Semi-classical trace formulas and heat expansions

Yves Colin de Verdière

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July 20, 2011

Introduction

There is a strong similarity between the expansions of the heat kernel as worked out by people in Riemannian geometry in the seventies (starting with the famous "Can one hear the shape of a drum" by Mark Kac [Kac], the Berger paper [Berger] and the Mc-Kean-Singer paper [McK-Si]) and the so-called semi-classical trace formulas developed by people in semi-classical analysis (starting with Helffer-Robert [He-Ro]). In fact, this is not only a similarity, but, as we will prove, each of these expansions, even if they differ when expressed numerically for some example, can be deduced from the other one as formal expressions of the fields.

Let us look first at the *heat expansion* on a smooth closed Riemannian manifold of dimension d, (X, g), with the (negative) Laplacian Δ_g[1]. The heat kernel $e(t, x, y)$, with $t > 0$ and $x, y \in X$, is the Schwartz kernel of $\exp(t\Delta_g)$: the solution of the heat equation $u_t - \Delta_g u = 0$ with initial datum u_0 is given by

$$u(t, x) = \int_X e(t, x, y) u_0(y) |dy|_g \ .$$

The function $e(t, x, x)$ admits, as $t \to 0^+$, the following asymptotic expansion:

$$e(t, x, x) \sim (4\pi t)^{-d/2} \left(1 + a_1(x)t + \cdots + a_l(x)t^l + \cdots \right) \ .$$

The a_l's are given explicitly in [Gilkey2], page 201, for $l \leq 3$ and are known for $l \leq 5$ [Avramidi, vdV]. See also the related works by Hitrik and Polterovich [Hi, Hi-Po-1, Hi-Po-2, Po]. They are universal polynomials in the components of the curvature tensor and its co-variant derivatives. For example $a_0 = 1$, $a_1 = \tau_g/6$ where τ_g is the scalar curvature.

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[1]In this note, we will not follow the usual sign convention of geometers, but the convention of analysts

The previous asymptotic expansion gives the expansion of the trace by integration over X and has been used as an important tool in spectral geometry:

$$\mathrm{trace}(e^{t\Delta_g}) = \int_X e(t,x,x)|dx|_g = \sum_{k=1}^{\infty} e^{\lambda_k t} ,$$

where $-\lambda_1 = 0 \leq -\lambda_2 \leq \cdots \leq -\lambda_k \leq \cdots$ is the sequence of eigenvalues of $-\Delta_g$ with the usual convention about multiplicities. If $d=2$, this gives

$$\mathrm{trace}(e^{t\Delta_g}) = \frac{1}{4\pi t}\left(\mathrm{Area}(X) + \frac{2\pi\chi(X)}{6}t + 0(t^2)\right) ,$$

where $\chi(X)$ is the Euler characteristic of X.

There is an extension of the previous expansion in the case of Laplace type operators on fiber bundles: the coefficients of the expansion are then polynomials in the co-variant derivatives of the curvature of the metric and of the connection on the fiber bundle. The heat expansion can be re-interpreted as an expansion of the Schwartz kernel of $f(-\hbar^2\Delta_g)$ on the diagonal $x=y$ in powers of $\hbar$ with $f(u)=\exp(-u)$ and $t=\hbar^2$. This is a particular case of the semi-classical trace.

Let us describe the semi-classical setting in the flat case: $\widehat{H_\hbar}$ is a self-adjoint $\hbar-$pseudo-differential operator with Weyl symbol $H(x,\xi)$ in some open domain X in $\mathbb{R}^d$, or more generally on a Riemannian manifold. Let $f \in \mathcal{S}(\mathbb{R})$ and look at $f(\widehat{H_\hbar})$. Under some suitable assumptions (ellipticity at infinity in ξ) on H, $f(\widehat{H_\hbar})$ is a pseudo-differential operator whose Weyl symbol $f^\star(H)$ is a formal power series in $\hbar$, given, using the Moyal product denoted by $\star$, by the following formula (see [Gracia] for explicit formulas and Section 4.2 for a proof, see also [Charles]) at the point $z_0 \in T^\star X$:

$$f^\star(H)(z_0) = (2\pi\hbar)^{-d}\left(\sum_{l=0}^{\infty}\frac{1}{l!}f^{(l)}(H(z_0))\,(H-H(z_0))^{\star\ l}\,(z_0)\right) . \qquad (1)$$

From the previous formula, we see that the symbol of $f(\widehat{H_\hbar})$ at the point z depends only of the Taylor expansions of H at the point z and of f at the point $H(z)$. In the paper [H-P], the authors study the case of the magnetic Schrödinger operator whose Weyl symbol is $H_{a,V}(x,\xi) = \sum_{j=1}^d (\xi_j - a_j(x))^2 + V(x)$ and show that the Schwartz kernel of $f(\widehat{H_{\hbar,a,V}})$ at the point (x,x) admits an asymptotic expansion of the form

$$[f(\widehat{H_{\hbar,a,V}})](x,x) = (2\pi\hbar)^{-d}\left[\sum_{j=0}^{\infty}\hbar^{2j}\left(\sum_{l=0}^{k_j}\int_{\mathbb{R}^d} f^{(l)}(\|\xi\|^2+V(x))Q_{j,l}^{a,V}(x,\xi)|d\xi|\right)\right]$$

where the $Q_{j,l}^{a,V}(x,\xi)$'s are polynomials in ξ calculated from the Taylor expansions of the magnetic field $B=da$ and V at the point x. The proof in [H-P] uses a pseudo-differential calculus adapted to the magnetic field.

We will give a simplified version of the expansion replacing the (non unique) $Q_{j,l}^{a,V}(x,\xi)$'s by functions $P_{j,l}^{B,V}(x)$'s which are uniquely defined and are given by universal $O(d)$-invariant polynomials of the Taylor expansions of B and V at the point x. We present then two ways to compute the $P_{j,l}^{B,V}$'s:

- we can first use Weyl's invariant theory (see Gilkey's book [Gilkey2]) in order to reduce the problem to the determination of a finite number of numerical coefficients; then simple examples, like harmonic oscillator and constant magnetic field, allow to determine (part of) these coefficients.
- The $P_{j,l}^{B,V}$'s are related in a very simple way to the coefficients of the heat expansion; it is possible to compute the $P_{j,l}^{B,V}$'s from the knowledge of the a_l's for $j+1 \leq l \leq 3j$. This is enough to re-compute the coefficient of $\hbar^2$ and also, in principle, the coefficients of $\hbar^4$ in the expansion, because the a_l's are known up to $l=6$ in the case of a flat metric (see [vdV]).

In this note, we will first describe precisely the semi-classical expansion for Schrödinger operators (in the case of an Euclidian metric) and the properties of the functions $P_{j,l}^{B,V}(x)$'s. Then, we will show how to compute the $P_{j,l}^{B,V}(x)$'s using an adaptation of the method used for the heat kernel (Weyl's Theorem on invariants and explicit examples). Finally, we will explain how the a_l's are related to the $P_{j,l}^{B,V}(x)$'s. This gives us two proofs of the main formula given by Helffer and Purice in [H-P]; this paper was the initial motivation to this work.

Acknowledgments

I thank the referee for his careful reading of the paper which forced me to make the statements and proofs more precise. Many thanks also to Johannes Sjöstrand for his help in clarifying some points of semi-classical analysis and for allowing me to present them in an Appendix to this paper.

1 Semi-classical trace for Schrödinger operators

In what follows, X is an open domain in $\mathbb{R}^d$, equipped with the canonical Euclidian metric, and $\Omega^k(X)$ will denote the space of smooth exterior differential forms in X. Let us give a Schrödinger operator, with a smooth magnetic field $B = \sum_{1\leq i<j\leq d} b_{ij} dx_i \wedge dx_j$ (a closed real 2-form) and a smooth electric potential V (a real valued smooth function) in X. We assume that V is bounded from below. We will assume also that the 2-form B is exact and can be written $B = da$ and we introduce the Schrödinger operator defined by

$$H_{\hbar,a,V} = \sum_{j=1}^{d} \left(\frac{\hbar}{i} \frac{\partial}{\partial x_j} - a_j(x) \right)^2 + V(x) \ .$$

The Weyl symbol of $H_{\hbar,a,V}$ is $H_{a,V}(x,\xi) = \|\xi - a(x)\|^2 + V(x)$. We denote by $\widehat{H_{\hbar,a,V}}$ a self-adjoint extension of $H_{\hbar,a,V}$ in $L^2(X,|dx|)$. Let us give $f \in \mathcal{S}(\mathbb{R})$ and $\phi \in C_o^\infty(X)$ and consider the trace of $\phi f(\widehat{H_{\hbar,a,V}})$ as a distribution on $X \times \mathbb{R}$ (the density of states):

$$\mathrm{Trace}(\phi f(\widehat{H_{\hbar,a,V}})) = \int_X Z_{\hbar,a,V}(g)(x)\phi(x)|dx| \ ,$$

where $Z_{\hbar,a,V}(g)(x)$ is the value at the point (x,x) of the Schwartz kernel of $f(\widehat{H_{\hbar,a,V}})$.

Theorem 1 *We have the following asymptotic expansion in power of $\hbar$:*

$$Z_{\hbar,a,V}(g)(x) \sim (2\pi\hbar)^{-d}\left[\int_{\mathbb{R}^d} f(\|\xi\|^2 + V(x))|d\xi| + \sum_{j=1}^{\infty}\hbar^{2j}\left(\sum_{l=j+1}^{l=3j} P_{j,l}^{B,V}(x)\int_{\mathbb{R}^d} f^{(l)}(\|\xi\|^2 + V(x))|d\xi|\right)\right]$$

We have the explicit formulas

$$P_{1,2}^{B,V} = -\frac{1}{6}\left(\Delta V + \|B\|^2\right) \ ,$$

$$P_{1,3}^{B,V} = -\frac{1}{12}\|\nabla V\|^2 \ ,$$

$$P_{2,3}^{B,V} = -\frac{1}{180}\left(8\|\nabla B\|^2 + \|d^\star B\|^2 + 12\langle \Delta B|B\rangle + 3\Delta^2 V\right) \ .$$

Here $\|B\|^2 = \sum_{1\le i<j\le d} b_{ij}^2$, $d^\star : \Omega^2(X) \to \Omega^1(X)$ is the formal adjoint of d used in the definition of the Hodge Laplacian on exterior forms. If $d = 3$, $\|B\|$ is the Euclidean norm of the vector field associated to B.

The $P_{j,l}^{B,V}(x)$ are polynomials of the derivatives of B and V at the point x. Moreover, if λ, μ, c are constants and we define $\lambda^\star(f)(x) = f(\lambda x)$, we have the following scaling properties:

1. *$P_{j,l}^{\lambda.\lambda^\star(B),\lambda^\star(V)}(x) = \lambda^{2j}P_{j,l}^{B,V}(\lambda x)$. This will be used with $x = 0$.*
2. *$P_{j,l}^{\mu B,\mu^2 V}(x) = \mu^{2(l-j)}P_{j,l}^{B,V}(x)$*
3. *$P_{j,l}^{B,V+c}(x) = P_{j,l}^{B,V}(x)$*
4. *$P_{j,l}^{-B,V}(x) = P_{j,l}^{B,V}(x)$.*
5. *The $P_{j,l}^{B,V}$'s are invariant by the natural action of the orthogonal group $O(d)$ on the Taylor expansions of B and V at the point x.*

Remark 1 *From the statement of the previous Theorem, we see that the expansion of the density of states is independent of the chosen self-adjoint extension.*

As a consequence, we can get the following full trace expansion under some more assumptions:

Corollary 1 *Let us assume that* $E_0 = \inf V < E_\infty = \liminf_{x\to\partial X} V(x)$ *and that we have chosen the Dirichlet boundary conditions. Let* $f \in C_o^\infty(]-\infty, E_\infty[)$, *then the trace of* $f(\widehat{H_{\hbar,a,V}})$ *admits the following asymptotic expansion*

$$\mathrm{Trace}(f(\widehat{H_{\hbar,a,V}})) \sim (2\pi\hbar)^{-d} \int_X \left(\int_{\mathbb{R}^d} f(\|\xi\|^2 + V(x))|d\xi| + \cdots \right.$$

$$\left. \cdots \sum_{j=1}^{\infty} \hbar^{2j} \sum_{l=j+1}^{l=3j} P_{j,l}^{B,V}(x) \int_{\mathbb{R}^d} f^{(l)}(\|\xi\|^2 + V(x))|d\xi| \right) |dx| \ ,$$

The coefficient of $\hbar^2$ *can be written as*

$$-\frac{1}{12} \int_{X\times\mathbb{R}^d} f^{(2)}(\|\xi\|^2 + V(x)) \left(\Delta V(x) + 2\|B(x)\|^2\right) |dx d\xi| \ .$$

The expansion follows from [He-Ro]. An integration by part in x gives

$$\int_X f^{(3)}(\|\xi\|^2 + V(x))\|\nabla V(x)\|^2|dx| = -\int_X f^{(2)}(\|\xi\|^2 + V(x))\Delta V(x)|dx| \ .$$

2 Existence of the $\hbar-$expansion of $Z_{\hbar,a,V}$

Using Theorem 2 in the Appendix, we can work in $\mathbb{R}^d$ with a and V compactly supported. The existence of the expansion is known in general from [He-Ro] and the calculus of the symbol of $f(\widehat{H_{\hbar,a,V}})$. We get

$$\int_X Z_{\hbar,a,V}(f)(x)\phi(x)|dx| = (2\pi\hbar)^{-d} \left(\sum_{j=0}^{\infty} \hbar^{2j} \sum_{l=0}^{k_j} \int \phi(x) f^{(l)}(H_{a,V}(x,\xi)) Q_{j,l}(x,\xi)|dx d\xi| \right)$$

where the $Q_{j,l}(x,\xi)$'s are polynomials in the Taylor expansion of $H_{a,V}$ at the point (x,ξ). The previous expansion is valid for any (admissible) pseudo-differential operator. In the case of Schrödinger operators we can make integrations by part in the integrals $\int f^{(l)}(H_{a,V}(x,\xi))Q_{j,l}(x,\xi)|d\xi|$ which reduces to a similar formula where we can replace the $Q_{j,l}(x,\xi)$'s by $P_{j,l}(x)$'s. This is based on the expansion of $Q_{j,l}$ as a polynomial in ξ in powers of $(\xi - a)$: odd powers give 0 and even powers can be reduced using

$$d_\xi \left((\xi_j - a_j) f^{(l)}(H_{a,V})\iota(\partial_{\xi_j})d\xi\right) = 2\|\xi_j - a_j\|^2 f^{(l+1)}(H_{a,V})d\xi + f^{(l)}(H_{a,V})d\xi \ .$$

We have only to check that the powers of ξ in $Q_{j,l}(x,\xi)$ are less than l: this is based on Equation (1). The coefficients of the $l-$th Moyal power of $H_{a,V}(z) - H_{a,V}(z_0)$ are homogeneous polynomials of degree l in the derivatives of $H_{a,V}(z)$. At the point $z = z_0$ only derivatives of order ≥ 1 are involved. They are all of degree ≤ 1 in ξ. Using Gauge invariance at the point x (Section 3), we can assume that $a(x) = 0$.

3 Gauge invariance

If $S : X \to \mathbb{R}$ is a smooth function, we have

$$\mathrm{Trace}(\phi e^{-iS(x)/\hbar} f(\widehat{H_{\hbar,a,V}}) e^{iS(x)/\hbar}) = \mathrm{Trace}(\phi f(\widehat{H_{\hbar,a,V}}))$$

and

$$e^{-iS(x)/\hbar} f(\widehat{H_{\hbar,a,V}}) e^{iS(x)/\hbar} = f(\widehat{H_{a+dS,V}}) \ .$$

Hence, we can chose any local gauge a in order to compute the expansion: using the synchronous gauge (see Section 4), we get the individual terms

$$\int f^{(l)}(H_{0,V}) P_{j,l}^{B,V}(x) |d\xi|$$

for the expansion, where the $P_{j,l}^{B,V}(x)$ depend only of the Taylor expansions of B and V at the point x.

4 The synchronous gauge

The main idea is to find an appropriate gauge a adapted to the point x_0 where we want to make the symbolic computation. In a geometric language, we use the trivialization of the bundle by parallel transportation along the rays: the potential a vanishes on the radial vector field [2]. Here, this is simply the fact that, for any closed 2-form B on $\mathbb{R}^2$, there exists an unique 1-form $a = \sum_{j=1}^{d} a_j dx_j$ so that $da = B$ and $\sum_{j=1}^{d} x_j a_j = 0$.

We will do that for the Taylor expansions degree by degree. In what follows we will use a decomposition for 1-forms, but it works also for $k-$forms.

Let us denote by Ω_N^k the finite dimensional vector space of k-differential forms on $\mathbb{R}^d$ whose coefficients are homogeneous polynomials of degree N and by $W = \sum_{j=1}^{d} x_j \frac{\partial}{\partial x_j}$ the radial vector field. The exterior differential induces a linear map from Ω_N^k into Ω_{N-1}^{k+1} and the inner product $\iota(W)$ a map from Ω_N^k into Ω_{N+1}^{k-1}. They define complexes which are exact except at $k = N = 0$. Moreover, we have a situation similar to Hodge theory:

$$\Omega_N^k = d\Omega_{N+1}^{k-1} \oplus \iota(W)\Omega_{N-1}^{k+1} \ .$$

This is due to Cartan's formula: the Lie derivative of a form $\omega \in \Omega_N^k$ satisfies, from the direct calculation, $\mathcal{L}_W \omega = (k+N)\omega$, and, by Cartan's formula, $\mathcal{L}_W \omega = d(\iota(W)\omega) + \iota(W)d\omega$. So

$$\omega = \frac{1}{k+N} \left(d(\iota(W)\omega) + \iota(W)d\omega \right) \ .$$

[2]This gauge is sometimes called the Fock-Schwinger gauge; in [A-B-P], it is called the synchronous framing

It remains to show that this is a direct sum: if $\omega = d\alpha = \iota(W)\gamma$, we have $\iota(W)\omega = 0$ and $d\omega = 0$; from the previous decomposition, we see that $\omega = 0$. Let us denote by $J^N\omega$, where ω is a differential form of degree k, the form in Ω^k_N which appears in the Taylor expansion of ω.

We get

Proposition 1 *If $P(J^0a, J^1a, \cdots, J^Na)$ is a polynomial in the Taylor expansion of the 1-form a at some order N which is invariant by $a \to a + dS$, P is independent of J^0a and*

$$P\left(J^1a, \cdots, J^Na\right) = P\left(\frac{1}{2}J^1\iota(W)B, \cdots, \frac{1}{N+1}J^N\iota(W)B\right)$$

is a polynomial of the Taylor expansion of B to the order $N-1$.

5 Properties of the $P_{j,l}$'s

5.1 Range of l for j fixed

From the scaling properties, we deduce that, in a monomial

$$D^{\alpha_1}B_{i_1,j_1}\cdots D^{\alpha_k}B_{i_k,j_k}D^{\beta_1}V\cdots D^{\beta_m}V\ ,$$

belonging to $P_{j,l}$, we have $k+2m = 2(l-j)$ and $k+|\alpha_1|+\cdots+|\alpha_k|+|\beta_1|+\cdots+|\beta_m| = 2j$. Moreover, for $j \geq 1$, $k+m \geq 1$ and $|\beta_p| \geq 1$. Hence $j+1 \leq l \leq 3j$. The previous bounds are sharp: take the monomials Δ^jV and $\|\nabla V\|^{2j}$ which give $l = j+1$ and $l = 3j$.

5.2 Invariance properties

1. Let us assume that we look at the point $x = 0$ and consider the operator $D_\mu(f)(x) = f(\mu x)$. We have

$$D_\mu \circ \hat{H}_{\hbar,A,V} \circ D_{1/\mu} = \hat{H}_{\hbar/\mu, A\circ D_\mu, V\circ D_\mu}\ .$$

The same relation is true for any function $f(\hat{H}_{\hbar,A,V})$ and then we have, looking at the Schwartz kernels and using the Jacobian μ^d of D_μ:

$$P^{B,V}_{j,l}(0)\int_{\mathbb{R}^d} f^{(l)}(\|\xi\|^2+V(0))|d\xi| = \mu^{-2j}P^{\mu.\mu^\star B,\mu^\star V}_{j,l}(0)\int_{\mathbb{R}^d} f^{(l)}(\|\xi\|^2+V(0))|d\xi|\ .$$

2. We have

$$\widehat{H}_{\hbar,\mu a,\mu^2V} = \mu^2\widehat{H}_{\frac{\hbar}{\mu},a,V}\ .$$

3. Changing V into $V+c$ gives a translation by c in the function f but does not change the $P_{j,l}^{B,V}$'s.
4. Changing B into $-B$ gives a complex conjugation in the computations. The final result is real valued.
5. Orthogonal invariance is clear: an orthogonal change of coordinates around the point x preserves the density of states.

5.3 The case $d = 2$

We deduce from the scaling properties and invariance by the orthogonal group, that there exists constants $a_d,\ b_d,\ c_d$ so that $P_{1,2}^{B,V}(x) = a_d \Delta V + b_d \|B\|^2,\ P_{1,3}(x) = c_d \|\nabla V\|^2$.

6 Explicit examples

The calculation for the harmonic oscillators and the constant magnetic fields allows to determine the constants $a_d,\ b_d,\ c_d$.

6.1 Harmonic oscillators

Let us consider $\Omega = -\hbar^2 \frac{d^2}{dx^2} + x^2$ with $d = 1$. The kernel of $P(t,x,y)$ of $\exp(-t\Omega)$ is given by the Mehler formula:

$$P(t,x,y) = (2\pi\hbar \sinh(2t\hbar))^{-\frac{1}{2}} \exp\left(-\frac{1}{2\hbar \sinh(2t\hbar)} \left(\cosh(2t\hbar)(x^2+y^2) - 2xy\right)\right) .$$

Hence

$$P(t,x,x) \sim (2\pi\hbar)^{-1} e^{-tx^2} \left(\int_{\mathbb{R}} e^{-t\xi^2} d\xi\right) \left(1 - \hbar^2(t^2 - t^3x^2)/3 + 0(\hbar^4)\right) .$$

Hence $P_{1,2}(x) = -V''(x)/6,\ P_{1,3}(x) = -V'(x)^2/12,.$

Similarly, in dimension $d > 1$, we get $P_{1,2}(x) = -\Delta V(x)/6,\ P_{1,3}(x) = -\|\nabla V\|^2/12,.$

6.2 Constant magnetic field

Let us consider the case of a constant magnetic field B in the plane and denote by $Q(t,x,y)$ the kernel of $\exp(-tH_{B,0})$. We have (see [A-H-S])

$$Q(t,x,x) = \frac{B}{4\pi\hbar \sinh Bt\hbar} .$$

Hence the asymptotic expansion

$$Q(t,x,x) = (2\pi\hbar)^{-2} \int \exp(-t\|\xi\|^2)|d\xi| \left(1 - t^2\hbar^2 B^2/6 + 0(\hbar^4)\right) ,$$

hence $P_{1,2}(x) = -B^2/6,\ P_{1,3}(x) = 0$.

Using the normal form $B = b_{12}dx_1 \wedge dx_2 + b_{34}dx_3 \wedge dx_4 + \cdots$, we get in dimension $d > 2$, $P_{1,2}(x) = -\|B\|^2/6,\ P_{1,3}(x) = 0$.

7 Heat expansion from the semi-classical expansions

We have $t\widehat{H_{1,a,V}} = \widehat{H_{\sqrt{t},\sqrt{t}a,tV}}$. Using the expansion of Theorem 1 with $f(E) = e^{-E}$, we get easily the point-wise expansion of the heat kernel on the diagonal as $t \to 0^+$:

$$[\exp(-t\widehat{H_{1,a,V}})](x,x) \sim \frac{1}{(4\pi t)^{d/2}} e^{-tV(x)} \left[\sum_{l=0}^{\infty} \left(\sum_{l/3 \leq j \leq l-1} P_{j,l}^{B,V}(x) \right) (-t)^l \right] .$$

In particular, $a_1(x) = -V(x)$ and the coefficient $a_2(x)$ is given by

$$a_2(x) = \frac{1}{2}V(x)^2 - \frac{1}{6}\Delta V(x) - \frac{1}{6}\|B(x)\|^2 .$$

This formula agrees with Equation (3) of Theorem 3.3.1 in [Gilkey2].

This gives another way to compute the $P_{j,l}$'s: if, as power series in t,

$$\sum_{l=0}^{\infty} (-1)^l b_l(x) t^l = e^{tV(x)} \left(\sum_{l=0}^{\infty} a_l(x) t^l \right) ,$$

we have

$$\sum_{l/3 \leq j \leq l-1} P_{j,l}^{B,V}(x) = b_l(x) .$$

$P_{j,l}^{B,V}$ is the sum of monomials homogeneous of degree $2(l-j)$ in b_l where B and its derivatives have weights 1 while V and its derivatives have weights 2.

The heat coefficients a_l on flat spaces are known for $l \leq 6$ from [vdV]. This is enough to check the term in $\hbar^2$ (uses a_2 and a_3) in [H-P] and to compute the term in $\hbar^4$ in the semi-classical expansion (uses the a_l's for $3 \leq l \leq 6$).

We have also a mixed expansion writing $t\widehat{H}_{\hbar,a,V} = \widehat{H}_{\sqrt{t}\hbar,\sqrt{t}a,tV}$, we get a power series expansion in powers of $\hbar$ and t valid in the domain $\hbar^2 t \to 0$ and $0 < t \leq t_0$ for the point-wise trace of $\exp(-t\widehat{H}_{\hbar,a,V})$:

$$Z_{t,\hbar}(x) \sim \frac{1}{(4\pi t)^{d/2}} e^{-tV(x)} \left(1 + \sum_{j \geq 1,\ j+1 \leq l \leq 3j} \hbar^{2j} (-t)^l P_{j,l}^{B,V}(x) \right) .$$

This shows that the integrals $\int_X V(x)^k |dx|$ and $\int_X P_{j,l}^{B,V}(x)|dx|$ are recoverable from the semi-classical spectrum.

Appendix: functional calculus in domains and self-adjoint extensions (after Johannes Sjöstrand)

The content of this Appendix is due to Johannes Sjöstrand. I thank him very much for this contribution.

Let $X \subset \mathbb{R}^d$ be an open set, we say that a linear operator A is a ΨDO in X, with Weyl symbol a, if, for any compact $K \subset X$, A acts on functions supported in K as a ΨDO of Weyl symbol a.

Theorem 2 *Let $H_{\hbar,a,V}$ be a Schrödinger operator with magnetic field given by*

$$H_{\hbar,a,V} = \sum_{j=1}^{d} \left(\frac{\hbar}{i} \frac{\partial}{\partial x_j} - a_j(x) \right)^2 + V(x) \ ,$$

defined in some open domain $X \subset \mathbb{R}^d$. We assume that a and V are smooth in X and that V is bounded from below, so that $H_{\hbar,a,V}$ admits some self-adjoint extensions on the Hilbert space $L^2(X, |dx|)$. One of them will be denoted by $\widehat{H_{\hbar,a,V}}$. Then, for any $f \in \mathcal{S}(\mathbb{R})$, $f(\widehat{H_{\hbar,a,V}})$, given by the functional calculus, is a semi-classical ΨDO in X whose symbol is given by Equation (1) and is independent of the chosen extension.

The proof uses a multi-commutator method already used by Helffer and Sjöstrand. *Proof.–*

We introduce, for $s \in \mathbb{R}$, the semi-classical ($\hbar$-dependent) Sobolev spaces

$$\mathcal{H}_\hbar^s := \{ u \in \mathcal{S}'(\mathbb{R}^d) \mid \|\mathrm{Op}_\hbar (1 + \|\xi\|^2)^{s/2} u\|_{L^2} < \infty \ \}$$

with the norm

$$\|u\|_s := \|\mathrm{Op}_\hbar (1 + \|\xi\|^2)^{s/2} u\|_{L^2} \ .$$

The ($\hbar$-dependent) norm $\|A\|_{s_1,s_2}$ is the norm of A as linear operator from $\mathcal{H}_\hbar^{s_1}$ to $\mathcal{H}_\hbar^{s_2}$. A linear operator K is smoothing if, for all $s_1, \ s_2$, $\|K\|_{s_1,s_2} = O(\hbar^\infty)$. This implies that the Schwartz kernel of K is smooth with all derivatives locally $O(\hbar^\infty)$. We have the

Lemma 1 *Let Y be an open set in $\mathbb{R}^d$. Let $P_j = P_j(\hbar)$, $j = 0, 1$ be two self-adjoint operators on Hilbert spaces $\mathcal{H}_j = L^2(X_j, |dx|)$ with*

$Y \subset\subset X_0 \subseteq X_1 \subseteq \mathbb{R}^d$ and with domains $\mathcal{D}_j$ so that $C_o^\infty(Y) \subset \mathcal{D}_j \subset \mathcal{H}_j$. Let us assume that, on $C_o^\infty(Y)$, $P_0 = P_1 = H_{\hbar,a,V}(= P)$.

Then, for any $f \in C_o^\infty(\mathbb{R})$, $f(P_0) - f(P_1)$ is smoothing on Y. In particular, the densities of states $[f(P_j)](x,x)$, $j = 0, 1$, coïncide in Y modulo $O(\hbar^\infty)$.

Assuming Lemma 1, Theorem 2 follows by extending a and V smoothly outside Y so that they have compact support in $\mathbb{R}^d$. We take $Y \subset\subset X = X_0 \subset \mathbb{R}^d = X_1$. It follows that P_1 is essentially self-adjoint and the functional calculus for P_1 follows then easily from [He-Ro]. The result is valid even for $f \in \mathcal{S}(\mathbb{R})$ because C_o^∞ is dense in $\mathcal{S}$ and the result of [He-Ro] is valid for $f \in \mathcal{S}$ and the resulting formulas for the symbols are continuous w.r. to the topology of $\mathcal{S}$.

□

Proof of Lemma 1.– If $\chi \in C_o^\infty(Y)$, then, for $z \notin \mathbb{R}$ and $j, k \in \{0, 1\}$, we have on $L^2(Y)$:

$$(P_j - z)^{-1} \circ \chi = \chi \circ (P_k - z)^{-1} - (P_j - z)^{-1}[P, \chi](P_k - z)^{-1} \tag{2}$$

Let $\chi_0 \leq \chi_1 \leq \cdots \leq \chi_N$ with, for $l = 0, \cdots, N$, $\chi_l \in C_o^\infty(Y)$ and, for $l = 0, \cdots, N-1$, $\chi_l(1 - \chi_{l+1}) \equiv 0$. By iterating Equation (2) and using $\chi_{l+1}[P, \chi_l] = [P, \chi_l]$, we find:

$$\begin{aligned}&(P_1 - z)^{-1} \circ \chi_0 = \chi_1 \circ (P_0 - z)^{-1}\chi_0 - \chi_2 \circ (P_0 - z)^{-1}[P, \chi_1](P_0 - z)^{-1}\chi_0 + \cdots \\ &\pm \chi_N (P_0 - z)^{-1}[P, \chi_{N-1}](P_0 - z)^{-1}[P, \chi_{N-2}] \cdots (P_0 - z)^{-1}\chi_0 \\ &\mp (P_1 - z)^{-1}[P, \chi_N](P_0 - z)^{-1} \cdots (P_0 - z)^{-1}\chi_0\end{aligned}$$

Let us give now χ_0, $\psi \in C_o^\infty(Y)$ with disjoints supports. By choosing the $\chi_l's$ for $l > 0$ with supports disjoint from the support of ψ, we see, using Equation (2), that, for any N,

$$\|\psi(P_1 - z)^{-1}\chi_0\|_{0,2} = O\left(\hbar^N |\Im z|^{-(N+1)}\right) .$$

The standard a priori elliptic estimates

$$\|u\|_{s+2,\Omega_1} \leq C\left(\|(P - z)u\|_{s,\Omega_2} + \|u\|_{s,\Omega_1}\right)$$

for $z \in K \subset\subset \mathbb{C}$ and $\Omega_1 \subset\subset \Omega_2 \subset\subset \mathbb{R}^d$, allow to prove that, for any N, s, there exists $M(N, s)$ so that

$$\|\psi(P_1 - z)^{-1}\chi_0\|_{s,s+N+2} = O(\hbar^N |\Im z|^{-M(N,s)}) \tag{3}$$

Let $\chi \in C_o^\infty(Y)$ so that $\chi \equiv 1$ on the support of χ_0. Let us apply a multiplication by χ_0 to the right and to the left to Equation (2) and choose ψ with support disjoint of χ_0 so that $[P,\chi]\psi = [P,\chi]$. Inserting ψ this way in Equation (2), we get, using Equation (3):

$$\chi_0(P_1 - z)^{-1}\chi_0 - \chi_0(P_0 - z)^{-1}\chi_0 = K$$

and, for any N, there exists $M(N)$ so that $\|K\|_{-N,N} = O(\hbar^N \Im z^{-M(N)})$. We now apply the formula (known to some people as the "Helffer-Sjöstrand formula", proved for example in the book [Di-Sj], p. 94–95), valid for $f \in C_o^\infty(\mathbb{R})$ and $\tilde{f}$ an almost holomorphic extension of f:

$$f(P_j) = \frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar{z}}\tilde{f}(z)(P_j - z)^{-1} dL(z) ,$$

where $dL(z)$ is the canonical Lebesgue measure in the complex plane. From this, we see that $f(P_0) - f(P_1)$ is smoothing in Y.

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