - C_1 \| u \|^2_{\mathcal{H}_{m}^A(\mathcal{X})}.$$
3.2. Semiclassical results

Let us now consider the dependence on $\hbar \in I$. We come back to (3.1) and analyze the $\hbar$-dependence of this product:

$$\left( \phi^{\hbar B}_{\hbar} \right)(X) = (\pi \hbar)^{-2d} \int_{\mathbb{R}^d} dY \int_{\mathbb{R}^d} dZ \, e^{-\left(2i/\hbar\right)\sigma(Y, Z)} \, e^{-\left(i/\hbar\right)\theta^{B}(x, y, z)} \phi(X - Y) \psi(X - Z)$$

with

$$\theta^B(x, y, z) := \int_{(x - y, x + y, x - y, z - y)} B$$

$$= 4 \sum_{jk} y_j z_k \int_0^1 ds \int_0^{1-s} dt B_{jk}(x + (2s - 1)y + (2t - 1)z).$$

Let us make the change of variables $(y, z) \mapsto (\hbar y, \hbar z)$ in order to obtain

$$\left( \phi^{\hbar B}_{\hbar} \psi \right)(X) = \pi^{-2d} \int_{\mathbb{R}^d} dY \int_{\mathbb{R}^d} dZ \, e^{-\left(2i/\hbar\right)\sigma(Y, Z)} \phi(x - \hbar y, \xi - \eta) \psi(x - \hbar z, \xi - \zeta).$$

(3.2)

with

$$\theta^B_{\hbar}(x, y, z) = 4 \sum_{jk} y_j z_k \int_0^1 ds \int_0^{1-s} dt B_{jk}(x + (2s - 1)\hbar y + (2t - 1)\hbar z).$$

We note that we can now obtain an asymptotic expansion of the $\phi^{\hbar B}_{\hbar}$-product with respect to $\hbar$ by using the Taylor formulas for $\phi, \psi$, like in the non-magnetic case, and for the exponential $e^{-\left(i/\hbar\right)\theta^B_{\hbar}(x, y, z)}$ and also for $B$ in the expression of $\theta^B_{\hbar}(x, y, z)$:

$$\phi(x - \hbar y, \xi - \eta) = \sum_{0 \leq v \leq N} \frac{(-\hbar)^v}{v!} \sum_{|\alpha| = v} \frac{\hbar^1}{\alpha!} \phi^0(x, \xi - \eta) + \mathcal{R}_{\phi, N},$$

$$\psi(x - \hbar z, \xi - \zeta) = \sum_{0 \leq \mu \leq N} \frac{(-\hbar)^\mu}{\mu!} \sum_{|\beta| = \mu} \mu^1 B_{\beta} \phi^0(x, \xi - \zeta) + \mathcal{R}_{\phi, N},$$

$$e^{-\left(i/\hbar\right)\theta^B_{\hbar}(x, y, z)} = \sum_{0 \leq \rho \leq N} \frac{(-\hbar)^\rho}{\rho!} \left[ \theta^B_{\hbar}(x, y, z) \right]^\rho + \mathcal{R}_{B, N},$$

$$\theta^B_{\hbar}(x, y, z) = \sum_{0 \leq \lambda \leq N} \frac{\hbar^1}{\lambda!} \left[ \sum_{|\gamma| = \lambda} \frac{\hbar^1}{\gamma!} \left( \sum_{jk} y_j z_k (\partial^\gamma B_{jk})(x) \right) \frac{\lambda^1}{\gamma!} \int_{-1}^1 ds \int_{-1}^{s} ds (s y + t z)^\gamma \right]^\lambda + \mathcal{R}_{B, N},$$

$$T^\gamma_{\delta} \phi := \int_{-1}^1 \phi^{(\delta)} ds \int_{-1}^{s} ds (s y + t z)^\gamma \prod_j C_{\gamma_j},$$

$T^\gamma_{\delta} \phi := \int_{-1}^1 \phi^{(\delta)} ds \int_{-1}^{s} ds (s y + t z)^\gamma \prod_j C_{\gamma_j},$
where for any $N \geq 1$ in $\mathbb{N}$ we have

$$\mathfrak{R}_{\phi,N}(\hbar, x, y, \xi, \eta) = (-\hbar)^{N+1} \sum_{|\alpha|=N+1} \frac{\chi_{\beta}}{\alpha!} \int_0^1 (\partial_{\alpha}^\beta \phi)(x - u\hbar y, \xi - \eta) \, du$$

$$= \sum_{|\beta|=N+1} \chi_{\beta} \mathfrak{R}_{\phi,N,\beta}(\hbar, x, y, \xi, \eta),$$

$$\mathfrak{R}_{\psi,N}(\hbar, x, z, \xi, \zeta) = (-\hbar)^{N+1} \sum_{|\beta|=N+1} \frac{\chi_{\beta}}{\beta!} \int_0^1 (\partial_{\beta}^\alpha \psi)(x - u\hbar z, \xi - \zeta) \, du$$

$$= \sum_{|\beta|=N+1} \chi_{\beta} \mathfrak{R}_{\psi,N,\beta}(\hbar, x, z, \xi, \zeta),$$

$$\mathfrak{R}_{B,N}(\hbar, x, y, z) = (-i\hbar)^{N+1} \left[ \theta_B(\hbar, x, y, z) \right]^{N+1} \int_0^1 du_1 \ldots \int_0^{u_N} e^{-iu_N h\hbar \theta_B(\hbar, x, y, z)} \, du_{N+1}$$

$$= \hbar^{N+1} \sum_{|\beta|=N+1} \chi_{\beta} \left[ \sum_{0 \leq j, k, \delta \leq N} \frac{h^j}{\lambda!} \sum_{|\gamma|=\delta} T^\gamma_{j,k} \bar{\psi}_{\gamma,\beta}(\hbar, x, y, z) \sum_{\delta \leq \gamma} \right]^{N+1}$$

$$\times \left( \sum_{jk} y_j z_k (\partial^\gamma B_{jk})(x) \right) + \tau_{B,N} \right]^{N+1}$$

$$\tau_{B,N}(\hbar, x, y, z) = \hbar^{N+1} \sum_{|\nu|=N+1} (\nu!)^{-1} \int_{-1}^1 ds \int_{-1}^{-s} dt \int_0^1 du$$

$$\times \sum_{jk} y_j z_k (\partial^\nu B_{jk})(x + \hbar u(sy + tz))(sy + tz)^\nu$$

$$= \hbar^{N+1} \sum_{jk} y_j z_k \sum_{|\nu|=N+1} (\nu!)^{-1} F^B_{\gamma,j,k}(\hbar, x, y, z) \sum_{\delta \leq \gamma} T^\gamma_{j,k} y^\delta z^{\gamma-\delta}.$$
and taking into account the differential operators contained in $J. \text{Phys. A: Math. Theor. 43 (2010) 474028 B Helffer and R Purice}.$

Let us discuss the remainders in the above expansion. First let us consider the factor $\left(\frac{\hbar}{2}\right)^{-N+1} \pi^{-2d} \int_{\mathbb{R}^d} dY \int_{\mathbb{R}^d} dZ e^{-\gamma(x,Y)} \left\{ \sum_{0 \leq \rho \leq N} \left(\frac{-\hbar}{\rho!}\right)^{\rho} \gamma(x) \sum_{0 \leq \lambda \leq N} \left(\frac{\hbar^\lambda}{4\lambda!}\right) \gamma^{\lambda}(x) \right\} \right.$

\begin{equation}
+ \pi^{-2d} \int_{\mathbb{R}^d} dY \int_{\mathbb{R}^d} dZ e^{-\gamma(x,Y)} \left\{ \sum_{0 \leq \rho \leq N} \left(\frac{-\hbar}{\rho!}\right)^{\rho} \gamma(x) \sum_{0 \leq \lambda \leq N} \left(\frac{\hbar^\lambda}{4\lambda!}\right) \gamma^{\lambda}(x) \right\} \right.

(3.4)

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+ \pi^{-2d} \int_{\mathbb{R}^d} dY \int_{\mathbb{R}^d} dZ e^{-\gamma(x,Y)} \left\{ \sum_{0 \leq \rho \leq N} \left(\frac{-\hbar}{\rho!}\right)^{\rho} \gamma(x) \sum_{0 \leq \lambda \leq N} \left(\frac{\hbar^\lambda}{4\lambda!}\right) \gamma^{\lambda}(x) \right\} \right.

(3.4)

(3.4)

(3.4)

(3.4)

(3.4)
\[
\begin{aligned}
&= \left(\frac{i}{2}\right)^{N+1} h^{(N+1)(\rho-\kappa)} \sum_{|\alpha|=\beta=\rho-\kappa} \int_{\mathbb{S}} dY \int_{\mathbb{S}} dZ \, e^{-2i\sigma(Y,Z)} G_{\alpha\beta}^B(\tilde{h}, x, y, z) \\
&\times \sum_{\delta \leq \gamma} (-1)^{N+1-|\delta|} T_\delta \delta^\alpha \delta^\beta \cdot T_{\delta^\gamma} (x) \cdot \cdots \cdot T_{\delta^\gamma} (x) \\
&\times \left(\partial^\beta \phi\right)(x - \tilde{h} y, \xi - \eta) \left(\partial^\gamma \psi\right)(x - \tilde{h} z, \xi - \zeta), (3.5)
\end{aligned}
\]

where \( G_{\alpha\beta}^B \) is a product of the \( \rho - \kappa \) functions of class \( BC^\infty(\mathcal{X}^3) \) uniformly for \( \tilde{h} \in (0, h_0] \) (in the sense that all the seminorms defining the topology of \( BC^\infty(\mathcal{X}^3) \) are bounded uniformly in \( \tilde{h} \in (0, h_0] \), depending only on the derivatives of order \( N + 1 \) of the magnetic field \( B \). Moreover, \( \partial^\beta \phi \in S_{1}^{m-|\beta|}(\mathcal{X}) \) and \( \partial^\gamma \psi \in S_{0}^{m-|\gamma|}(\mathcal{X}) \) uniformly in \( \tilde{h} \in (0, h_0] \) so that integral (3.5) defines an element in \( S_{1}^{N+1,m-2(N+1)}(\mathcal{X}) \) for any \( \rho - \kappa \geq 1 \).

Let us consider the second contribution:

\[
\begin{aligned}
&\int_{\mathbb{S}} dY \int_{\mathbb{S}} dZ \, e^{-2i\sigma(Y,Z)} \mathcal{R}_{\beta,N}(h, x, y, z) \phi(x - \tilde{h} y, \xi - \eta) \psi(x - \tilde{h} z, \xi - \zeta) \\
&= (-i)^{N+1} \int_{\mathbb{S}} dY \int_{\mathbb{S}} dZ \left( \int_{0}^{1} du \cdots \int_{0}^{1} du_{N+1} \right) e^{-iu_{N+1}h\phi(x, y, z)} \cdots \cdots e^{-iu_{1}h\phi(x, y, z)} \\
&\times e^{-2i\sigma(Y,Z)} \left( \partial^\beta_{N+1}(x, y, z) \right)^{N+1} \phi(x - \tilde{h} y, \xi - \eta) \psi(x - \tilde{h} z, \xi - \zeta)
\end{aligned}
\]

so that a similar procedure to the one used for (3.5) proves that this integral defines a function of class \( S_{1}^{N+1,m-2(N+1)}(\mathcal{X}) \).

For any \( \phi \in S^m(\mathcal{X}) \) the rest \( \mathcal{R}_{\phi,N,\alpha} \) is a function of class \( S_{1}^{N+1,m-2(N+1)}(\mathcal{X}) \), \( \forall \alpha \in \mathbb{N}^d \) so that it is easy to note that the last contribution to the rest,

\[
\begin{aligned}
&\pi^{-2d} \int_{\mathbb{S}} dY \int_{\mathbb{S}} dZ \, e^{-2i\sigma(Y,Z)} \left\{ \sum_{0 \leq \rho \leq N} \frac{(-i)^{\rho}}{\rho!} \left( \sum_{0 \leq \lambda \leq N} \frac{h^{\lambda}}{4\lambda!} \left( \frac{i}{2} \right)^{\lambda} \mathcal{R}_{\rho}(x) \right)^{\rho} \\
&\times \left[ \left( \frac{i}{2} \right)^{N+1} \sum_{|\alpha|=N+1} \left( \mathcal{R}_{\rho,\phi,N,\alpha}(\partial_{N+1}^{\gamma} \phi)(x, y, z) + (-1)^{N+1} \mathcal{R}_{\rho,\phi,N,\alpha}(\partial_{N+1}^{\gamma} \phi) \right) \\
&\times (x - \tilde{h} y, \xi - \eta) - (-1)^{N+1} \left( \frac{i}{2} \right)^{2(N+1)} \sum_{|\rho|=N+1} \sum_{|\alpha|=N+1} (-1)^{N+1} (\partial_{N+1}^{\gamma} \mathcal{R}_{\rho,\phi,N,\alpha})(\tilde{h}, x, y, z, \xi, \zeta),
\end{aligned}
\]

defines an element of \( S_{1}^{N+1,m_1,m_2-2(N+1)}(\mathcal{X}) \).

Let us now concentrate on the main terms in expansion (3.4):

\[
\begin{aligned}
&\pi^{-2d} \int_{\mathbb{S}} dY \int_{\mathbb{S}} dZ \, e^{-2i\sigma(Y,Z)} \left\{ \sum_{0 \leq \rho \leq N} \frac{(-i)^{\rho}}{\rho!} \left( \sum_{0 \leq \lambda \leq N} \frac{h^{\lambda}}{4\lambda!} \left( \frac{i}{2} \right)^{\lambda} \mathcal{R}_{\rho}(x) \right)^{\rho} \\
&\times \left[ \sum_{0 \leq \nu \leq N} \frac{(-i)^{\nu}}{\nu!} \sum_{|\alpha|=\nu} \frac{1}{\alpha!} \left( (i/2) \partial_{v} \right)^{\alpha} (\partial_{N+1}^{\gamma} \phi)(x, \xi - \eta) \right] \\
&\times \left[ \sum_{0 \leq \mu \leq N} \frac{(-i)^{\mu}}{\mu!} \sum_{|\beta|=\mu} \frac{1}{\beta!} \left( (-1/2) \partial_{\beta} \right)^{\beta} (\partial_{N+1}^{\gamma} \psi)(x, \xi - \zeta) \right]
\end{aligned}
\]

\[
= \pi^{-2d} \int_{\mathbb{S}} dY \int_{\mathbb{S}} dZ \, e^{-2i\sigma(Y,Z)}
\]
order \leq \lambda_{1}\ldots \lambda_{p}.

Starting from the above result in what follows we work with functions of class $S^{0,m_{2}-N}_{1}(\mathcal{X})$, thus admitting asymptotic expansions in $h \in \mathcal{I}$ of the form given in the above proposition.

4. The magnetic Schrödinger operator

4.1. Preliminaries

Let us note that the magnetic Schrödinger operator defined in (1.1) satisfies

$$P^{A}(\hbar) = \mathcal{D}p^{A}_{\hbar}(\xi^{2} + V).$$

(4.1)
We suppose that the magnetic field has components of class $BC^\infty(\mathcal{X})$, that the vector potential has been chosen of class $C_0^\infty(\mathcal{X})$ and that $V$ is a real $BC^\infty(\mathcal{X})$ function. Hence $F := \xi^2 + V \in S_2^1(\mathcal{X})$ and all the results in section 3 can be applied in order to conclude that (taking also into account that $V$ is a bounded self-adjoint perturbation of $P_0^B(\xi) := \Omega p_0^B(\xi^2)$ and the Neumann series expansion of the resolvent):

**Proposition 4.1.**

1. $P^A(\xi)$ defined in (4.1) is essentially self-adjoint on $S(\mathcal{X})$ and its self-adjoint extension, denoted $H_0^A$, has the domain $H^A_0(\mathcal{X})$.

2. The resolvent $(H_0^A - \lambda)^{-1}$ is well defined for $\lambda \in \mathbb{C} \setminus \{ \xi \in \mathbb{R} \mid \xi \geq a \}$ for some $a \in \mathbb{R}$ and has the form $(H_0^A - \lambda)^{-1} = \Omega p_0^B(\xi^2)$ with $r_B^A(\xi) \in S^{(0,-2)}_1(\mathcal{X})$.

3. There exists $a_0 \geq a$ depending on $B$ and $V$ and $h_0 > 0$ such that $\sigma_{ess}(H_0^A) \subset [a_0, \infty)$ for any $\lambda \in (0, h_0]$.

4.2. The resolvent

We concentrate now on the asymptotic expansion of the symbol $r_B^A(\xi)$ with respect to $\xi \in \mathcal{X}$. In fact, as the case without the magnetic field is well known, we will only be interested in the ‘magnetic’ contribution to the terms of the $h$-asymptotic expansion, specifically in putting them in a manifestly gauge-invariant form. For this purpose we use our parametrix-type construction [22] in order to express $r_B^A$ in terms of $(F - \xi)^{-1}$. In fact we know that $(F - \xi) r_B^A = 1$. In order to shorten our notations we denote by $p_j := F - \xi$. Let us compute

$$p_j^A p_j^{-1} = 1 + \gamma^A_j(p_j, p_j^{-1}) = 1 + \sum_{k=1}^{N-1} \hbar^k \zeta^A_k(p_j, p_j^{-1}) + \hbar^N \zeta^A_N(p_j, p_j^{-1})$$

with $\zeta^A_k(p_j, p_j^{-1}) \in S^{(0,-N)}_1(\mathcal{X})$ and $\zeta^A_N(p_j, p_j^{-1}) \in S^{(1,-N)}_1(\mathcal{X})$. Thus

$$r_B^A = p_j^{-1} - r_B^A \gamma^A_j(p_j, p_j^{-1})$$

$$= \sum_{0 \leq j \leq M-1} (-1)^j p_j^{-1} \gamma^A_j(p_j, p_j^{-1})^j + (-1)^M r_B^A \gamma^A_j(p_j, p_j^{-1})^M$$

$$= \sum_{0 \leq j \leq M-1} (-1)^j p_j^{-1} \gamma^A_j \left[ \sum_{k=1}^{N-1} \hbar^k \zeta^A_k(p_j, p_j^{-1}) + \hbar^N \zeta^A_N(p_j, p_j^{-1}) \right]$$

$$+ (-1)^M r_B^A \gamma^A_j \left[ \sum_{k=1}^{N-1} \hbar^k \zeta^A_k(p_j, p_j^{-1}) + \hbar^N \zeta^A_N(p_j, p_j^{-1}) \right]^M. \quad (4.2)$$

Let us first study the corrections $\zeta^A_k(p_j, p_j^{-1})$. We use the general formulas (3.8), (3.7) and obtain

$$\zeta^A_k(p_j, p_j^{-1})(x, \xi) = (2\pi)^{-2d} \sum_{1 \leq j_1 < \cdots < j_d \leq 1 \leq \rho \leq k} \sum_{1 \leq e_1 < \cdots < e_{\rho} \leq \rho} \frac{(-1)^{e_1 + \cdots + e_{\rho}}}{4^\rho \rho!} \sum_{l_1+\cdots+l_\rho=k} \left( \frac{i}{2} \right)^{l_1+\cdots+l_\rho} t^1_{l_1+\cdots+l_\rho} \frac{1}{\alpha!\beta!}$$

$$\times \sum_{\substack{1 \leq j_1 < \cdots < j_d \leq 1 \leq \rho \leq k \\\text{and} \\\text{any} \\\text{order}}} \cdot \left( \partial^{\rho/2} B_{j_1j_2} \right) \left( x \right) \left( \partial_{j_1} \cdots \partial_{j_d} \partial_{\xi}^{\rho/2} \partial_{\xi}^{\rho/2} \partial_{p_j} \right)(x, \xi)$$

$$\times \left( \partial_{x_1} \cdots \partial_{x_d} \partial_{\eta}^{\rho/2} \partial_{\eta}^{\rho/2} \partial_{\eta} \right)(x, \xi).$$
An important observation is that all the derivatives of the symbols \( p_j \) and \( p_j^{-1} \) have a very special dependence on \( z \). More precisely we have

1. \( (\partial^a_x p_j)(x, \xi) = (\partial^a_x F)(x, \xi) = (\partial^a_x V)(x) \);
2. \( (\partial^a_v p_j)(x, \xi) = (\partial^a_v F)(x, \xi) = 2\xi; \quad (\partial^a_v \partial^a_k p_j)(x, \xi) = 2\delta_{jk}; \quad (\partial^a_x p_j)(x, \xi) = 0, \quad \forall |\alpha| \geq 3; \)
3. \( (\partial^a_v \partial^a_k p_j)(x, \xi) = 0, \quad \text{for } |\alpha| \geq 1, |\beta| \geq 1. \)

### Lemma 4.2.

For any multindices \( \alpha \) and \( \beta \) we have that

\[
(\partial^a_x \partial^a_v \partial^a_k p_j^{-1})(x, \xi) = \sum_{0 \leq k \leq N} q_k(x, \xi) p_j^{-1-k}(x, \xi)
\]

where \( q_k(x, \xi) \) are the polynomials of degree at most \( k \) in \( z \) with coefficient functions of \( x \) depending only on the first \( |\alpha| \) derivatives of \( V(x) \).

**Proof.**

In fact we have

\[
(\partial_{\xi j} p_j^{-1})(x, \xi) = -p_j^{-2}(x, \xi)(\partial_{\xi j} F)(x, \xi) = -p_j^{-2}(x, \xi)(\partial_{\xi j} V)(x);
\]

\[
(\partial_{\xi j} p_j^{-1})(x, \xi) = -p_j^{-2}(x, \xi)(\partial_{\xi j} F)(x, \xi) = -2\xi_j p_j^{-2}(x, \xi) .
\]

Thus, the statement of the lemma is true for \( |\alpha| + |\beta| = 1 \) and we proceed by induction on \( |\alpha| + |\beta| \). Suppose the statement has been proved for \( |\alpha| + |\beta| = N \) and let us compute the next derivatives:

\[
(\partial_{\xi j} \partial^a_x \partial^a_v \partial^a_k p_j^{-1})(x, \xi) = \partial_{\xi j} \left[ \sum_{0 \leq k \leq N} q_k(x, \xi) p_j^{-1-k}(x, \xi) \right] (x, \xi)
\]

\[
= \sum_{0 \leq k \leq N} (\partial_{\xi j} q_k)(x, \xi) p_j^{-1-k}(x, \xi) - (1 + k) 
\]

\[
\times \sum_{0 \leq k \leq N} q_k(x, \xi)(\partial_{\xi j} p_j)(x, \xi) p_j^{-1-(k+1)}(x, \xi) 
\]

\[
= \sum_{0 \leq k \leq N} \left[ (\partial_{\xi j} q_k)(x, \xi) - k q_{k-1}(x, \xi) (\partial_{\xi j} V)(x) \right] p_j^{-1-k}(x, \xi) 
\]

\[
- (1 + N)q_N(x, \xi)(\partial_{\xi j} V)(x) p_j^{-1-(N+1)}(x, \xi); 
\]

\[
(\partial_{\xi j} \partial^a_x \partial^a_v \partial^a_k p_j)(x, \xi) = \partial_{\xi j} \left[ \sum_{0 \leq k \leq N} q_k(x, \xi) p_j^{-1-k}(x, \xi) \right] (x, \xi)
\]

\[
= \sum_{0 \leq k \leq N} (\partial_{\xi j} q_k)(x, \xi) p_j^{-1-k}(x, \xi) - (1 + k) 
\]

\[
\times \sum_{0 \leq k \leq N} q_k(x, \xi)(\partial_{\xi j} p_j)(x, \xi) p_j^{-1-(k+1)}(x, \xi) 
\]

\[
= \sum_{0 \leq k \leq N} \left[ (\partial_{\xi j} q_k)(x, \xi) - 2k \xi_j q_{k-1}(x, \xi) \right] p_j^{-1-k}(x, \xi) 
\]

\[
- 2(1 + N)\xi_j q_N(x, \xi) p_j^{-1-(N+1)}(x, \xi).
\]

Thus, the formula is also valid for \( |\alpha| + |\beta| = N + 1 \) with coefficients having obviously the same structure. \( \square \)
Remark 4.3. Some simple computation proves that
\[ c^B_j(p_j, p_j^{-1}) = 0, \]
\[ c^B_j(p_j, p_j^{-1})(x, \xi) = \frac{1}{2} p_{j-2}(x, \xi)(\Delta V)(x) - \frac{1}{2} p_j^{-2}(x, \xi) |(\nabla V)(x)|^2 - 2 p_j^{-3}(x, \xi) \sum_{lm} \left(1 - \frac{1}{2} \delta_{lm}\right) (\partial_x \partial_x \partial_x V)(x) \xi_l \xi_m + \frac{1}{2} p_j^{-2}(x, \xi) B(x)^2 \]
\[ = 2 p_j^{-3}(x, \xi) \sum_{jkm} B_{jk}(x) B_{jm}(x) \xi_k \xi_m + \frac{2}{3} p_j^{-2}(x, \xi) \sum_{jk} (\partial_x B_{jk}(x)) \xi_k \]
\[ - 2 p_j^{-3}(x, \xi) \sum_{jk} B_{jk}(x) \xi_k (\partial_x V)(x). \]

Developing successively each \( \sharp B \)-product in (4.2) and using proposition 3.7, one gets the following statement.

Proposition 4.4. The 'magnetic' symbol \( r^B \) admits for any \( N \in \mathbb{N} \) an asymptotic expansion in \( \hbar \) of the form
\[ r^B(X) = p^{-1}_j + \sum_{1 \leq j \leq N} \hbar^j c_j^{B} (\hbar; X) + \hbar^N c_N^{B} (\hbar; X) \]
where the terms \( c_j^{B} (\hbar; X) \) only depend on the magnetic field \( B \) and its derivatives up to order \( j + 1 \) evaluated at \( X \), and the rest \( c_N^{B} (\hbar; X) \) only depends on the magnetic field \( B \) (in a non-local way). Moreover, \( c_j^{B} (\hbar; X) \in S_1^{1j} (X) \) and \( c_N^{B} (\hbar) \in S_1^{0, -N^j} (X) \).

Considering (4.2) we obtain the following expansion of \( r^B \) in powers of \( \hbar \):
\[ r^B \sim p^{-1}_j + \sum_{1 \leq j \leq N} \hbar^j \sum_{1 \leq k \leq j} (-1)^k \sum_{1 \leq l \leq k-1} p^{-1}_j \hbar^l c_j^{B} (p_j, p_j^{-1}) \hbar^l c_{j-l}^{B} (p_j, p_j^{-1}) \]
(4.3)
and developing further each \( \hbar \)-dependent \( \sharp B \)-product, one has
\[ r^B \sim p^{-1}_j + \sum_{1 \leq j \leq k \leq j} (-1)^k \sum_{1 \leq l \leq k-1} \hbar^l c_{j-l}^{B} (p_j, p_j^{-1}) \]
\[ \times (p^{-1}_j, c_j^{B} (p_j, p_j^{-1}), \ldots, c_k^{B} (p_j, p_j^{-1})) \]
\[ = p^{-1}_j + \sum_{1 \leq j \leq N} \hbar^j \sum_{1 \leq k \leq j} (-1)^k \sum_{1 \leq l \leq k-1} c_j^{B} (p_j, p_j^{-1}) \]
\[ \times \left( c_{j-l}^{B} (p_j, p_j^{-1}), \ldots, c_{j}^{B} (p_j, p_j^{-1}) \right) \]
where
\[ c_j^{B} (f, g_1, \ldots, g_k) := c_{\mu_j, \ldots, \mu_k}^{B} (f, g_1, \ldots, g_k). \]

Putting together all these formulas we conclude that:

Proposition 4.5. Each term \( c_j^{B} (\hbar; X) \) for \( j \geq 1 \) is a finite sum of the form
\[ c_j^{B} (\hbar; x, \xi) = \sum_{0 \leq p < j} z_p^{B} (x, \xi) p^{-2-p} (x, \xi) \]
where $f^h(x, \xi)$ are polynomials in $\xi$ of degree at most $p$ whose coefficients are $C^\infty$ functions of $x$ depending only on a finite number of partial derivatives of $V$ and $B$ at the given point $x$.

**Remark 4.6.** Some tedious computation gives

\begin{align*}
\tau^h_0(\xi) &= p_s^{-1} \\
\tau^h_1(\xi) &= -p_s^{-1}c^h(p_s, p_s^{-1}) = 0 \\
\tau^h_2(\xi) &= -p_s^{-1}c^h(p_s, p_s^{-1}) + p_s^{-1}c^h(p_s, p_s^{-1})c^h(p_s, p_s^{-1}) - c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) \\
&= -p_s^{-1}c^h(p_s, p_s^{-1}) = -\frac{1}{2}p^{-3}(x, \xi)(\nabla V)(x) + \frac{1}{2}p^{-3}(x, \xi)|V(x)|^2 \\
&+ \frac{1}{2}p^{-3}(x, \xi) \sum_{im} \left(1 - \frac{1}{2}\delta_{im}\right)(\partial_{\xi_i}\partial_{\xi_m}^V)(x)\xi_i\xi_m - \frac{1}{2}p^{-3}(x, \xi)|B(x)|^2 \\
&+ \frac{1}{2}p^{-3}(x, \xi) \sum_{jkm} B_{jk}(x)B_{jm}(x)\xi_j\xi_k - \frac{2}{3}p^{-3}(x, \xi) \sum_{j} (\partial_j B_{jk}) (x)\xi_k \\
&+ 2p^{-3}(x, \xi) \sum_{jk} B_{jk}(x)\xi_k(\partial_j, V)(x);
\end{align*}

\begin{align*}
\tau^h_3(\xi) &= -p_s^{-1}c^h(p_s, p_s^{-1}) + 2p_s^{-1}c^h(p_s, p_s^{-1})c^h(p_s, p_s^{-1}) \left[c^h(p_s, p_s^{-1})\right]^3 \\
&+ c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) - c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) \\
&= -p_s^{-1}c^h(p_s, p_s^{-1}) - c^h(p_s^{-1}, c^h(p_s, p_s^{-1}));
\end{align*}

\begin{align*}
\tau^h_4(\xi) &= -p_s^{-1}c^h(p_s, p_s^{-1}) + 2p_s^{-1}c^h(p_s, p_s^{-1})c^h(p_s, p_s^{-1}) + p_s^{-1}c^h(p_s, p_s^{-1}) \\
&- 3p^{-1}c^h(p_s, p_s^{-1})^3 - c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) \\
&+ 2c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) - c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) \\
&+ 2c^h(p_s^{-1}, c^h(p_s, p_s^{-1})c^h(p_s, p_s^{-1}) - c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) \\
&+ c^h(p_s^{-1}, c^h(p_s, p_s^{-1}), c^h(p_s, p_s^{-1})) \\
&= -p_s^{-1}c^h(p_s, p_s^{-1}) + p_s^{-1}c^h(p_s, p_s^{-1})^3 - c^h(p_s^{-1}, c^h(p_s, p_s^{-1})) \\
&- c^h(p_s^{-1}, c^h(p_s, p_s^{-1})).
\end{align*}
Proposition 4.7. The 'magnetic' symbol \( \tilde{g}(F)_h \) admits for any \( K \in \mathbb{N} \) an asymptotic expansion in \( h \) of the form

\[
\tilde{g}(F)_h (X) = \sum_{0 \leq j \leq K-1} h^j g^B_j[F](X) + h^K g^B_K[F](\hbar, X)
\]

where the terms \( g^B_j[F](X) \) only depend on the magnetic field \( B \) and its derivatives up to order \( j \). Moreover, \( g^B_j[F] \in S((-\infty, 0] \times \mathcal{X}) \) and \( g^B_K[F] \in S((-\infty, 0] \times \mathcal{X}) \).

Due to the diamagnetism inequality, \( a_0 \geq \Sigma_V \); let \( g \in C^\infty(\mathbb{R}) \) be with support \( \Sigma_g \subset \mathbb{R} \). As \( \sigma(H_\hbar) \) is discrete in this region, and \( \Sigma_g \) is compact, we deduce that \( g(H_\hbar) \) is of finite rank and thus trace-class. Moreover, \( g(H_\hbar) = \mathbb{D}^A(\tilde{g}(F)_h) \) is an integral operator having the integral kernel (see [21])

\[
K^A[g(H_\hbar)](x, y) := (e^{-\frac{1}{2} \cdot \cdot \cdot A^2}) \tilde{g}^{-1} \tilde{g}(F)_h \left(\frac{x+y}{2}, x-y\right)
\]

with \( \tilde{g}^{-1} \) the inverse Fourier transform in the second variable (as defined on distributions on \( \mathbb{R} = \mathcal{X} \times \mathcal{X} \)). In order to study the regularity properties of this integral kernel we use our formula (4.4) and write that

\[
r^B_{x+yj\mu}(X) = (F - (\lambda + i\mu))^{-1}(X) + \tilde{x}^B_{x+yj\mu}(X)
\]

where

\[
-\pi^{-1} \lim_{\epsilon \to 0} \int_{|\lambda| \geq \epsilon} \frac{\partial \tilde{g}}{\partial \xi_\lambda}(\lambda, \mu) (F - (\lambda + i\mu))^{-1} \, d\lambda \, d\mu = (g \circ F) \in C^\infty(\mathbb{R})
\]

and

\[
\tilde{x}^B_{x+yj\mu} = r^B_{x+yj\mu} - (F - (\lambda + i\mu))^{-1}
\]

\[
= r^B_{x+yj\mu} - (1 - (F - (\lambda + i\mu))^{-1}) - S_1^{(-2, -2)}(X)
\]

due to our proposition 3.3 applied to \( 1 - (F - (\lambda + i\mu))^{-1} \). Let us remark that in two or three dimensions, \( \tilde{g}^{-1} \tilde{S}_1^{(-2, -2)}(X) \) is contained in the space of jointly continuous functions on \( \mathcal{X} \times \mathcal{X} \) (by the Riemann–Lebesgue lemma). Let us recall that for trace-class operators with continuous integral kernels we have the following property.

Proposition 4.8. Suppose \( T \in \mathfrak{B}(L^2(\mathcal{X})) \) has an integral kernel \( K[T] \in C(\mathcal{X} \times \mathcal{X}) \). Then the following limit exists and we have the equality

\[
\lim_{R \to \infty} \int_{|x| \leq R} dx \, K[T](x, x) = \text{Tr} T.
\]

Let us discuss now the case \( d \geq 4 \). We come back to formula (4.4) and use proposition 4.4 with the above observations:

\[
\tilde{g}(F)_h (X) = -\pi^{-1} \lim_{\epsilon \to 0} \int_{|\lambda| \geq \epsilon} \frac{\partial \tilde{g}}{\partial \xi_\lambda}(\lambda, \mu) \, r^B_{x+yj\mu}(X) \, d\lambda \, d\mu
\]
\[
= -\pi^{-1} \lim_{\epsilon \to 0^+} \int_{|\mu| \geq \epsilon} \frac{\hat{g}}{\hat{z}}(\lambda, \mu) \times \left[ \sum_{0 \leq j \leq N - 1} \hat{g} \left( \lambda + i\mu ; X \right) + \hat{g} \left( \lambda + i\mu ; \hat{h}, X \right) \right].
\]

(4.5)

Taking now \( N > d \) and taking into account proposition 4.4 we conclude that \( \hat{g} \left( \lambda + i\mu ; \hat{h} \right) \in S(0, -N) \) and by the Riemann–Lebesgue lemma it has a continuous Fourier transform (with respect to the \( \xi \) variable). Let us consider the main terms in expansion (4.5) for \( N > d \). Taking into account proposition 4.5 we have to study integrals of the form

\[
\lim_{\epsilon \to 0^+} \int_{|\mu| \geq \epsilon} \frac{\hat{g}}{\hat{z}}(\lambda, \mu) f_{\hat{B}}(x, \xi) \left[ \sum_{0 \leq j \leq N - 1} \hat{g} \left( \lambda + i\mu ; X \right) + \hat{g} \left( \lambda + i\mu ; \hat{h}, X \right) \right].
\]

We can evidently use again the Riemann–Lebesgue lemma to obtain continuity of the Fourier transform (with respect to the \( \xi \) variable). Putting all these results together we obtain the following statement.

**Proposition 4.9.** For \( B \) a magnetic field with components of class \( BC^\infty(X) \) and \( H_{\hat{h}} \) the self-adjoint operator defined in proposition 4.1, if \( g \in C^\infty_0(\mathbb{R}) \) has compact support \( \Sigma_g \subset \mathbb{R} \) and \( H_{\hat{h}} \), then \( g(H_{\hat{h}}) \) is a trace-class operator\(^4\) and we have the formula

\[
\text{Tr} \ g(H_{\hat{h}}) = \int_X dX \mathfrak{g}(\mathfrak{g}^{-1}(x, 0) = \int_X dX \mathfrak{g}(\mathfrak{g}^{-1}(x, 0),
\]

so that \( \text{Tr} \ g(H_{\hat{h}}) \) only depends on the magnetic field.

4.4. End of the proof of the semiclassical trace formula

4.4.1. Comparison of the theorems using Agmon estimates. We are now ready to consider the semiclassical expansion of the trace formula starting from proposition 4.9 and using the semiclassical expansions computed previously. Before doing that let us look in more detail at the remark in [8] that due to the exponential decay of the eigenfunctions (Agmon estimates [1]) one can modify the potential outside a compact region by polynomially bounded terms with only an exponentially small change (of order \( \exp(-c/\hat{h}) \)) in the eigenvalues situated in any compact part of the discrete spectrum [9, 10]. A simple inspection of the proof in [1] shows that the same exponential decay estimates can be obtained for the magnetic Schrödinger operator so that we can apply the same arguments from [8] to our ‘magnetic’ situation. Here is the basic proposition.

**Proposition 4.10.** Let \((A, V)\) and \((\hat{A}, \hat{V})\) be two pairs of electro-magnetic potentials satisfying hypotheses 1.1 and 1.2. Let \( E \) verify

- \( E < \min(\Sigma_V, \Sigma_{\hat{V}}) \),
- \( U_E := V^{-1}([-\infty, E]) = \hat{V}^{-1}([-\infty, E]) \),
- \( V = \hat{V} \) on \( U_E \) and \( A = \hat{A} \) on \( U_E \).

\(^4\) In fact it is even finite rank.
and let $H_h$ and $\hat{H}_h$ be the corresponding magnetic Schrödinger operators. Then for any $g \in C_0^\infty(\mathbb{R})$, such that $\text{supp } g \subset \left[ -\infty, \infty \right]$, $E[\text{Tr } g(H_h)]$ and $\text{Tr } g(\hat{H}_h)$ have the same semiclassical expansion modulo $O(\hbar^{\infty})$.

It is enough to observe that, for any $\epsilon > 0$, the eigenfunctions corresponding to eigenvalues of $H_h$ (resp. $\hat{H}_h$) less than $E - \epsilon$ decay exponentially in any compact outside of $U_{E-\epsilon}$.

This can be used in the following way.

**Proposition 4.11.** Let $(A, V)$ satisfy hypotheses 1.1 and 1.2 and let $E < \Sigma V$; then there exists a pair $(\hat{A}, \hat{V})$ such that the assumptions of proposition 4.10 are satisfied with in addition $\hat{A}$ and $\hat{V}$ bounded (with all the derivatives).

The proof is easy. We can indeed consider a $C^\infty$ increasing function $\chi$ on $\mathbb{R}$ such that $\chi(t) = t$ on $[-\infty, \frac{1}{2}(E + \Sigma V)]$, $\chi'(t) = 0$ on $[\frac{1}{2}(E + 2\Sigma V), +\infty[.$

We can then take $\hat{V} = \chi(V)$. It is not difficult to modify $A$ outside $V - \frac{1}{2}(E + \Sigma V)$ to get a $C^\infty$ bounded magnetic potential.

As a consequence, it is enough for proving theorem 1.3 to prove it with $A$ and $V$ of class $C^\infty$ and bounded. Hence we can work at the intersection of the two calculi and use either the results of Weyl’s calculus or of the adapted magnetic calculus.

### 4.4.2. The case with boundary.

Let us consider the case of the Dirichlet realization in a bounded open set $\Omega$; then it is easy to modify the comparison argument of the previous subsubsection in order to obtain the following theorem.

**Theorem 4.12.** Let $A$ and $V$ be $C^\infty$ potentials on $\Omega$ and assume that

$$\inf_{x \in \Omega} V(x) < \inf_{x \in \partial \Omega} V(x).$$

Then, with $H_h$ the Dirichlet realization of $P_A$ in $\Omega$, there exists a sequence of distributions $T^j_B \in \mathcal{D}'(\mathbb{R})$, $(j \in \mathbb{N})$, such that, for any $\epsilon > 0$, for any $N \in \mathbb{N}$, there exist $C_N$ and $h_N$, such that if

$$g \in C_0^\infty(\mathbb{R}), \text{ with } \text{supp } g \subset \left[ -\infty, \inf_{x \in \partial \Omega} V - \epsilon \right],$$

then

$$\left| (2\pi \hbar)^d \text{Tr } g(H_h) - \sum_{0 \leq j \leq N} h^j T^j_B(g) \right| \leq C_N h^{N+1}, \forall h \in [0, h_N] \cap \mathcal{I}. \quad (4.6)$$

More precisely there exists $k_j \in \mathbb{N}$ and universal polynomials $P_k(u_\alpha, v_\beta, j, k)$ depending on a finite number of variables, indexed by $\alpha \in \mathbb{N}^{2d}$ and $\beta \in \mathbb{N}^d$, such that the distributions

$$T^j_B(g) = \sum_{0 \leq \ell \leq k_j} \int g^{(\ell)}(F(x, \xi)) P_\ell(\partial_{\xi}^{\alpha} F(x, \xi), \partial_{x}^{\beta} B_{jk}(x)) \, dx \, d\xi. \quad (4.7)$$

Finally, $T^j_B = 0$ for $j$ odd.

**Remark 4.13.** The polynomials are the same as in theorem 1.3. In particular they are independent of $\Omega$.

Using a (small extension of) the comparison proposition, one can modify the potentials in the neighborhood of $\partial \Omega$ and then extend outside of $\Omega$ without modifying the asymptotic of $\text{Tr } g(H_h)$ and use the results obtained in the case of $\mathbb{R}^d$. 19
**Remark 4.14.** Note that we have not done any assumptions on the topology of $\Omega$. Hence we also have that this expansion depends only on the magnetic field for cases where one can get various generating magnetic potentials which are not in the same cohomology class.

### 4.4.3. The odd coefficients vanish.
To prove this result, one first observes that we have

$$
|h|^0 \text{Tr} \left( g \left( H_h \right) \right) - \sum_{0 \leq j \leq N} \hbar^j T^B_j (g) \leq C_N \hbar^{N+1}, \forall \hbar \in [-\hbar_N, \hbar_N] \setminus \{0\}
$$

(the $\hbar$-pseudodifferential calculus can be extended to $\hbar < 0$) and using the complex conjugation one obtains that the trace of $g(H_h)$ is unchanged when $\hbar \mapsto -\hbar$. Hence the odd coefficients are 0.

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