Magnetic calculus and semiclassical trace formulas.

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Abstract

The aim of these notes is to show how the magnetic calculus developed in [MP, IMP1, IMP2, MPR, LMR] permits to give a 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 [HR2].

1 Introduction

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

$$P^A(\hbar) = \sum_{j=1}^{d} (\hbar D_{x_j} - A_j(x))^2 + V(x) , \qquad (1.1)$$

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

Hypothesis 1.1

- $\hbar \in \mathcal{I} \subset]0, +\infty[$, *with $\mathcal{I}$ a bounded set having 0 as accumulation point,*

- $A = (A_1, \dots, A_d)$ *with $A_j \in C^\infty(\mathbb{R}^d)$,*

- $V \in C^\infty$, $V \geq -C$.

It is known that the operator associated with $P^A(\hbar)$ on $C_0^\infty(\mathbb{R}^d)$ admits a unique selfadjoint extension on $L^2(\mathbb{R}^d)$, which can be defined as the Friedrichs extension. We denote by $\widetilde{P^A}(\hbar)$ this extension. For any function $g \in C_0^\infty(\mathbb{R})$, we can define by the abstract functional calculus $g(\widetilde{P^A}(\hbar))$.

We shall also make the following assumption concerning the potential function V:

Hypothesis 1.2

$$\Sigma_V := \liminf_{|x| \to \infty} V(x) > \inf V .$$

It is known in this case by Persson's Theorem (see for example [Ag]) that the spectrum is discrete in $]-\infty, \Sigma_V[$ and using the max-min principle one shows easily that the spectrum is non empty for $\hbar$ small enough. In particular, for $\operatorname{supp} g \subset\subset]-\infty, \liminf V[$, one can consider $\operatorname{Tr} g(\widetilde{P^A}(\hbar))$. Our goal is to analyze the expansion of this trace as a power series in $\hbar$ and the dependence of the coefficients on the magnetic field, i.e. the two-form $B := d(\sum_j A_j dx_j)$. Of course if we have two vector potentials A and $\hat{A}$, such that $dA = d\hat{A} = B$, we know that there exists $\phi \in C^\infty(\mathbb{R}^d)$ such that : $A = \hat{A} + d\phi$, and the conjugation by the multiplication operator by $\exp \frac{i}{\hbar}\phi$ gives a unitary equivalence between $\widetilde{P^A}(\hbar)$ and $\widetilde{P^{\hat{A}}}(\hbar)$. Hence $\operatorname{Tr} g(\widetilde{P^A}(\hbar))$ 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 $H = \widetilde{P^A}(\hbar)$, 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 $\operatorname{supp} g \subset]-\infty, \Sigma_V[$ and for any $N \in \mathbb{N}$, there exist C_N and h_N, such that:

$$\left| (2\pi\hbar)^d \operatorname{Tr} g(H) - \sum_{0 \leq j \leq N} \hbar^j T_j^B(g) \right| \leq C_N \hbar^{N+1} , \ \forall \hbar \in]0, h_N] \cap \mathcal{I}. \qquad (1.2)$$

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

$$T_j^B(g) = \sum_{0 \leq \ell \leq k_j} \int g^{(\ell)}(F(x,\xi)) P_\ell(\partial_{x,\xi}^\alpha F(x,\xi), \partial_x^\beta B_{jk}(x)) \, dx d\xi , \qquad (1.3)$$

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 [HR1], 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 $dA = B$. Tricky calculations permitted after to recover a gauge invariant expression for the three first terms :

$$T_0^B(g) := \int_\Xi dx \, d\xi g(F(x,\xi)), \quad T_1^B(g) := 0, \quad T_2^B(g) := -\frac{1}{12} \int_\Xi dx \, d\xi g''(F(x,\xi)) \left[(\Delta V)(x) + \|B(x)\|^2 \right]. \quad (1.4)$$

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The approach of [HR1] did not permit to recover the same kind of result for any term of the expansion. On the contrary, we will show that, when it can be applied the magnetic calculus permits to give naturally this expression. To state the results at the intersection of the domains of validity of the two calculi is actually unnecessary. Following essentially arguments presented in [HMR] in the case without magnetic potential, we will show how we can use the Agmon exponential decay estimates in order to modify the behaviour of V and A at infinity, without changing the asymptotic behavior of $\operatorname{Tr} g(\widetilde{P^A(h)})$, in order to enter simultaneously in Helffer-Robert's class and in the magnetic pseudodifferential calculus of [IMP1, IMP2, MP, MPR].

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 [IMP1, IMP2, MP, MPR]. The last section will give the proof of the main theorem.

We shall constantly use the notations $\mathcal{X} \cong \mathbb{R}^d$, $\Xi := \mathcal{X} \times \mathcal{X}'$, with $\mathcal{X}'$ the dual of $\mathcal{X}$. The points of Ξ will be denoted as $X = (x, \xi)$. Recall that Ξ 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 $C_{\mathsf{pol}}^\infty(\mathcal{Y})$ the space of C^∞-functions on the vector space $\mathcal{Y}$ having at most polynomial growth at infinity together with all their derivatives. We denote by $C_{\mathsf{pol,u}}^\infty(\mathcal{Y})$ the subspace of functions having a unique polynomial upper bound for all their derivatives.

2   The $\hbar$-pseudodifferential Weyl calculus and trace formulas

To any Schwartz test function $\phi \in \mathcal{S}(\Xi)$ we associate a bounded linear operator $\mathfrak{Op}_{\hbar}(\phi)$ on the Hilbert space $\mathcal{H} := L^2(\mathcal{X})$:

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

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

$$\|\mathfrak{Op}_{\hbar}(\phi)\|_{\mathbb{B}(\mathcal{H})} \leq \int_\mathcal{X} dx \|[\mathfrak{F}^- \phi](x, \cdot)\|_\infty$$

where $\mathfrak{F}^-$ denotes the inverse Fourier transform with respect to the second variable. Moreover it is not hard to prove, by using Schur's Lemma, that $\mathfrak{Op}_{\hbar} : \mathcal{S}(\Xi) \to \mathbb{B}(\mathcal{H})$ extends to an isomorphism of topological vector spaces $\mathfrak{Op}_{\hbar} : \mathcal{S}'(\Xi) \to \mathbb{B}(\mathcal{S}(\mathcal{X}); \mathcal{S}'(\mathcal{X}))$. We can transport the operator multiplication from $\mathbb{B}(\mathcal{H})$ back to a non-commutative product on $\mathcal{S}(\Xi)$

$$\mathfrak{Op}_{\hbar}(\phi)\mathfrak{Op}_{\hbar}(\psi) =: \mathfrak{Op}_{\hbar}(\phi\sharp_{\hbar}\psi), \quad \forall (\phi, \psi) \in [\mathcal{S}(\Xi)]^2.$$

Explicitely we have

$$(\phi\sharp_{\hbar}\psi)(X) := (\pi\hbar)^{-2d} \int_\Xi dY \int_\Xi dZ \exp\left[-(2i/\hbar)\,\sigma(Y, Z)\right] \phi(X - Y)\psi(X - Z). \tag{2.1}$$

One can prove that

$$\mathfrak{Op}_{\hbar}[\mathcal{S}(\Xi)] = \mathbb{B}(\mathcal{S}(\mathcal{X}); \mathcal{S}(\mathcal{X})) = \mathbb{B}(\mathcal{S}'(\mathcal{X}); \mathcal{S}'(\mathcal{X}))$$

so that one can consider products of the form $\mathfrak{Op}_{\hbar}(\Phi)\mathfrak{Op}_{\hbar}(\phi)$ and $\mathfrak{Op}_{\hbar}(\phi)\mathfrak{Op}_{\hbar}(\Phi)$ for $(\Phi, \phi) \in \mathcal{S}'(\Xi) \times \mathcal{S}(\Xi)$ and define the Moyal algebra

$$\mathfrak{M}(\Xi) := \left\{ \Phi \in \mathcal{S}'(\Xi) \mid \Phi\sharp_{\hbar}\phi \in \mathcal{S}(\Xi), \phi\sharp_{\hbar}\Phi \in \mathcal{S}(\Xi), \forall \phi \in \mathcal{S}(\Xi) \right\},$$

that is obviously an algebra for the $\sharp_{\hbar}$-multiplication and even a $*$-algebra for the anti-involution given by complex conjugation of distributions.

The limit $\hbar \to 0$, that has a rather singular behaviour, 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 [La]), but is out of our aims in this paper. On the contrary, the asymptotics $\hbar \to 0$, known as the semi-classical asymptotics, and considered in the frame of asymptotic series in $\hbar$ is an important problem and we shall concentrate on some of its aspects when magnetic fields are present.

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

$$S_1^m(\mathcal{X}) := \left\{ F \in C^\infty(\Xi) \mid \sup_{(x,\xi) \in \Xi} <\xi>^{-m+|\alpha|} \left| (\partial_x^a \partial_\xi^\alpha F)(x,\xi) \right| < \infty \right\}.$$

A symbol $F \in S_1^m(\mathcal{X})$ of strictly positive order $m > 0$ satisfying

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

is called *elliptic* and has the property that it exists a positive constant $a \geq 0$ such that for any $\mathfrak{z} \in \mathbb{C} \setminus \mathbb{R} \cup (\infty, -a)$ the distribution $\mathfrak{z} + F$ has an inverse $(\mathfrak{z} + F)^-$ with respect to the $\sharp_\hbar$-product and this inverse belongs to the class $S_1^{-m}(\mathcal{X})$. In other words, the operator $\mathfrak{Op}_\hbar(F)$ has a self-adjoint extension with a resolvent that has a symbol of Hörmander class $S_1^{-m}(\mathcal{X})$. An important problem is how to relate this pseudodifferential calculus (defined by the Moyal product $\sharp_\hbar$) with the usual functional calculus for self-adjoint operators, when these operators are of the form $\mathfrak{Op}_\hbar(F)$ with $F \in S_1^m(\mathcal{X})$ 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 $\sharp_\hbar$ has a 'suitable' behaviour with respect to such asymptotic series. More precisely, let us consider the space $S_1^{(s,m)}(\mathcal{X})$ of $\hbar$-symbols of the form $F : \mathcal{I} \times \Xi \to \mathbb{C}$ such that

$$F(\hbar) \in C^\infty(\Xi), \ \forall \hbar \in \mathcal{I}, \quad \sup_{\mathcal{I} \times \Xi} \hbar^{-s} < \xi >^{-m+|\alpha|} \left| (\partial_x^a \partial_\xi^\alpha F)(\hbar, \xi, x) \right| < \infty.$$

We refer to [Rob, He2] for a systematic discussion and for more general $\hbar$-symbols. In the frame of these symbol classes, the Moyal product $\sharp_\hbar$ has the following property (see [Rob, He2]):

$$\forall(F,G) \in S_1^{(s_1, m_1)}(\mathcal{X}) \times S_1^{(s_2, m_2)}(\mathcal{X}), \quad F\sharp_\hbar G \in S_1^{(s_1+s_2, m_1+m_2)}(\mathcal{X}) \text{ and}$$

$$F\sharp_\hbar G - FG \in S_1^{(s_1+s_2+1, m_1+m_2-1)}(\mathcal{X}).$$

We shall usually work with elements $F \in S_1^{(s,m)}(\mathcal{X})$ having an asymptotic expansion of the form:

$$F(\hbar, \xi, x) \sim \hbar^s \sum_{k \in \mathbb{N}} \hbar^k F_k(x, \xi), \quad \text{with } F_k \in S_1^{m-k}(\mathcal{X}). \tag{2.2}$$

The symbol $\hbar^s F_0 \in S_1^{(s,m)}(\mathcal{X})$ is then called *the principal symbol of F*.

What is important here is to find a class of functions (actually essentially C_0^∞) such that $g(F)$ is a nice pseudodifferential operator with simple rules of computation for the principal symbol. We are starting from the general Dynkin-Helffer-Sjöstrand formula (see [DiSj])

$$g(P) = -\pi^{-1} \lim_{\epsilon \to 0^+} \iint_{|\mu| \geq \epsilon} \frac{\partial \tilde{g}}{\partial \bar{z}}(\lambda, \mu) \, (\lambda + i\mu - P)^{-1} d\lambda \, d\mu \,, \tag{2.3}$$

which is true for any selfadjoint operator P and any g in $C_0^\infty(\mathbb{R})$.
Here the function $(\lambda, \mu) \mapsto \tilde{g}(\lambda, \mu)$ is a compactly supported, almost analytic extension of g to $\mathbb{C}$. This means that $\tilde{g} = g$ on $\mathbb{R}$ and that for any $N \in \mathbb{N}$ there exists a constant C_N such that $|\frac{\partial \tilde{g}}{\partial \bar{z}}(\lambda, \mu)| \leq C_N |\mu|^N$.
The main result due to Helffer-Robert (see also [DiSj] and references therein) is that, for $P = \mathfrak{Op}_\hbar(F)$ a self-adjoint operator with a 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 a $\hbar$-pseudodifferential operator of the form $\mathfrak{Op}_\hbar(\widetilde{g_\hbar}(F))$, whose Weyl symbol $\widetilde{g_\hbar}(F)(\hbar, \xi, x)$ admits a formal asymptotic expansion in $\hbar$

$$\widetilde{g_\hbar}(F)(\hbar, \xi, x) \sim \sum_{k \geq 0} h^k g_k(F)(x, \xi) \,, \tag{2.4}$$

with

$$\begin{aligned} g_0(F) &= g(F_0) \,, \\ g_1(F) &= F_1 \cdot g'(F_0) \,, \\ g_k(F) &= \sum_{l=1}^{2k-1} d_{k,l} g^{(l)}(F_0) \,, \ \forall k \geq 2 \,, \end{aligned} \tag{2.5}$$

where the $d_{k,l}$ are 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

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

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with

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

$$p_{2,3}(x,\xi) = \frac{1}{24} \sum_{j,k} \left(2\partial^2_{x_k \xi_j} F_0 \cdot \partial_{x_j} F_0 \cdot \partial_{\xi_k} F_0 - \partial^2_{x_j x_k} F_0 \cdot \partial_{\xi_j} F_0 \cdot \partial_{\xi_k} F_0 - \partial^2_{\xi_j \xi_k} F_0 \cdot \partial_{x_j} F_0 \cdot \partial_{x_k} F_0 \right). \tag{2.8}$$

The main point in the proof is that one can construct for $\Im z \neq 0$ a parametrix (= approximate inverse) for $(P - z)$ with a nice control as $\Im z$ tends to 0. The constants controlling the estimates on the symbols are exploding as $\Im z \to 0$ but the choice of the almost analytic extension of f absorbs any negative power of $|\Im z|$.

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

$$F_0^{-1}(I + [-\epsilon_0, \epsilon_0]) \text{ is compact}, \tag{2.9}$$

then the spectrum of $\mathfrak{Op}_\hbar(F_0)$ 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 $\mathfrak{Op}_\hbar(F_0)$ is discrete ($\mathfrak{Op}_\hbar(F_0)$ has compact resolvent). In fact one gets more precisely the following theorem (due to Helffer-Robert).

Theorem 2.1 :
Let $P = \mathfrak{Op}_\hbar(F)$ be a self-adjoint operator with a $\hbar$-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 $C_0^\infty(]E_1, E_2[)$, we have the following expansion in powers of $\hbar$:

$$\mathrm{Tr} \left[g\big(\mathfrak{Op}_\hbar(F)\big) \right] \sim (2\pi\hbar)^{-d} \sum_{j \geq 0} \hbar^j \, T_j(g), \tag{2.10}$$

where $g \mapsto T_j(g)$ are distributions in $\mathcal{D}'(]E_1, E_2[)$.
In particular we have, when $F_1 = F_2 = 0$,

$$\begin{aligned} T_0(g) &= \iint g(F_0(x,\xi)) \, dx \, d\xi, \\ T_1(g) &= 0, \\ T_2(g) &= -\frac{1}{24} \iint g''(F_0(x,\xi)) \sum_{j,k} \left(\frac{\partial^2 F_0}{\partial \xi_j \partial \xi_k} \frac{\partial^2 F_0}{\partial x_j \partial x_k} - \frac{\partial^2 F_0}{\partial x_j \partial \xi_k} \frac{\partial^2 F_0}{\partial \xi_j \partial x_k} \right) dx d\xi. \end{aligned} \tag{2.11}$$

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

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

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

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 ([Ho1], [Ho4] and [Iv]) 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: $g_{s,E}(t) := \max\{0, (E-t)\}^s$ (for some $s \geq 0$ and $E \in (E_1, E_2)$), we shall get a better expansion when s is large.

Under some assumptions on A and V, including the condition $\mathrm{div}\, A = 0$, one can show that $P_A(\hbar)$ is an $\hbar$-pseudodifferential operator whose total Weyl-symbol is $F(x,\xi) = (\xi - A)^2 + V$ in some class of [HR1]. More prcsely, we have to assume that for any $\alpha \in \mathbb{N}^d$, we have

$$|\partial_x^\alpha V(x)| \leq C_\alpha (V(x) + C + 1), \tag{2.13}$$

and, for $j = 1 \dots, d$, the following non gauge covariant conditions:

$$|\partial_x^\alpha A_j(x)| \leq C_\alpha (V(x) + C + 1)^{\frac{1}{2}}. \tag{2.14}$$

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3 The $\hbar$-magnetic quantization

3.1 Results for fixed $\hbar$

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 Ξ

$$\sigma^B_{(x,\xi)}((y,\eta),(\zeta,z)) := \eta(z) - \zeta(y) + B_x(y,z),$$

that may be used to define the classical Hamiltonian system in the given magnetic field. For the quantum description we shall also consider the Hilbert space $\mathcal{H} = L^2(\mathcal{X})$, we shall choose a smooth vector potential A, i.e. a 1-form satisfying the equality $B = dA$ and we shall define the following gauge covariant representation, for all $\phi \in \mathcal{S}(\Xi)$ and all $u \in \mathcal{S}(\Xi)$,

$$\left[\mathfrak{Op}^A_\hbar(\phi)u\right](x) : (2\pi\hbar)^{-d} \int_\mathcal{X} \int_{\mathcal{X}'} dy\, d\eta\, e^{\frac{i}{\hbar}\eta(x-y)} e^{-\frac{i}{\hbar}\int_{[x,y]} A} \phi\left(\frac{x+y}{2},\eta\right) u(y),$$

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 to define a 'magnetic' Moyal product $\sharp^B_\hbar$

$$
\begin{aligned}
\left(\phi \sharp^B_\hbar \psi\right)(X) \quad &:= (\pi\hbar)^{-2d} \int_\Xi dY \int_\Xi dZ \exp\left[-(2i/\hbar)\,\sigma^B_x(Y,Z)\right] \phi(X-Y)\psi(X-Z) \\
&= (\pi\hbar)^{-2d} \int_\Xi dY \int_\Xi dZ\, e^{-(2i/\hbar)\sigma(Y,Z)} e^{-(i/\hbar)\theta^B(x,y,z)} \phi(X-Y)\psi(X-Z) \\
&= (\pi\hbar)^{-2d} \int_\Xi dY \int_\Xi dZ\, e^{-(2i/\hbar)\sigma(X-Y,X-Z)} e^{-(i/\hbar)\widetilde{\theta^B}(x,y,z)} \phi(Y)\psi(Z).
\end{aligned}
\tag{3.1}
$$

$$\theta^B(x,y,z) := \int_{<x-y-z,x+y-z,x-y+z>} B \quad , \quad \widetilde{\theta^B}(x,y,z) := \int_{<x-y+z,y-z+x,z-x+y>} B \quad .$$

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 two form on the given oriented triangle. Associated with this product we can define a 'magnetic' Moyal algebra for the magnetic field B:

$$\mathfrak{M}^B(\Xi) := \left\{ \Phi \in \mathcal{S}'(\Xi) \mid \Phi \sharp^B_\hbar \phi \in \mathcal{S}(\Xi), \phi \sharp^B_\hbar \Phi \in \mathcal{S}(\Xi), \forall \phi \in \mathcal{S}(\Xi) \right\},$$

This 'magnetic' Moyal calculus preserves a large number of the nice features of the usual Moyal calculus and we shall recall some of them that are useful for our analysis of semiclassical trace formulas.

Proposition 3.1 *(Propositions 3.5 and 3.10 in [MP])*
For any magnetic field B with components of class $C^\infty_{\mathsf{pol}}(\mathcal{X})$, one can find a vector potential A with components also of class $C^\infty_{\mathsf{pol}}(\mathcal{X})$ and then the application $\mathfrak{Op}^A_\hbar : \mathcal{S}(\Xi) \to \mathbb{B}(L^2(\mathcal{X}))$ extends to an isomorphism of vector spaces $\mathfrak{Op}^A_\hbar : \mathcal{S}'(\Xi) \to \mathbb{B}(\mathcal{S}(\mathcal{X}); \mathcal{S}'(\mathcal{X}))$. The above isomorphism has a restriction $\mathfrak{Op}^A_\hbar : L^2(\Xi) \to \mathbb{B}_2(L^2(\mathcal{X}))$ 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 [MP] and Lemma 1.2 in [IMP1])*
For any magnetic field B with components of class $C^\infty_{\mathsf{pol}}(\mathcal{X})$, we have the following inclusions:

$$C^\infty_{\mathsf{pol},\mathsf{u}}(\Xi) \subset \mathfrak{M}^B(\Xi); \qquad S^m_1(\mathcal{X}) \subset \mathfrak{M}^B(\Xi).$$

Proposition 3.3 *(Theorem 2.11 in [LMR])*
For any magnetic field B with components of class $BC^\infty(\mathcal{X})$ the 'magnetic' Moyal product defines a continuous map

$$S^{m_1}_1(\mathcal{X}) \times S^{m_2}_1(\mathcal{X}) \ni (F,G) \mapsto F \sharp^B_\hbar G \in S^{m_1+m_2}_1(\mathcal{X}),$$

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

$$F \sharp^B_\hbar G = \sum_{j=0}^{N-1} H_j + R_N, \quad \text{with } H_j \in S^{m_1+m_2-j}_1(\mathcal{X}), R_N \in S^{m_1+m_2-N}_1(\mathcal{X})$$

in which $H_0 = F \cdot G$.

Proposition 3.4 *(Theorem 3.1 in [IMP1])*
For any magnetic field B with components of class $BC^\infty(\mathcal{X})$ we have that for any associated vector potential A,

$$\mathfrak{Op}_\hbar^A\big[S_1^0(\mathcal{X})\big] \subset \mathbb{B}(L^2(\mathcal{X}))$$

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

$$\left\|\mathfrak{Op}_\hbar^A(F)\right\|_{\mathbb{B}(L^2(\mathcal{X}))} \leq c \sup_{|a|\leq p}\big(\sup_{|\alpha|\leq p}\big(\sup_{(x,\xi)\in\Xi} <\xi>^{|\alpha|}\big|\big(\partial_x^a\partial_\xi^\alpha F\big)(x,\xi)\big|\big)\big).$$

Proposition 3.5 *(Theorems 4.1 and 4.3 in [IMP1] and Proposition 6.31 in [IMP2])*
Suppose the magnetic field B is of class $BC^\infty(\mathcal{X})$; then

- *if $F \in S_1^0(\mathcal{X})$ is a real function, $\mathfrak{Op}_\hbar^A(F)$ is a bounded self-adjoint operator on $L^2(\mathcal{X})$ for any vector potential A of B; then the resolvent of $\mathfrak{Op}_\hbar^A(F)$ has a 'magnetic' symbol of class $S_1^0(\mathcal{X})$;*

- *if $F \in S_1^m(\mathcal{X})$ is a real elliptic symbol with $m > 0$, then $\mathfrak{Op}_\hbar^A(F)$ 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 $S_1^{-m}(\mathcal{X})$; if we choose A with components of class $C^\infty_{\mathrm{pol}}(\mathcal{X})$ then $\mathfrak{Op}_\hbar^A(F)$ is essentially self-adjoint on $\mathcal{S}(\mathcal{X})$ and its self-adjoint extension has as domain the 'magnetic' Sobolev space:*

$$\mathcal{H}_m^A(\mathcal{X}) := \Big\{u \in L^2(\mathcal{X}) \mid \mathfrak{Op}_\hbar^A(p_m)u \in L^2(\mathcal{X}), \text{ where } p_m(x,\xi) := <\xi>^m\Big\};$$

- *if $F \in S_1^m(\mathcal{X})$, 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 $u \in \mathcal{H}_\infty^A(\mathcal{X})$ we have*

$$\Re <u, \mathfrak{Op}^A(F)u>_{L^2(\mathcal{X}} \geq C_0\|u\|_{\mathcal{H}_{m/2}^A(\mathcal{X})} - C_1\|u\|_{\mathcal{H}_s^A(\mathcal{X})}.$$

Proposition 3.6 *(Proposition 6.33 in [IMP2])*
Suppose the magnetic field B has components of class $BC^\infty(\mathcal{X})$ and $\Phi \in C_0^\infty(\mathbb{R})$, then, for any real $F \in S_1^m(\mathcal{X})$ with $m \geq 0$, F elliptic for $m > 0$, and for any A such that $dA = B$, the operator $\Phi\big(\mathfrak{Op}_\hbar^A(F)\big)$, defined by the functional calculus for self-adjoint operators has a 'magnetic' symbol of class $S_1^{-m}(\mathcal{X})$.

3.2 Semiclassical results

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

$$\big(\phi\sharp_\hbar^B\psi\big)(X) = (\pi\hbar)^{-2d}\int_\Xi dY\int_\Xi dZ\, e^{-(2i/\hbar)\sigma(Y,Z)}e^{-(i/\hbar)\theta^B(x,y,z)}\phi(X-Y)\psi(X-Z)$$

with

$$\theta^B(x,y,z) := \int_{<x-y-z,x+y-z,x-y+z>} B \qquad = 4\sum_{jk}y_jz_k\int_0^1 ds\int_0^{1-s}dt\, B_{jk}\big(x+(2s-1)y+(2t-1)z\big).$$

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

$$\big(\phi\sharp_\hbar^B\psi\big)(X) \tag{3.2}$$

$$= \pi^{-2d}\int_\Xi dY\int_\Xi dZ\, e^{-2i\sigma(Y,Z)}e^{-(i\hbar)\theta_\hbar^B(x,y,z)}\phi(x-\hbar y,\xi-\eta)\psi(x-\hbar z,\xi-\zeta),$$

with

$$\theta_\hbar^B(x,y,z) = 4\sum_{jk}y_jz_k\int_0^1 ds\int_0^{1-s}dt\, B_{jk}\big(x+(2s-1)\hbar y+(2t-1)\hbar z\big).$$

We notice that we can now obtain an asymptotic expansion of the $\sharp_\hbar^B$-product with respect to $\hbar$ by using the Taylor formulas for ϕ, ψ, like in the non-magnetic case, and for the exponential $e^{-(i\hbar)\theta_\hbar^B(x,y,z)}$ and also for B in the expression of $\theta_\hbar^B(x,y,z)$:

$$\phi(x-\hbar y,\xi-\eta) = \sum_{0\leq\nu\leq N}\frac{(-\hbar)^\nu}{\nu!}\sum_{|\alpha|=\nu}\frac{\nu!}{\alpha!}y^\alpha\big(\partial_x^\alpha\phi\big)(x,\xi-\eta) + \mathfrak{R}_{\phi,N},$$

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$$\psi(x - \hbar z, \xi - \zeta) = \sum_{0 \le \mu \le N} \frac{(-\hbar)^\mu}{\mu!} \sum_{|\beta|=\mu} \frac{\mu!}{\beta!} z^\beta \left(\partial_x^\beta \psi\right)(x, \xi - \zeta) + \mathfrak{R}_{\psi,N},$$

$$e^{-(i\hbar)\theta_\hbar^B(x,y,z)} = \sum_{0 \le \rho \le N} \frac{(-i\hbar)^\rho}{\rho!} \left[\theta_\hbar^B(x,y,z)\right]^\rho + \mathfrak{R}_{B,N},$$

$$\theta_\hbar^B(x,y,z) = \sum_{0 \le \lambda \le N} \frac{\hbar^\lambda}{\lambda!} \left[\sum_{|\gamma|=\lambda} \left(\sum_{jk} y_j z_k \left(\partial^\gamma B_{jk}\right)(x)\right) \frac{\lambda!}{\gamma!} \int_{-1}^1 ds \int_{-1}^{-s} dt (sy+tz)^\gamma\right] + \mathfrak{r}_{B,N}$$

$$= \sum_{0 \le \lambda \le N} \frac{\hbar^\lambda}{\lambda!} \left[\sum_{|\gamma|=\lambda} \sum_{\delta \le \gamma} \boldsymbol{T}_\delta^\gamma \, y^\delta z^{\gamma-\delta} \left(\sum_{jk} y_j z_k \left(\partial^\gamma B_{jk}\right)(x)\right)\right] + \mathfrak{r}_{B,N},$$

where for any $N \ge 1$ in $\mathbb{N}$ we have

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

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

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

$$= \hbar^{N+1} \chi_{N+1}^B(\hbar, x, y, z) \left[\sum_{0 \le \lambda \le N} \frac{\hbar^\lambda}{\lambda!} \left[\sum_{|\gamma|=\lambda} \sum_{\delta \le \gamma} \boldsymbol{T}_\delta^\gamma \, y^\delta z^{\gamma-\delta} \left(\sum_{jk} y_j z_k \left(\partial^\gamma B_{jk}\right)(x)\right)\right] + \mathfrak{r}_{B,N}\right]^{N+1}$$

$$\mathfrak{r}_{B,N}(\hbar, x, y, z) = \hbar^{N+1} \sum_{|\gamma|=N+1} (\gamma!)^{-1} \int_{-1}^1 ds \int_{-1}^{-s} dt \int_0^1 du \sum_{jk} y_j z_k \left(\partial^\gamma B_{jk}\right)\left(x + \hbar u(sy+tz)\right)(sy+tz)^\gamma$$

$$= \hbar^{N+1} \sum_{jk} y_j z_k \sum_{|\gamma|=N+1} (\gamma!)^{-1} F_{\gamma,j,k}^B(\hbar, x, y, z) \sum_{\delta \le \gamma} \boldsymbol{T}_\delta^\gamma \, y^\delta z^{\gamma-\delta}.$$

Let us observe first that the powers y^α and z^β appearing in the Taylor expansions of ϕ and ψ are dealt by integration by parts, using the 'oscillatory' exponential $e^{-2i\sigma(Y,Z)}$ and transformed in ζ-derivatives of ψ and respectively in η-derivatives of ϕ. A similar procedure may be used to get rid of the factors $y^\delta z^\gamma$ appearing in the expansions of $\theta_\hbar^B(x,y,z)^\rho$; in fact we have

$$y^\alpha e^{-2i\sigma(Y,Z)} = (-i/2)^{|\alpha|} \partial_\zeta^\alpha e^{-2i\sigma(Y,Z)}; \qquad z^\beta e^{-2i\sigma(Y,Z)} = (i/2)^{|\beta|} \partial_\eta^\beta e^{-2i\sigma(Y,Z)}.$$

Thus, denoting by

$$\mathfrak{T}_\lambda^B(x) := \sum_{\substack{|\gamma|=\lambda \\ \delta \le \gamma}} \sum_{jk} (-1)^{\lambda-|\delta|} \boldsymbol{T}_\delta^\gamma \left(\partial^\gamma B_{jk}\right)(x) \partial_\zeta^\delta \partial_{\zeta_j} \partial_\eta^{\gamma-\delta} \partial_{\eta_k}, \tag{3.3}$$

one has

$$(\phi \sharp_\hbar^B \psi)(X) = \pi^{-2d} \int_\Xi dY \int_\Xi dZ \, e^{-2i\sigma(Y,Z)} \times$$

$$\times \left\{\sum_{0 \le \rho \le N} \frac{(-i\hbar)^\rho}{\rho!} \left[\sum_{0 \le \lambda \le N} \frac{\hbar^\lambda}{4\lambda!} \left(\frac{i}{2}\right)^\lambda \mathfrak{T}_\lambda^B(x) + \mathfrak{r}_{B,N}\right]^\rho + \mathfrak{R}_{B,N}\right\} \times$$

$$\times \left[\sum_{0 \le \nu \le N} \frac{(-\hbar)^\nu}{\nu!} \sum_{|\alpha|=\nu} \frac{\nu!}{\alpha!} \left((i/2)\partial_\zeta\right)^\alpha \left(\partial_x^\alpha \phi\right)(x, \xi - \eta) + \mathfrak{R}_{\phi,N}\right] \times$$

$$\times \left[\sum_{0 \le \mu \le N} \frac{(-\hbar)^\mu}{\mu!} \sum_{|\beta|=\mu} \frac{\mu!}{\beta!} \left((-i/2)\partial_\eta\right)^\beta \left(\partial_x^\beta \psi\right)(x, \xi - \zeta) + \mathfrak{R}_{\psi,N}\right]$$

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$$= (2\pi)^{-2d} \left\{ \sum_{0 \le \rho \le N} \frac{(-i\hbar)^\rho}{\rho!} \left[\sum_{0 \le \lambda \le N} \frac{\hbar^\lambda}{4\lambda!} \left(\frac{i}{2} \right)^\lambda \mathfrak{T}_\lambda^B(x) \right]^\rho \right\} \times \qquad (3.4)$$

$$\times \left[\sum_{\substack{0 \le \nu \le N \\ 0 \le \mu \le N}} \frac{(i)^{\nu+\mu}(-1)^\mu(\hbar)^{\nu+\mu}}{2^{\nu+\mu}\nu!\mu!} \sum_{\substack{|\alpha|=\nu \\ |\beta|=\mu}} \frac{\nu!}{\alpha!}\frac{\mu!}{\beta!}(\partial_\xi^\beta \partial_x^\alpha \phi)(x,\xi)(\partial_\xi^\alpha \partial_x^\beta \psi)(x,\xi) \right] +$$

$$+\pi^{-2d} \int_\Xi dY \int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \left[\mathfrak{r}_{B,N}(\hbar,x,y,z) \mathfrak{Z}_N^B(\hbar,x,y,z) + \mathfrak{R}_{B,N}(\hbar,x,y,z) \right] \phi(x-\hbar y, \xi-\eta)\psi(x-\hbar z, \xi-\zeta)+$$

$$+\pi^{-2d} \int_\Xi dY \int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \left\{ \sum_{0 \le \rho \le N} \frac{(-i\hbar)^\rho}{\rho!} \left[\sum_{0 \le \lambda \le N} \frac{\hbar^\lambda}{4\lambda!} \left(\frac{i}{2} \right)^\lambda \mathfrak{T}_\lambda^B(x) \right]^\rho \right\} \times$$

$$\times \left[\left(\frac{i}{2} \right)^{N+1} \sum_{|\alpha|=N+1} \left(\widetilde{\mathfrak{R}}_{\phi,N,\alpha}\big(\partial_\zeta^\alpha \psi\big)(x-\hbar z, \xi-\zeta) + (-1)^{N+1}\widetilde{\mathfrak{R}}_{\psi,N,\alpha}\big(\partial_\eta^\alpha \phi\big)(x-\hbar y, \xi-\eta) \right) - \right.$$

$$\left. -(-1)^{N+1} \left(\frac{i}{2} \right)^{2(N+1)} \sum_{|\alpha|=N+1} \sum_{|\beta|=N+1} \big(\partial_\eta^\beta \widetilde{\mathfrak{R}}_{\phi,N,\alpha}\big)(\hbar,x,y,z,\xi,\eta)\big(\partial_\zeta^\alpha \widetilde{\mathfrak{R}}_{\psi,N,\beta}\big)(\hbar,x,y,z,\xi,\zeta) \right]$$

Let us discuss the remainders in the above expansion. First let us consider the factor $\mathfrak{Z}_N^B(\hbar,x,y,z)$.

$$\mathfrak{Z}_N^B(\hbar,x,y,z) = \sum_{1 \le \rho \le N} \frac{(-i\hbar)^\rho}{\rho!} \sum_{0 \le \kappa \le \rho-1} C_\rho^\kappa \mathfrak{r}_{B,N}(\hbar,x,y,z)^{\rho-\kappa} \left[\sum_{0 \le \lambda \le N} \frac{\hbar^\lambda}{4\lambda!} \left(\frac{i}{2} \right)^\lambda \mathfrak{T}_\lambda^B(x) \right]^\kappa$$

and taking into account the differential operators contained in $\mathfrak{T}_\lambda^B(x)$ (see (3.3)) let us compute for $\rho \ge 1$ and $0 \le \kappa \le \rho-1$ one of the terms appearing in the above sum (with $0 \le \lambda_j \le N$ for $1 \le j \le \kappa$)

$$\int_\Xi dY \int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \mathfrak{r}_{B,N}(\hbar,x,y,z)^{\rho-\kappa}\mathfrak{T}_{\lambda_1}^B(x)\cdots\mathfrak{T}_{\lambda_\kappa}^B(x)\phi(x-\hbar y,\xi-\eta)\psi(x-\hbar z,\xi-\zeta)$$

$$= \hbar^{(N+1)(\rho-\kappa)} \int_\Xi dY \int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \left[\sum_{jk} y_j z_k \sum_{|\gamma|=N+1} (\gamma!)^{-1} F_{\gamma,j,k}^B(\hbar,x,y,z) \sum_{\delta \le \gamma} \boldsymbol{T}_\delta^\gamma \; y^\delta z^{\gamma-\delta} \right]^{\rho-\kappa} \times$$

$$\times \mathfrak{T}_{\lambda_1}^B(x)\cdots\mathfrak{T}_{\lambda_\kappa}^B(x)\phi(x-\hbar y,\xi-\eta)\psi(x-\hbar z,\xi-\zeta)$$

$$= \left(\frac{i}{2} \right)^{N+1} \hbar^{(N+1)(\rho-\kappa)} \sum_{|\alpha|=|\beta|=\rho-\kappa} \int_\Xi dY \int_\Xi dZ \; e^{-2i\sigma(Y,Z)} G_{\alpha\beta}^B(\hbar,x,y,z) \times$$

$$\times \sum_{\delta \le \gamma} (-1)^{N+1-|\delta|}\boldsymbol{T}_\delta^\gamma \partial_\zeta^\delta \partial_\eta^{\gamma-\delta}\mathfrak{T}_{\lambda_1}^B(x)\cdots\mathfrak{T}_{\lambda_\kappa}^B(x)\big(\partial_\xi^\beta \phi\big)(x-\hbar y,\xi-\eta)\big(\partial_\xi^\alpha \psi\big)(x-\hbar z,\xi-\zeta) \qquad (3.5)$$

where $G_{\alpha\beta}^B$ is a product of $\rho-\kappa$ functions of class $BC^\infty(\mathcal{X}^3)$ uniformly for $\hbar \in (0,\hbar_0]$, depending only on the derivatives of order $N+1$ of the magnetic field B. Moreover $\partial_\xi^\beta \phi \in S_1^{m_1-|\beta|}(\mathcal{X})$ and $\partial_\xi^\alpha \psi \in S_1^{m_2-|\alpha|}(\mathcal{X})$ uniformly in $\hbar \in (0,\hbar_0]$ so that the integral (3.5) defines an element in $S_1^{(N+1,m_1+m_2-2-(N+1))}(\mathcal{X})$ for any $\rho-\kappa \ge 1$.

Let us consider the second contribution:

$$\int_\Xi dY \int_\Xi dZ \; e^{-2i\sigma(Y,Z)}\mathfrak{R}_{B,N}(\hbar,x,y,z)\phi(x-\hbar y,\xi-\eta)\psi(x-\hbar z,\xi-\zeta) \qquad (3.6)$$

$$= (-i\hbar)^{N+1} \left(\int_0^1 du_1 \ldots \int_0^{u_N} e^{-iu_{N+1}\hbar\theta_\hbar^B(x,y,z))} du_{N+1} \right) \times$$

$$\times \int_\Xi dY \int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \left[\theta_\hbar^B(x,y,z)) \right]^{N+1} \phi(x-\hbar y,\xi-\eta)\psi(x-\hbar z,\xi-\zeta)$$

so that a similar procedure with the one used for (3.5) proves that this integral defines a function of class $S_1^{(N+1,m_1+m_2-2(N+1))}(\mathcal{X})$.

For any $\phi \in S^m(\mathcal{X})$ the rest $\widetilde{\mathfrak{R}}_{\phi,N,\alpha}$ is a function of class $S_1^{(N+1,m-(N+1))}(\mathcal{X})$, $\forall \alpha \in \mathbb{N}^d$ so that it is easy to notice that the last contribution to the rest:

$$+\pi^{-2d} \int_\Xi dY \!\!\int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \left\{ \sum_{0\leq\rho\leq N} \frac{(-i\hbar)^\rho}{\rho!} \left[\sum_{0\leq\lambda\leq N} \frac{\hbar^\lambda}{4\lambda!} \left(\frac{i}{2}\right)^\lambda \mathfrak{T}_\lambda^B(x) \right]^\rho \right\} \times$$

$$\times \left[\left(\frac{i}{2}\right)^{N+1} \sum_{|\alpha|=N+1} \left(\widetilde{\mathfrak{R}}_{\phi,N,\alpha}\big(\partial_\zeta^\alpha \psi\big)(x-\hbar z,\xi-\zeta) + (-1)^{N+1}\widetilde{\mathfrak{R}}_{\psi,N,\alpha}\big(\partial_\eta^\alpha \phi\big)(x-\hbar y,\xi-\eta) \right) - \right.$$

$$\left. -(-1)^{N+1} \left(\frac{i}{2}\right)^{2(N+1)} \sum_{|\alpha|=N+1}\sum_{|\beta|=N+1} \big(\partial_\eta^\beta\widetilde{\mathfrak{R}}_{\phi,N,\alpha}\big)(\hbar,x,y,z,\xi,\eta)\big(\partial_\zeta^\alpha\widetilde{\mathfrak{R}}_{\psi,N,\beta}\big)(\hbar,x,y,z,\xi,\zeta) \right]$$

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 the expansion (3.4):

$$\pi^{-2d} \int_\Xi dY \!\!\int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \left\{ \sum_{0\leq\rho\leq N} \frac{(-i\hbar)^\rho}{\rho!} \left[\sum_{0\leq\lambda\leq N} \frac{\hbar^\lambda}{4\lambda!} \left(\frac{i}{2}\right)^\lambda \mathfrak{T}_\lambda^B(x) \right]^\rho \right\} \times$$

$$\times \left[\sum_{0\leq\nu\leq N} \frac{(-\hbar)^\nu}{\nu!} \sum_{|\alpha|=\nu} \frac{\nu!}{\alpha!} ((i/2)\partial_\zeta)^\alpha \big(\partial_x^\alpha \phi\big)(x,\xi-\eta) \right] \left[\sum_{0\leq\mu\leq N} \frac{(-\hbar)^\mu}{\mu!} \sum_{|\beta|=\mu} \frac{\mu!}{\beta!} ((-i/2)\partial_\eta)^\beta \big(\partial_x^\beta \psi\big)(x,\xi-\zeta) \right]$$

$$= \pi^{-2d} \int_\Xi dY \!\!\int_\Xi dZ \; e^{-2i\sigma(Y,Z)} \left\{ \sum_{0\leq\rho\leq N} \frac{(-i\hbar)^\rho}{4^\rho\rho!} \sum_{\substack{\{\lambda_1,\dots,\lambda_\rho\}\\ 0\leq\lambda_j\leq\rho\\ 1\leq j\leq\rho}} \left(\frac{i\hbar}{2}\right)^{\lambda_1+\dots+\lambda_\rho} \frac{1}{\lambda_1!\cdots\lambda_\rho!} \mathfrak{T}_{\lambda_1}^B(x)\cdots\mathfrak{T}_{\lambda_\rho}^B(x) \right\} \times$$

$$\times \sum_{\substack{0\leq\nu\leq N\\ 0\leq\mu\leq N}} (-1)^\mu \left(\frac{i\hbar}{2}\right)^{\nu+\mu} \sum_{\substack{|\alpha|=\nu\\ |\beta|=\mu}} \left[\frac{1}{\alpha!\beta!} \big(\partial_\xi^\beta\partial_x^\alpha\phi\big)(x,\xi-\eta)\big(\partial_\xi^\alpha\partial_x^\beta\psi\big)(x,\xi-\zeta) \right]$$

$$= \sum_{0\leq k\leq N} \hbar^k \sum_{\substack{l_1+l_2+l=k\\ 0\leq l_1\leq k\\ 0\leq l_2\leq k\\ 0\leq l\leq k}} \sum_{\substack{\rho+\lambda_1+\dots+\lambda_\rho=l\\ 0\leq\rho\leq l\\ 0\leq\lambda_j\leq l\\ 1\leq j\leq\rho}} \frac{(-1)^{\rho+l_2}i^\rho}{4^\rho\rho!} \sum_{\substack{|\alpha|=l_1\\ |\beta|=l_2}} \left(\frac{i}{2}\right)^{l_1+l_2+\lambda_1+\dots+\lambda_\rho} \frac{1}{\alpha!\beta!} \times \qquad (3.7)$$

$$\times \sum_{\substack{|\gamma_1|=\lambda_1\\ \delta_1\leq\gamma_1}} \cdots \sum_{\substack{|\gamma_\rho|=\lambda_\rho\\ \delta_\rho\leq\gamma_\rho}} (-1)^{|\delta_1|+\dots+|\delta_\rho|} T_{\delta_1}^{\gamma_1}\cdots T_{\delta_\rho}^{\gamma_\rho} \big(\partial^{\gamma_1} B_{j_1 k_1}\big)(x)\cdots\big(\partial^{\gamma_\rho} B_{j_\rho k_\rho}\big)(x) \times$$

$$\times \left(\partial_{\xi_{k_1}}\cdots\partial_{\xi_{k_\rho}} \partial_\xi^{\beta+\gamma_1-\delta_1+\dots+\gamma_\rho-\delta_\rho}\partial_x^\alpha\phi \right)(x,\xi) \left(\partial_{\xi_{j_1}}\cdots\partial_{\xi_{j_\rho}} \partial_\xi^{\alpha+\delta_1+\dots+\delta_\rho}\partial_x^\beta\psi \right)(x,\xi) \;+\; R_N(\hbar;\phi,\psi)(x,\xi),$$

where $R_N \in S_1^{(N+1,m_1+m_2-(N+1))}(\mathcal{X})$.

Using these expansions one gets the following statement.

Proposition 3.7
If the magnetic field B has components of class $BC^\infty(\mathcal{X})$ and $\phi \in S_1^{m_1}(\mathcal{X})$, $\psi \in S_1^{m_2}(\mathcal{X})$ then there exists a sequence $\{\mathfrak{c}_k^B(\phi,\psi)\}_{k\in\mathbb{N}}$ such that $\mathfrak{c}_k^B(\phi,\psi) \in S_1^{m_1+m_2-k}(\mathcal{X})$ and, for any $N \geq 1$ in $\mathbb{N}$, we have:

$$\hbar^{-N}\left(\phi \sharp_\hbar^B \psi - \sum_{k=0}^{N-1} \hbar^k \mathfrak{c}_k^B(\phi,\psi) \right) \in S_1^{m_1+m_2-N}(\mathcal{X})$$

uniformly for $\hbar \in \mathcal{I}$. For $k=0$, we have $\mathfrak{c}_0^B(\phi,\psi) = \phi\cdot\psi$. Moreover, for any $k \in \mathbb{N}$, the function $\mathfrak{c}_k^B(\phi,\psi;X)$ only depends on values of the magnetic field B and its derivatives of order $\leq j-1$ evaluated at x.

We shall use the notation

$$\gamma_\hbar^B(\phi, \psi) := \phi \sharp_\hbar^B \psi - \phi \cdot \psi = \sum_{k=1}^{N-1} \hbar^k \mathfrak{c}_k^B(\phi, \psi) + \hbar^N \mathfrak{t}_N^B(\phi, \psi), \tag{3.8}$$

with $\mathfrak{t}_N^B(\phi, \psi) \in S_1^{(0, m_1 + m_2 - N)}(\mathcal{X})$.

Starting from the above result we shall work in the sequel with functions of class $S_1^{(s,m)}(\mathcal{X})$, thus admitting asymptotic expansions in $\hbar \in \mathcal{I}$ of the form given in the above proposition.

4 The magnetic Schrödinger operator

4.1 Preliminaries

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

$$P^A(\hbar) = \mathfrak{Op}_\hbar^A(\xi^2 + V), . \tag{4.1}$$

We shall suppose that the magnetic field has components of class $BC^\infty(\mathcal{X})$, that the vector potential has been chosen of class $C_{\mathsf{pol}}^\infty(\mathcal{X})$ and that V is a real $BC^\infty(\mathcal{X})$ function. Hence $F := \xi^2 + V \in S_1^2(\mathcal{X})$ 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 $P_0^A(\hbar) := \mathfrak{Op}_\hbar^A(\xi^2)$ and the Neumann series expansion of the resolvent) :

Proposition 4.1

1. $P^A(\hbar)$ defined in (4.1) is essentially self-adjoint on $\mathcal{S}(\mathcal{X})$ and its self-adjoint extension, denoted H, has the domain $\mathcal{H}_2^A(\mathcal{X})$.

2. The resolvent $(H - \mathfrak{z})^{-1}$ is well defined for $\mathfrak{z} \in \mathbb{C} \setminus \{\mathfrak{r} \in \mathbb{R} \mid \mathfrak{r} \geq \mathfrak{a}\}$ for some $\mathfrak{a} \in \mathbb{R}$ and has the form $(H - \mathfrak{z})^{-1} = \mathfrak{Op}_\hbar^A(r_\mathfrak{z}^B)$ with $r_\mathfrak{z}^B \in S_1^{(0,-2)}(\mathcal{X})$.

3. There exists $\mathfrak{a}_0 \geq \mathfrak{a}$ depending on B and V such that $\sigma_{\mathsf{ess}}(H) \subset [\mathfrak{a}_0, \infty)$.

4.2 The resolvent

We shall concentrate now on the asymptotic expansion of the symbol $r_\mathfrak{z}^B \in S_1^{(0,-2)}(\mathcal{X})$ with respect to $\hbar \in \mathcal{I}$. In fact, as the case witout magnetic field is well-known, we shall only be interested in the 'magnetic' contribution to the terms of the $\hbar$-asymptotic expansion, specifically in putting them in a manifestly gauge invariant form. For this purpose we shall use our parametrix type construction of [MPR] in order to express $r_\mathfrak{z}^B$ in terms of $(F - \mathfrak{z})^{-1}$. In fact we know that $(F - \mathfrak{z}) \sharp_\hbar^B r_\mathfrak{z}^B = 1$. In order to shorten our notations we shall denote by $p_\mathfrak{z} := F - \mathfrak{z}$. Let us compute

$$p_\mathfrak{z} \sharp_\hbar^B p_\mathfrak{z}^{-1} = 1 + \gamma_\hbar^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) = 1 + \sum_{k=1}^{N-1} \hbar^k \mathfrak{c}_k^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + \hbar^N \mathfrak{t}_N^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})$$

with $\mathfrak{c}_k^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) \in S_1^{-j}(\mathcal{X})$ and $\mathfrak{t}_N^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) \in S_1^{(0,-N)}(\mathcal{X})$. Thus

$$r_\mathfrak{z}^B = p_\mathfrak{z}^{-1} - r_\mathfrak{z}^B \sharp_\hbar^B \gamma_\hbar^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})$$

$$= \sum_{0 \leq j \leq M-1} (-1)^j p_\mathfrak{z}^{-1} \sharp_\hbar^B \gamma_\hbar^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})^{\sharp_\hbar^B j} + (-1)^M r_\mathfrak{z}^B \sharp_\hbar^B \gamma_\hbar^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})^{\sharp_\hbar^B M} \tag{4.2}$$

$$= \sum_{0 \leq j \leq M-1} (-1)^j p_\mathfrak{z}^{-1} \sharp_\hbar^B \left[\sum_{k=1}^{N_1-1} \hbar^k \mathfrak{c}_k^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + \hbar^{N_1} \mathfrak{t}_{N_1}^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) \right]^{\sharp_\hbar^B j} +$$

$$+ (-1)^M r_\mathfrak{z}^B \sharp_\hbar^B \left[\sum_{k=1}^{N_2-1} \hbar^k \mathfrak{c}_k^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + \hbar^{N_2} \mathfrak{t}_{N_2}^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) \right]^{\sharp_\hbar^B M} .$$

Let us first study the corrections $\mathfrak{c}_k^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})$. We use the general formulae (3.8), (3.7) and obtain:

$$\mathfrak{c}_k^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) = (2\pi)^{-2d} \sum_{\substack{l_1+l_2+l=k \\ 0 \leq l_1 \leq k \\ 0 \leq l_2 \leq k \\ 0 \leq l \leq k}} \sum_{\substack{\rho+\lambda_1+\ldots+\lambda_\rho=l \\ 0 \leq \rho \leq l \\ 0 \leq \lambda_j \leq l \\ 1 \leq j \leq \rho}} \frac{(-1)^{\rho+l_2} i^\rho}{4^\rho \rho!} \sum_{\substack{|\alpha|=l_1 \\ |\beta|=l_2}} \left(\frac{i}{2}\right)^{l_1+l_2+\lambda_1+\ldots+\lambda_\rho} \frac{1}{\alpha!\beta!} \times$$

$$\times \sum_{\substack{|\gamma_1|=\lambda_1 \\ \delta_1 \leq \gamma_1}} \cdots \sum_{\substack{|\gamma_\rho|=\lambda_\rho \\ \delta_\rho \leq \gamma_\rho}} (-1)^{|\delta_1|+\ldots+|\delta_\rho|} T_{\delta_1}^{\gamma_1} \cdots T_{\delta_\rho}^{\gamma_\rho} \left(\partial^{\gamma_1} B_{j_1 k_1}\right)(x) \cdots \left(\partial^{\gamma_\rho} B_{j_\rho k_\rho}\right)(x) \times$$

$$\times \left(\partial_{\xi_{k_1}} \cdots \partial_{\xi_{k_\rho}} \partial_\xi^{\beta+\gamma_1-\delta_1+\ldots+\gamma_\rho-\delta_\rho} \partial_x^\alpha p_\mathfrak{z}\right)(x,\xi) \left(\partial_{\xi_{j_1}} \cdots \partial_{\xi_{j_\rho}} \partial_\xi^{\alpha+\delta_1+\ldots+\delta_\rho} \partial_x^\beta (p_\mathfrak{z}^{-1})\right)(x,\xi).$$

An important observation is that all the derivatives of the symbols $p_\mathfrak{z}$ and $p_\mathfrak{z}^{-1}$ have a very special dependence on $\mathfrak{z}$. More precisely we have:

- $\left(\partial_x^\alpha p_\mathfrak{z}\right)(x,\xi) = \left(\partial_x^\alpha F\right)(x,\xi) = \left(\partial_x^\alpha V\right)(x)$;

- $\left(\partial_{\xi_j} p_\mathfrak{z}\right)(x,\xi) = \left(\partial_{\xi_j} F\right)(x,\xi) = 2\xi_j$; $\quad \left(\partial_{\xi_j}\partial_{\xi_k} p_\mathfrak{z}\right)(x,\xi) = 2\delta_{jk}$; $\quad \left(\partial_\xi^\alpha p_\mathfrak{z}\right)(x,\xi) = 0$, $\quad \forall |\alpha| \geq 3$;

- $\left(\partial_x^\alpha \partial_\xi^\beta p_\mathfrak{z}\right)(x,\xi) = 0$, $\quad$ for $|\alpha| \geq 1, |\beta| \geq 1$.

Lemma 4.2 *For any multiindices α and β we have that:*

$$\left(\partial_x^\alpha \partial_\xi^\beta p_\mathfrak{z}\right)(x,\xi) = \sum_{0 \leq k \leq |\alpha|+|\beta|} \mathfrak{q}_k(x,\xi) p_\mathfrak{z}^{-1-k}(x,\xi)$$

where $\mathfrak{q}_k(x,\xi)$ are polynomials of degree at most k in ξ with coefficients functions of x depending only on the first $|\alpha|$ derivatives of $V(x)$.

Proof.
In fact we have:
$\left(\partial_{x_j} p_\mathfrak{z}^{-1}\right)(x,\xi) = -p_\mathfrak{z}^{-2}(x,\xi)\left(\partial_{x_j} F\right)(x,\xi) = -p_\mathfrak{z}^{-2}(x,\xi)\left(\partial_{x_j} V\right)(x)$;
$\left(\partial_{\xi_j} p_\mathfrak{z}^{-1}\right)(x,\xi) = -p_\mathfrak{z}^{-2}(x,\xi)\left(\partial_{\xi_j} F\right)(x,\xi) = -2\xi_j p_\mathfrak{z}^{-2}(x,\xi)$.
Thus the statement of the Lemma is true for $|\alpha|+|\beta|=1$ and we shall proceed by induction on $|\alpha|+|\beta|$. Suppose the statement has been proved for $|\alpha|+|\beta|=N$ and let us compute the next derivatives.

$$\left(\partial_{x_j}\partial_x^\alpha \partial_\xi^\beta p_\mathfrak{z}\right)(x,\xi) = \partial_{x_j}\left[\sum_{0 \leq k \leq N} \mathfrak{q}_k p_\mathfrak{z}^{-1-k}\right](x,\xi)$$

$$= \sum_{0 \leq k \leq N} \left(\partial_{x_j}\mathfrak{q}_k\right)(x,\xi) p_\mathfrak{z}^{-1-k}(x,\xi) - (1+k) \sum_{0 \leq k \leq N} \mathfrak{q}_k(x,\xi)\left(\partial_{x_j} p_\mathfrak{z}\right)(x,\xi) p_\mathfrak{z}^{-1-(k+1)}(x,\xi)$$

$$= \sum_{0 \leq k \leq N} \left[\left(\partial_{x_j}\mathfrak{q}_k\right)(x,\xi) - k\mathfrak{q}_{k-1}(x,\xi)\left(\partial_{x_j} V\right)(x)\right] p_\mathfrak{z}^{-1-k}(x,\xi) - (1+N)\mathfrak{q}_N(x,\xi)\left(\partial_{x_j} V\right)(x) p_\mathfrak{z}^{-1-(N+1)}(x,\xi);$$

$$\left(\partial_{\xi_j}\partial_x^\alpha \partial_\xi^\beta p_\mathfrak{z}\right)(x,\xi) = \partial_{\xi_j}\left[\sum_{0 \leq k \leq N} \mathfrak{q}_k p_\mathfrak{z}^{-1-k}\right](x,\xi)$$

$$= \sum_{0 \leq k \leq N} \left(\partial_{\xi_j}\mathfrak{q}_k\right)(x,\xi) p_\mathfrak{z}^{-1-k}(x,\xi) - (1+k) \sum_{0 \leq k \leq N} \mathfrak{q}_k(x,\xi)\left(\partial_{\xi_j} p_\mathfrak{z}\right)(x,\xi) p_\mathfrak{z}^{-1-(k+1)}(x,\xi)$$

$$= \sum_{0 \leq k \leq N} \left[\left(\partial_{\xi_j}\mathfrak{q}_k\right)(x,\xi) - 2k\xi_j \mathfrak{q}_{k-1}(x,\xi)\right] p_\mathfrak{z}^{-1-k}(x,\xi) - 2(1+N)\xi_j\mathfrak{q}_N(x,\xi) p_\mathfrak{z}^{-1-(N+1)}(x,\xi).$$

Thus the formula is valid also for $|\alpha|+|\beta|=N+1$ with coefficients having obviously the same structure. $\blacksquare$

Remark 4.3 *Some simple computation proves that:*

$$\mathfrak{c}_1^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1}) = 0,$$

$$\mathfrak{c}_2^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1}) = \frac{1}{2}p_{\mathfrak{z}}^{-2}(x,\xi)\big(\Delta V\big)(x) - \frac{1}{2}p_{\mathfrak{z}}^{-3}(x,\xi)\big|(\nabla V)(x)\big|^2 -$$

$$- 2p_{\mathfrak{z}}^{-3}(x,\xi)\sum_{lm}\left(1 - \frac{1}{2}\delta_{lm}\right)\big(\partial_{x_l}\partial_{x_m}V\big)(x)\xi_l\xi_m +$$

$$+ \frac{1}{2}p_{\mathfrak{z}}^{-2}(x,\xi)\,|B(x)|^2 - 2p_{\mathfrak{z}}^{-3}(x,\xi)\sum_{jkm}B_{jk}(x)B_{jm}(x)\xi_k\xi_m + \frac{2}{3}p_{\mathfrak{z}}^{-2}(x,\xi)\sum_{jk}\big(\partial_j B_{jk}\big)(x)\xi_k -$$

$$- 2p_{\mathfrak{z}}^{-3}(x,\xi)\sum_{jk}B_{jk}(x)\xi_k\big(\partial_{x_j}V\big)(x).$$

Developing successively each $\sharp_\hbar^B$-product in (4.2) and using Proposition 3.7, one gets the following statement.

Proposition 4.4
The 'magnetic' symbol $r_{\mathfrak{z}}^B$ admits for any $N \in \mathbb{N}$ an asymptotic expansion in $\hbar$ of the form

$$r_{\mathfrak{z}}^B(X) = p_{\mathfrak{z}}^{-1} + \sum_{1 \le j \le N-1}\hbar^j\mathfrak{r}_j^B(\mathfrak{z}; X) + \hbar^N\widetilde{\mathfrak{r}_N^B}(\mathfrak{z}; \hbar, X)$$

where the terms $\mathfrak{r}_j^B(\mathfrak{z}; X)$ only depend on the magnetic field B and its derivatives up to order $j-1$ evaluated at X, and the rest $\widetilde{\mathfrak{r}_N^B}(\mathfrak{z}; \hbar, X)$ only depends on the magnetic field B (in a non-local way). Moreover $\mathfrak{r}_j^B(\mathfrak{z}) \in S_1^{-j}(\mathcal{X})$ and $\widetilde{\mathfrak{r}_N^B}(\mathfrak{z}) \in S_1^{(0,-N)}(\mathcal{X})$.

Considering (4.2) we obtain the following expansion of $r_{\mathfrak{z}}^B$ in powers of $\hbar$

$$r_{\mathfrak{z}}^B \sim p_{\mathfrak{z}}^{-1} + \sum_{1 \le j}\hbar^j\sum_{1 \le k \le j}(-1)^k\sum_{\substack{\lambda_1 + \ldots + \lambda_k = j \\ 1 \le \lambda_l \le j \\ 1 \le l \le k}}p_{\mathfrak{z}}^{-1}\sharp_\hbar^B\mathfrak{c}_{\lambda_1}^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1})\sharp_\hbar^B \cdots \sharp_\hbar^B\mathfrak{c}_{\lambda_k}^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1}) \tag{4.3}$$

and developing further each $\hbar$-dependent $\sharp_\hbar^B$-product, one has

$$r_{\mathfrak{z}}^B \sim p_{\mathfrak{z}}^{-1} + \sum_{1 \le j}\sum_{1 \le k \le j}(-1)^k\sum_{\substack{\lambda_1 + \ldots + \lambda_k = j \\ 1 \le \lambda_l \le j \\ 1 \le l \le k}}\sum_{\substack{0 \le \mu_l \\ 1 \le l \le k}}\hbar^{j+\mu_1+\ldots+\mu_k}\mathfrak{C}_{\mu_k,\ldots\mu_1}^B\big(p_{\mathfrak{z}}^{-1}, \mathfrak{c}_{\lambda_1}^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1}), \ldots, \mathfrak{c}_{\lambda_k}^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1})\big)$$

$$= p_{\mathfrak{z}}^{-1} + \sum_{1 \le n}\hbar^n\sum_{1 \le j \le n}\sum_{1 \le k \le j}(-1)^k\sum_{\substack{\lambda_1 + \ldots + \lambda_k = j \\ 1 \le \lambda_l \le j \\ 1 \le l \le k}}\sum_{\substack{j + \mu_1 + \ldots + \mu_k = n \\ 0 \le \mu_l \\ 1 \le l \le k}}\mathfrak{C}_{\mu_k,\ldots\mu_1}^B\big(p_{\mathfrak{z}}^{-1}, \mathfrak{c}_{\lambda_1}^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1}), \ldots, \mathfrak{c}_{\lambda_k}^B(p_{\mathfrak{z}}, p_{\mathfrak{z}}^{-1})\big)$$

where

$$\mathfrak{C}_{\mu_k,\ldots\mu_1}^B\big(f, g_1, \ldots, g_k\big) := \mathfrak{c}_{\mu_k}^B(\mathfrak{c}_{\mu_{k-1}}^B(\ldots\mathfrak{c}_{\mu_1}^B(f, g_1), g_2), \ldots, g_k)$$

Putting together all these formulae we conclude that:

Proposition 4.5
Each term $\mathfrak{r}_j^B(\mathfrak{z})$ for $j \ge 1$ is a finite sum of the form

$$\mathfrak{r}_j^B(\mathfrak{z}) = \sum_{0 \le p \le j}\mathfrak{f}_p^B(x,\xi)p_{\mathfrak{z}}^{-2-p}(x,\xi)$$

where $\mathfrak{f}_p^B(x,\xi)$ are polynomials in ξ of degree at most p whose coefficients are C^∞ 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:*

$\mathfrak{r}_0^B(\mathfrak{z}) = p_\mathfrak{z}^{-1}$;

$\mathfrak{r}_1^B(\mathfrak{z}) = -p_\mathfrak{z}^{-1}\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) = 0$;

$$
\begin{aligned}
\mathfrak{r}_2^B(\mathfrak{z}) &= -p_\mathfrak{z}^{-1}\mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + p_\mathfrak{z}^{-1}\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) - \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) \\
&= -p_\mathfrak{z}^{-1}\mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) \\
&= -\tfrac{1}{2}p_\mathfrak{z}^{-3}(x,\xi)\left(\Delta V\right)(x) + \tfrac{1}{2}p_\mathfrak{z}^{-4}(x,\xi)\left|(\nabla V)(x)\right|^2 \\
&\quad + 2p_\mathfrak{z}^{-4}(x,\xi)\sum_{lm}\left(1 - \tfrac{1}{2}\delta_{lm}\right)\left(\partial_{x_l}\partial_{x_m}V\right)(x)\xi_l\xi_m \\
&\quad - \tfrac{1}{2}p_\mathfrak{z}^{-3}(x,\xi)\left|B(x)\right|^2 + 2p_\mathfrak{z}^{-4}(x,\xi)\sum_{jkm}B_{jk}(x)B_{jm}(x)\xi_k\xi_m - \tfrac{2}{3}p_\mathfrak{z}^{-3}(x,\xi)\sum_{jk}\left(\partial_j B_{jk}\right)(x)\xi_k \\
&\quad + 2p_\mathfrak{z}^{-4}(x,\xi)\sum_{jk}B_{jk}(x)\xi_k\left(\partial_{x_j}V\right)(x);
\end{aligned}
$$

$$
\begin{aligned}
\mathfrak{r}_3^B(\mathfrak{z}) &= -p_\mathfrak{z}^{-1}\mathfrak{c}_3^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + 2p_\mathfrak{z}^{-1}\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) - p_\mathfrak{z}^{-1}\left[\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^3 + p_\mathfrak{z}^{-1}\mathfrak{c}_1^B\left(\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}), \mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) \\
&\quad - \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) - \mathfrak{c}_2^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) + \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \left[\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^2\right) \\
&= -p_\mathfrak{z}^{-1}\mathfrak{c}_3^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) - \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right);
\end{aligned}
$$

$$
\begin{aligned}
\mathfrak{r}_4^B(\mathfrak{z}) &= -p_\mathfrak{z}^{-1}\mathfrak{c}_4^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + 2p_\mathfrak{z}^{-1}\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\mathfrak{c}_3^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + p_\mathfrak{z}^{-1}\left[\mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^2 - 3p_\mathfrak{z}^{-1}\left[\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^2\mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) \\
&\quad + p_\mathfrak{z}^{-1}\left[\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^4 - \mathfrak{c}_3^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) - \mathfrak{c}_2^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) \\
&\quad + 2\mathfrak{c}_2^B\left(p_\mathfrak{z}^{-1}, \left[\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^2\right) - \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_3^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) \\
&\quad + 2\mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) - \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \left[\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^3\right) + \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_1^B\left(\mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}), \mathfrak{c}_1^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right)\right) \\
&= -p_\mathfrak{z}^{-1}\mathfrak{c}_4^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1}) + p_\mathfrak{z}^{-1}\left[\mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right]^2 - \mathfrak{c}_2^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_2^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right) - \mathfrak{c}_1^B\left(p_\mathfrak{z}^{-1}, \mathfrak{c}_3^B(p_\mathfrak{z}, p_\mathfrak{z}^{-1})\right).
\end{aligned}
$$

4.3 The functional calculus with the magnetic Schrödinger operator

Using the results recalled in Section 3 we conclude that for any function $g \in C_0^\infty(\mathbb{R})$, we can define by the functional calculus for self-adjoint operators a bounded operator $g(H)$ that can be computed using Formula (2.3). Then, using the fact that $(H - \mathfrak{z})^{-1} = \mathfrak{Op}_\hbar^A(r_\mathfrak{z}^B)$, we conclude that we can compute directly the symbol of $g(H) =: \mathfrak{Op}_\hbar^A(\widetilde{g(F)}_\hbar^B)$,

$$
\widetilde{g(F)}_\hbar^B(X) = -\pi^{-1}\lim_{\epsilon \to 0^+}\iint_{|\mu| \geq \epsilon}\frac{\partial\tilde{g}}{\partial\bar{z}}(\lambda, \mu)\, r_{\lambda+i\mu}^B(X)d\lambda\,d\mu, \quad \forall X \in \Xi, \tag{4.4}
$$

defining a function of class $S_1^{(0,-2)}(\mathcal{X})$. Using our previous Proposition 4.4 we obtain:

Proposition 4.7
The 'magnetic' symbol $\widetilde{g(F)}_\hbar^B$ admits for any $K \in \mathbb{N}$ an asymptotic expansion in $\hbar$ of the form

$$
\widetilde{g(F)}_\hbar^B(X) = \sum_{0 \leq j \leq K-1}\hbar^j g_j^B[F](X) + \hbar^K\widetilde{g_K^B}[F](\hbar, X)
$$

where the terms $g_j^B[F](X)$ only depend on the magnetic field B and its derivatives up to order $j-1$ evaluated at X, and the rest $\widetilde{g_K^B}[F](\hbar, X)$ only depends on the magnetic field B (in a non-local way). Moreover $g_j^B[F] \in S_1^{-j}(\mathcal{X})$ and $\widetilde{g_K^B}[F] \in S_1^{(0,-K)}(\mathcal{X})$.

Let us consider a function $g \in C_0^\infty(\mathbb{R})$ such that its support Σ_g is contained in $]-\infty, \mathfrak{a}_0[$. As the spectrum of H is discrete in this region, and Σ_g is a compact subset of $]-\infty, \mathfrak{a}_0[$, we deduce that $g(H)$ is finite rank and thus trace-class. Moreover, $g(H) = \mathfrak{Op}^A(\widetilde{g(F)}_\hbar^B)$ is an integral operator having the integral kernel (see [MP])

$$
K^A[g(H)](x, y) := \left(e^{-\frac{i}{\hbar}\int_{[x,y]}A}\right)\mathfrak{F}^-\left[\widetilde{g(F)}_\hbar^B\right]\left(\frac{x+y}{2}, x-y\right)
$$

with $\mathfrak{F}^-$ the inverse Fourier transform in the second variable (as defined on distributions on $\Xi = \mathcal{X} \times \mathcal{X}'$). In order to study the regularity properties of this integral kernel we shall use our formula (4.4) and write that

$$
r_{\lambda+i\mu}^B(X) = (F - (\lambda + i\mu))^{-1}(X) + \mathfrak{X}_{\lambda+i\mu}^B(X)
$$

where

$$
-\pi^{-1}\lim_{\epsilon \to 0^+}\iint_{|\mu| \geq \epsilon}\frac{\partial\tilde{g}}{\partial\bar{z}}(\lambda, \mu)\,(F - (\lambda + i\mu))^{-1}d\lambda\,d\mu = (g \circ F) \in C_0^\infty(\Xi)
$$

and

$$
\mathfrak{X}_{\lambda+i\mu}^B = r_{\lambda+i\mu}^B - (F - (\lambda + i\mu))^{-1} = r_{\lambda+i\mu}^B\sharp_\hbar^B\left(1 - (F - (\lambda + i\mu))\sharp_\hbar^B(F - (\lambda + i\mu))^{-1}\right) \in S_1^{-2-2}(\mathcal{X})
$$

due to our Proposition 3.3 applied to $1 - (F - (\lambda + i\mu)) \sharp_\hbar^B (F - (\lambda + i\mu))^{-1}$. Let us remark that in 2 or 3 dimensions, $\mathfrak{F}^- S_1^{-4}(\mathcal{X})$ 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 $T \in \mathbb{B}_1(L^2(\mathcal{X}))$ *has an integral kernel* $K[T] \in C(\mathcal{X} \times \mathcal{X})$. *Then the following limit exists and we have the equality*

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

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.

$$\widetilde{g(F)}_\hbar^B(X) = -\pi^{-1} \lim_{\epsilon \to 0^+} \iint_{|\mu| \geq \epsilon} \frac{\partial \tilde{g}}{\partial \bar{z}}(\lambda, \mu) \, r_{\lambda + i\mu}^B(X) d\lambda \, d\mu$$

$$= -\pi^{-1} \lim_{\epsilon \to 0^+} \iint_{|\mu| \geq \epsilon} \frac{\partial \tilde{g}}{\partial \bar{z}}(\lambda, \mu) \left[\sum_{0 \leq j \leq N-1} \hbar^j \mathfrak{r}_j^B(\lambda + i\mu; X) + \hbar^N \widetilde{\mathfrak{r}_N^B}(\lambda + i\mu; \hbar, X) \right]. \tag{4.5}$$

Taking now $N > d$ and taking into account Proposition 4.4 we conclude that $\widetilde{\mathfrak{r}_N^B}(\lambda + i\mu; \hbar) \in S_1^{(0, -N)}$ and by the Riemann-Lebesgue Lemma it has a continuous Fourier transform (with respect to the ξ variable). Let us consider the main terms in the expansion (4.5) for $N > d$. Taking into account Proposition 4.5 we have to study integrals of the form

$$\lim_{\epsilon \to 0^+} \iint_{|\mu| \geq \epsilon} \frac{\partial \tilde{g}}{\partial \bar{z}}(\lambda, \mu) \, \mathfrak{f}_p^B(x, \xi) p_{\lambda + i\mu}^{-2-p}(x, \xi) = \mathfrak{f}_p^B(x, \xi) \frac{1}{(2 + p - 1)!} \lim_{\epsilon \to 0^+} \iint_{|\mu| \geq \epsilon} \frac{\partial \tilde{g}}{\partial \bar{z}}(\lambda, \mu) \big(\partial_\lambda^{p+1} p_{\lambda + i\mu}^{-1} \big)(x, \xi)$$

$$= \frac{(-1)^{p+1}}{(2 + p - 1)!} \mathfrak{f}_p^B(x, \xi) \big[\big(\partial_\lambda^{p+1} g \big) \circ F \big](x, \xi).$$

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

Proposition 4.9
For B *a magnetic field with components of class* $BC^\infty(\mathcal{X})$ *and* H *the self-adjoint operator defined in Proposition 4.1, if* $g \in C_0^\infty(\mathbb{R})$ *has compact support* $\Sigma_g \subset (-\infty, \mathfrak{a}_0)$, *then* $g(H)$ *is a trace-class operator*[1] *and we have the formula*

$$\operatorname{Tr} g(H) = \int_{\mathcal{X}} dx \, \mathfrak{F}^- \left[\widetilde{g(F)}_\hbar^B \right](x, 0) = \int_\Xi dX \, \widetilde{g(F)}_\hbar^B(x, \xi),$$

so that $\operatorname{Tr} g(H)$ *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 come back more in detail at the remark in [HMR] that due to the exponential decay of the eigenfunctions (Agmon estimates [Ag]) one can modify the potential outside a compact region by polynomially bounded terms with only an exponentially small change (of order $\exp\{-c/\hbar\}$) in the eigenvalues situated in any compact part of the discrete spectrum. A simple inspection of the proof in [Ag] shows that the same exponential decay estimates can be obtained for the magnetic Schrödinger operator so that we can apply the same arguments from [HMR] to our 'magnetic' situation. Here is the basic proposition.

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

- $E < \min(\Sigma_V, \Sigma_{\widehat{V}})$,

- $U_E := V^{-1}(] - \infty, E[) = \widehat{V}^{-1}(] - \infty, E[)$,

---

[1] In fact it is even finite-rank.

- $V = \widehat{V}$ on U_E and $A = \widehat{A}$ on U_E,

and let H and $\widehat{H}$ the corresponding magnetic Schrödinger operators. Then for any $g \in C_0^\infty(\mathbb{R})$, such that $\operatorname{supp} g \subset]-\infty, E[$, then $\operatorname{Tr} g(H)$ and $\operatorname{Tr} g(\widehat{H})$ have the same semiclassical expansion modulo $\mathcal{O}(\hbar^\infty)$.

It is enough to observe that, for any $\epsilon > 0$, the eigenfunctions corresponding to eigenvalues of H (resp. $\widehat{H}$) less than $E - \epsilon$) decay exponentially in any compact outside of $U_{E-\frac{\epsilon}{2}}$.

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 $(\widehat{A}, \widehat{V})$ such that the assumptions of Proposition 4.10 are satisfied with in addition $\widehat{A}$ and $\widehat{V}$ bounded (with all the derivatives).

The proof is easy. We can indeed consider a C^∞ increasing function χ on $\mathbb{R}$ such that

$$\chi(t) = t \text{ on }]-\infty, \tfrac{1}{2}(E + \Sigma_V)[\,, \ \chi'(t) = 0 \text{ on }]\tfrac{1}{3}(E + 2\Sigma_V), +\infty[\,.$$

We can then take $\widehat{V} = \chi(V)$. It is not difficult to modify A outside $V^{-1}(]-\infty, \tfrac{1}{2}(E + \Sigma_V)[)$ to get a C^∞ bounded magnetic potential.

As a consequence, it is enough for proving Theorem 1.3 to prove it with A and V of class C^∞ and bounded. Hence we can work at the intersection of the two calculi and use either the results of the 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 Ω, 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^∞ potentials on $\overline{\Omega}$ and assume that

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

Then, with H the Dirichlet realization of P_A in Ω, 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 exists C_N and h_N, such that if

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

then, :

$$\left| (2\pi\hbar)^d \operatorname{Tr} g(H) - \sum_{0 \le j \le N} \hbar^j T_j^B(g) \right| \le C_N \hbar^{N+1}\,, \ \forall \hbar \in]0, h_N] \cap \mathcal{I}\,. \tag{4.6}$$

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

$$T_j^B(g) = \sum_{0 \le \ell \le k_j} \int g^{(\ell)}(F(x,\xi)) P_\ell(\partial_{x,\xi}^\alpha F(x,\xi), \partial_x^\beta B_{jk}(x)) \, dx d\xi\,, \tag{4.7}$$

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 Ω.*

Using a (small extension of) the comparison proposition, one can modify the potentials in the neighborhood of $\partial\Omega$ and then extend outside of Ω without modify the asymptotic of $\operatorname{Tr} g(H)$ and then use the results obtained in the case of $\mathbb{R}^d$.

Remark 4.14 *Note that we have not done any assumptions on the topology of Ω. Hence we have also 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

$$\left| |\hbar|^d \mathbb{T}\mathrm{r}\ g(H) - \sum_{0 \leq j \leq N} \hbar^j T_j^B(g) \right| \leq C_N \hbar^{N+1}\,, \forall \hbar \in [-h_N, h_N] \setminus \{0\}\,.$$

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

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