Bohr-Sommerfeld rules to all orders

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1 Introduction

The goal of this paper is to give a rather simple algorithm which computes the Bohr-Sommerfeld quantization rules to all orders in the semi-classical parameter h for a semi-classical Hamiltonian $\widehat{H}$ on the real line. The formula gives the high order terms in the expansion in powers of h of the *semi-classical action* using only integrals on the energy curves of quantities which are *locally computable* from the Weyl symbol. The recipe uses only the knowledge of the *Moyal formula* expressing the star product of Weyl symbols. It is important to note that our method assumes already the existence of Bohr-Sommerfeld rules to any order (which is usually shown using some precise Ansatz for the eigenfunctions, like the WKB-Maslov Ansatz) and the problem we adress here is only about ways to compute these corrections.

Our way to get these high order corrections is inspired by A. Voros's thesis (1977) [9], [10]. The reference [1], where a very similar method is sketched, was given to us by A. Voros. We use also in an essential way the nice formula of Helffer-Sjöstrand expressing $f(\widehat{H})$ in terms of the resolvent.

[1]Keywords: Bohr-Sommerfeld rules, Moyal formula, functional calculus, pseudo-differential operator, spectral theory, quantization rules
[2]MSC 2000: 34E05, 35P15, 35S99, 81Q10

2 The setting and the main result

Let us give a smooth classical Hamiltonian $H : T^\star\mathbb{R} \to \mathbb{R}$, where the symbol H admits the formal expansion $H \sim H_0 + hH_1 + \cdots + h^k H_k + \cdots$; following [4] p.101, we will assume that

- H belongs to the space of symbols $S^o(m)$ for some order function m (for example $m = (1 + |\xi|^2)^p$)
- $H + i$ is elliptic

and define $\widehat{H} = \mathrm{Op}_{\mathrm{Weyl}}(H)$ with [3]

$$\mathrm{Op}_{\mathrm{Weyl}}(H)u(x) = \int_{\mathbb{R}^2} e^{i(x-y)\xi/h} H(\frac{x+y}{2}, \xi)u(y) \left|\frac{dyd\xi}{2\pi h}\right| .$$

The operator $\widehat{H}$ is then essentially self-adjoint on $L^2(\mathbb{R})$ with domain the Schwartz space $\mathcal{S}(\mathbb{R})$.

In general, we will denote by $\sigma_{\mathrm{Weyl}}(A)$ the Weyl symbol of the operator A.

The hypothesis:

- We fix some compact intervall $I = [E_-, E_+] \subset \mathbb{R},\ E_- < E_+$, and we assume that there exists a topological ring $\mathcal{A}$ such that $\partial\mathcal{A} = A_- \cup A_+$ with $A_\pm$ a connected component of $H_0^{-1}(E_\pm)$.
- We assume that H_0 has no critical point in $\mathcal{A}$
- We assume that A_- is included in the disk bounded by A_+. If it is not the case, we can always change H to $-H$.

We define the *well* W as the disk bounded by A_+.

Definition 1 *Let $H_W : T^\star\mathbb{R} \to \mathbb{R}$ be equal to H in W, $> E_+$ outside W and bounded. Then $\widehat{H_W} = \mathrm{Op}_{\mathrm{Weyl}}(H_W)$ is a self-adjoint bounded operator. The* semi-classical spectrum associated to the well W, *denoted by σ_W, is defined as follows:*

$$\sigma_W = \mathrm{Spectrum}(\widehat{H_W}) \cap]-\infty, E_+] .$$

The previous definition is usefull because σ_W is independent of H_W mod $O(h^\infty)$. Moreover, if $H_0^{-1}(]-\infty, E^+]) = W_1 \cup \cdots \cup W_N$ (connected components), then

$$\mathrm{Spectrum}(\widehat{H}) \cap]-\infty, E^+] = \cup \sigma_{W_l} + O(h^\infty) .$$

[3] Contrary to the usual notation, we denote by $|dx_1 \cdots dx_n|$ the Lebesgue measure on $\mathbb{R}^n$ in order to avoid confusions related to orientations problems.

The spectrum $\sigma_W \cap [E_-, E_+]$ is then given mod $O(h^\infty)$ by the following **Bohr-Sommerfeld rules**

$$\mathcal{S}_\mathbf{h}(\mathbf{E_n}) = \mathbf{2\pi nh}$$

where $\mathbf{n} \in \mathbb{Z}$ is the *quantum number* **and the formal series**

$$\mathcal{S}_\mathbf{h}(\mathbf{E}) = \sum_{\mathbf{j=0}}^{\infty} \mathbf{S_j(E)h^j}$$

is called the *semi-classical action.*

Our goal is to give an algorithm for computing the functions $S_j(E),\ E \in I$.

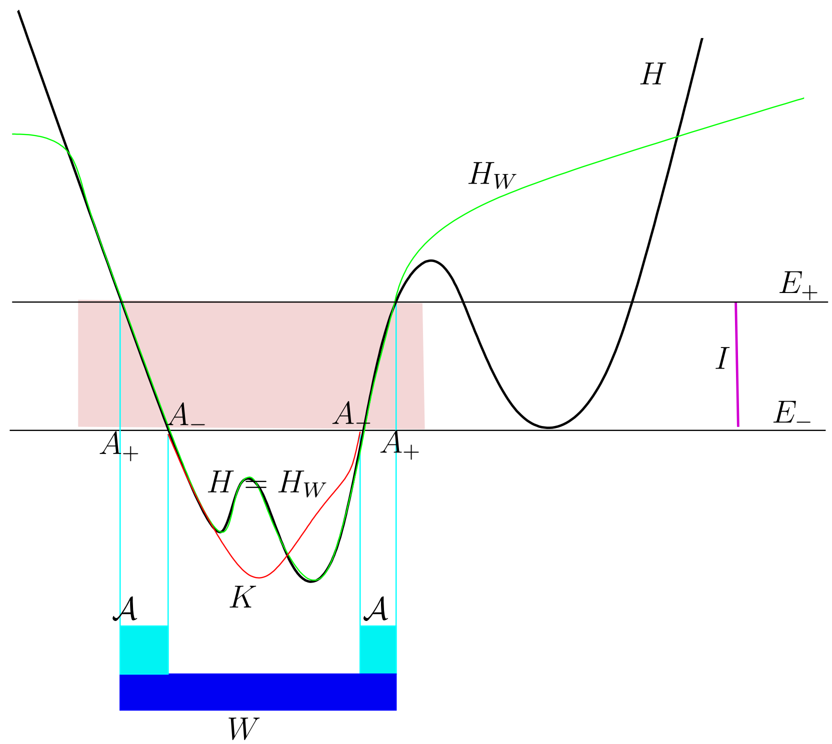

Figure 1: the phase space

In fact $\exp(i\mathcal{S}_h(E)/h)$ is the holonomy of the WKB-Maslov microlocal solutions of $(\hat{H} - E)u = 0$ around the trajectory $\gamma_E = H^{-1}(E) \cap \mathcal{A}$.

It is well known that:

- $S_0(E) = \int_{\gamma_E} \xi dx = \int_{\{H_0 \leq E\} \cap W} |dx d\xi|$ is the *action integral*
- $S_1(E) = \pi - \int_{\gamma_E} H_1 |dt|$ includes the *Maslov correction* and the *subprincipal term.*

Our main result is:

Theorem 1 *If H satisfies the previous hypothesis, we have: for $j \geq 2$,*

$$S_j(E) = \sum_{2 \leq l \leq L(j)} \frac{(-1)^{l-1}}{(l-1)!} \left(\frac{d}{dE}\right)^{l-2} \int_{\gamma_E} P_{j,l}(x,\xi)|dt|$$

where

- *t is the parametrization of γ_E by the time evolution*

$$dx = (H_0)_\xi dt,\ d\xi = -(H_0)_x dt$$

- *The $P_{j,l}$'s are locally (in the phase space) computable quantities: more precisely each $P_{j,l}(x,\xi)$ is a universal polynomial evaluated on the partial derivatives $\partial^\alpha H(x,\xi)$.*

  The $P_{j,l}$'s are given from the Weyl symbol of the resolvent (see Proposition (1)):

$$\sigma_{\mathrm{Weyl}}\left((z-\hat{H})^{-1}\right) = \frac{1}{z-H_0} + \sum_{j=1}^{\infty} h^j \sum_{l=2}^{L(j)} \frac{P_{j,l}}{(z-H_0)^l}\ .$$

If $H = H_0$, $S_{2j+1}(E) = 0$ for $j > 0$. In that case, the polynomial $P_{j,l}(\partial^\alpha H)$ is homogeneous of degree $l-1$ w.r. to H and the total weight of the derivatives is $2j$, so that all monomials in $P_{j,l}$ are of the form

$$\Pi_{k=1}^{l-1} \partial^{\alpha_k} H$$

with $\sum_{k=1}^{l-1} |\alpha_k| = 2j$ and $\forall k,\ |\alpha_k| \geq 1$.

Remark 1 *We have also the following nice formula [4]: for any $l \geq 2$,*

$$\sum_j h^j P_{j,l}(x_0,\xi_0) = (H - H_0(x_0,\xi_0))^{\star(l-1)}(x_0,\xi_0)\ ,$$

where the power $(l-1)$ is taken w.r. to the star product.
Proof.–

Let us denote $h_0 = H_0(x_0,\xi_0)$. We have

$$z - \hat{H} = (z-h_0) - (\hat{H} - h_0)$$

and

$$(z-\hat{H})^{-1} = \sum_{l=1}^{\infty} (z-h_0)^{-l} (\hat{H}-h_0)^{l-1}$$

The formula follows then by identification of both expressions of the Weyl symbol of the resolvent at (x_0,ξ_0).

A less formal derivation is given by applying formula (3) to $f(E) = (E-h_0)^{l-1}$ and computing Weyl symbols at the point (x_0,ξ_0).

□

[4] I learned this formula from Laurent Charles

3 Moyal formula

Let us define the Moyal product $a \star b$ of the semi-classical symbols a and b by the rule:

$$\mathrm{Op}_{\mathrm{Weyl}}(\mathrm{a}) \circ \mathrm{Op}_{\mathrm{Weyl}}(b) = \mathrm{Op}_{\mathrm{Weyl}}(a \star b)$$

We have the well known "Moyal formula" (see [4]):

$$a \star b = \sum_{j=0}^{\infty} \frac{1}{j!} \left(\frac{h}{2i} \right)^j \{a, b\}_j$$

where

$$\{a, b\}_j(z) = [(\partial_\xi \partial_{x_1} - \partial_x \partial_{\xi_1})^j (a(z) \otimes b(z_1))]_{|z_1 = z}$$

with $z = (x, \xi)$, $z_1 = (x_1, \xi_1)$.

In particular $\{a, b\}_0 = ab$ and $\{a, b\}_1$ is the usual Poisson bracket.

From the Moyal formula, we deduce the following:

Proposition 1 *The Weyl symbol $\sum_j h^j R_j(z)$ of the resolvent $(z - \hat{H})^{-1}$ of $\hat{H}$ is given by*

$$\sum_{j=0}^{\infty} h^j R_j(z) = \frac{1}{z - H_0} + \sum_{j=1}^{\infty} h^j \sum_{l=2}^{L(j)} \frac{P_{j,l}}{(z - H_0)^l} \tag{1}$$

where the $P_{j,l}(x, \xi)$ are universal polynomials evaluated on the Taylor expansion of H at the point (x, ξ).

If $H = H_0$, only even powers of j occur: $R_{2j} = 0$.

Proof.–

The proposition follows directly from the evaluation by Moyal formula of the left-hand side of

$$(z - H) \star \left(\sum_{j=0}^{\infty} h^j R_j \right) = 1 \ .$$

The important point is that the poles at $z = H$ are at least of multiplicity 2 for $j \geq 1$.

Using

$$(z - H) \star \left(\sum_{j=0}^{\infty} h^j R_j \right) = \left(\sum_{j=0}^{\infty} h^j R_j \right) \star (z - H) = 1 \ ,$$

and the fact that $\{.,.\}_j$ are symmetric for even j's and antisymmetric for odd j's, we can prove the second statement by induction on j.

□

4 The method

Let $f \in C_o^\infty(I)$ and let us compute the trace $D(f) := \mathrm{Trace}(f(\widehat{H_W}))$ mod $O(h^\infty)$ in 2 different ways:

1. Using the eigenvalues given by Bohr-Sommerfeld rules we get:

$$\mathrm{Trace}(f(\widehat{H_W})) = \sum_{n \in \mathbb{Z}} f(S_h^{-1}(2\pi h n)) + O(h^\infty)$$

and, because $f \circ S_h^{-1}$ is a smooth function converging in the C_o^∞ topology to $f \circ S_0^{-1}$ we can apply Poisson summation formula and we get

$$D(f) = \frac{1}{2\pi h} \int_{\mathbb{R}} f(S_h^{-1}(u))|du| + O(h^\infty)$$

and

$$D(f) = \frac{1}{2\pi h} \int_{\mathbb{R}} f(E)\mathcal{S}'_h(E)|dE| + O(h^\infty)$$

or using Schwartz distributions:

$$\textbf{(a) } \mathbf{D} = \frac{\mathbf{1}}{\mathbf{2\pi h}} \mathcal{S}'_{\mathbf{h}}(\mathbf{E}) + \mathbf{O}(\mathbf{h}^\infty)$$

2. On the other hand, we compute the Weyl symbol of $f(\widehat{H})$ using Helffer-Sjöstrand's trick (see [4] p. 93):

$$f(\widehat{H}) = -\frac{1}{\pi} \int_{\mathbb{C}_{z=x+iy}} \frac{\partial F}{\partial \bar{z}}(z)(z - \widehat{H})^{-1}|dxdy| \qquad (2)$$

where $F \in C_0^\infty(\mathbb{C})$ is a *quasi-analytic extension of* f, i.e. F admits the Taylor expansion

$$F(x + \zeta) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x)\zeta^k$$

at any real x.

We start with the Weyl symbol of the resolvent (1).

We get then the symbol of $f(\hat{H})$ by puting Equation (1) into (2):

$$[f(\hat{H}) = \mathrm{Op_{Weyl}}\left(f(H_0) + \sum_{j \geq 1, l \geq 2} \frac{h^j}{(l-1)!} f^{(l-1)}(H_0) P_{j,l} \right) . \qquad (3)$$

The justification of this formal step is done in [4].

We then compute the trace by using

$$\mathrm{Tr}\left(\mathrm{Op}_{\mathrm{Weyl}}(a)\right) = \frac{1}{2\pi h}\int_{T^\star\mathbb{R}} a(x,\xi)|dxd\xi|\ .$$

We get:

$$D(f) = \frac{1}{2\pi h}\int_{T^\star\mathbb{R}}\left(f(H_0) + \sum_{j\geq 1, l\geq 2} h^j \frac{1}{(l-1)!} f^{(l-1)}(H_0)P_{j,l}\right)|dxd\xi|$$

We can rewrite using $|dtdE| = |dxd\xi|$ and integrating by parts:

$$(\mathbf{b})\ \mathbf{D} = \frac{\mathbf{1}}{\mathbf{2\pi h}}\left(\mathbf{T(E)} + \sum_{\mathbf{j\geq 1, l\geq 2}} \mathbf{h^j}\frac{(\mathbf{-1})^{\mathbf{l-1}}}{(\mathbf{l-1})!}\left(\frac{\mathbf{d}}{\mathbf{dE}}\right)^{\mathbf{l-1}}\int_{\gamma_{\mathbf{E}}} \mathbf{P_{j,l}|dt|}\right)$$

So we get, because $l \geq 2$, by identification of (a) and (b), for $j \geq 1$:

$$S_j(E) - \sum_{l\geq 2}\frac{(-1)^{l-1}}{(l-1)!}\left(\frac{d}{dE}\right)^{l-2}\int_{\gamma_E} P_{j,l}|dt| = C_j \tag{4}$$

where the C_j's are independent of E.

Proposition 2 *In the previous formula (4), the C_j's are also independent of the operator.*

Proof.–

We can assume that $(0,0)$ is in the disk whose boundary is A_-. Let us choose an Hamiltonian K which coïncides with H_W outside the disk bounded by A_- and with the harmonic oscillator

$$\hat{\Omega} = \mathrm{Op}_{\mathrm{Weyl}}(\frac{1}{2}(x^2+\xi^2))$$

near the origine. We can assume that K has no other critical values than 0.

We claim: for all $j \geq 1$,

1. $C_j(\hat{K}) = C_j(\hat{\Omega})$
2. $C_j(\hat{H}) = C_j(\hat{K})$

Both claims come from the following facts: let us give 2 Hamiltonians whose Weyl symbols coïncide in some ring $\mathcal{B}$, then

(i) The $P_{j,l}$ are the same for 2 operators in the ring $\mathcal{B}$ where both have the same Weyl symbol, because they are locally computed from the symbols which are the same.

(ii) The $S_j(E)$'s are the same for both operators because they have the same eigenvalues in the corresponding well modulo $O(h^\infty)$: both operators have the same WKB-Maslov quasi-modes in $\mathcal{B}$.

□

5 The case of the harmonic oscillator

Proposition 3 *For the harmonic oscillator, $C_1 = \pi$ and, for $j \geq 2$, $C_j = 0$.*

Proof.–

If $\hat{\Omega} = \mathrm{Op}_{\mathrm{Weyl}}(\frac{1}{2}(x^2 + \xi^2))$ is the harmonic oscillator we have:

$$S_h(E) = 2\pi E + \pi h$$

because $E_n = (n - \frac{1}{2})h$ for $n = 1, \cdots$.

It remains to compute the $P_{j,l}$'s. Let us put $\rho = \frac{1}{2}(x^2 + \xi^2)$, and

$$\sigma_{\mathrm{Weyl}}\left((z - \hat{\Omega})^{-1}\right) = \sum_{j=0}^{\infty} h^j R_j$$

It is clear that the R_j's are functions $f_j(\rho, z)$ and from Moyal formula we get:

$$f_{j+2} = -\frac{1}{4(z-\rho)}(f_j' + \rho f_j'')$$

and by induction on j:

$f_{2j+1} = 0$ and

$$f_{2j}(\rho, z) = \sum_{l=2j+1}^{l=3j+1} \frac{a_{l,j}\rho^{l-2j-1}}{(z-\rho)^l} \ ,$$

with $a_{j,l} \in \mathbb{R}$. The result comes from

$$\left(\frac{d}{dE}\right)^{l-2} \int_{\gamma_E} \rho^{l-2j-1} |dt| = 0 \ ,$$

if $l \geq 2j + 1$.

□

6 The term S_2

Let us assume first that $H = H_0$. From the Moyal formula, we have

$$R_2 = -\frac{1}{z - H_0}\{H_0, \frac{1}{z - H_0}\}_2 = -\frac{\Delta}{4(z - H_0)^3} - \frac{\Gamma}{4(z - H_0)^4}$$

with

$$\Delta = (H_0)_{xx}(H_0)_{\xi\xi} - ((H_0)_{x\xi})^2$$

and

$$\Gamma = (H_0)_{xx}((H_0)_\xi)^2 + (H_0)_{\xi\xi}((H_0)_x)^2 - 2(H_0)_{x\xi}(H_0)_x(H_0)_\xi \ .$$

Using formulae (1) and (4), we get:

$$S_2(E) = -\frac{1}{8}\frac{d}{dE}\int_{\gamma_E} \Delta|dt| + \frac{1}{24}\left(\frac{d}{dE}\right)^2 \int_{\gamma_E} \Gamma|dt| \tag{5}$$

Theorem 2 • *If $H = H_0$, we have*

$$S_2 = -\frac{1}{24}\frac{d}{dE}\int_{\gamma_E} \Delta|dt| \tag{6}$$

• *In the general case, we have:*

$$S_2 = -\frac{1}{24}\frac{d}{dE}\int_{\gamma_E} \Delta|dt| - \int_{\gamma_E} H_2|dt| + \frac{1}{2}\frac{d}{dE}\int_{\gamma_E} H_1^2|dt| \ .$$

Formula (5) were obtained in [1], formula (3.12), and formula (6) by Robert Littlejohn [6] using completely different methods.

Proof.–

Γdt is the restriction to γ_E of the 1-form α in $\mathbb{R}^2$ with

$$\alpha = ((H_0)_{xx}(H_0)_\xi - (H_0)_{x\xi}(H_0)_x)dx + ((H_0)_{x\xi}(H_0)_\xi - (H_0)_{\xi\xi}(H_0)_x)d\xi \ .$$

Orienting γ_E along the Hamiltonian flow, we get using Stokes formula:

$$\int_{\gamma_E} \Gamma|dt| = \int_{\gamma_E} \alpha = -\int_{D_E} d\alpha$$

where $\partial D_E = \gamma_E$ and D_E is oriented by $dx \wedge d\xi$. We have

$$d\alpha = -2\Delta dx \wedge d\xi$$

and hence:

$$\int_{\gamma_E} \Gamma|dt| = 2\int_{D_E} \Delta|dxd\xi| \ .$$

From $|dtdE| = |dxd\xi|$, we get:

$$\frac{d}{dE}\int_{D_E} \Delta|dxd\xi| = \int_{\gamma_E} \Delta|dt| \ .$$

So that:

$$\frac{d}{dE}\int_{\gamma_E} \Gamma|dt| = 2\int_{\gamma_E} \Delta|dt|$$

from which Theorem 2 follows easily.

□

7 Quantum numbers

Theorem 3 *The quantum number "n" in the Bohr-Sommerfeld rules corresponds exactly to the n'th eigenvalue in the corresponding well, i.e. the n'th eigenvalue of $\widehat{H_W}$.*

Proof.–

It is clear that the labelling of the eigenvalues of $\widehat{H_W}$ is invariant by homotopies leaving the symbol constant in $\mathcal{A}$. We can then change $\widehat{H_W}$ to $\hat{K}$ for which the result is clear because the quantization rules give then exactly all eigenvalues.

□

8 Extensions

8.1 2d phase spaces

The method applies to any 2d phase space using only 3 things:

- The star product
- The fact that the trace of operators is given by $(1/2\pi h)\times$ (the integral of their symbols)
- An example where you know enough to compute the C_j's

The power of our method is that it avoides the use of any Ansatz. Maslov contributions come only from the computation of an explicit example.

8.2 The cylinder $\mathbf{T}^\star(\mathbb{R}/\mathbb{Z})$

In that case, we replace the hypothesis by the following:

- We fix some compact intervall $I = [E_-, E_+] \subset \mathbb{R},\ E_- < E_+$, and we assume there exists a topological ring $\mathcal{A}$, *homotopic to the zero section of* $T^\star(\mathbb{R}/\mathbb{Z})$, such that $\partial\mathcal{A} = A_- \cup A_+$ with $A_\pm$ a connected component of $H^{-1}(E_\pm)$.
- We assume that H has no critical point in $\mathcal{A}$
- We assume that A_- is "below" A_+ (see Figure 2).

We will use the Weyl quantization for symbols which are of period 1 in x. *Then Theorem 1 holds.* The only change is S_1 which is now 0. The proof is the same except that the reference operator is now $\frac{h}{i}\partial_x$ instead of the harmonic oscillator.

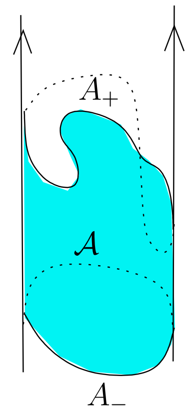

Figure 2: the cylinder

8.3 Other extensions

It should be nice to extend the previous method to the case of Toeplitz operators on 2-dimensional symplectic phase spaces, in the spirit of [2] and [3], and to the case of systems starting from the analysis in [5].

As remarked by Littlejohn, our method does not obviously extend to semi-classical completely integrable systems $\widehat{H_1}, \cdots, \widehat{H_d}$ with $d \geq 2$ degrees of freedom. The reason for that is that, using the same lines, we will get only the jacobian determinant of the d BS actions which is not enough to recover the actions even up to constants.

9 Relations with KdV

Let us consider the periodic Schrödinger equation $\hat{H} = -\partial_x^2 + q(x)$ with $q(x+1) = q(x)$. Let us denote by $\lambda_1 < \lambda_2 \leq \lambda_3 < \lambda_4 \leq \cdots$ the eigenvalues of the periodic problem for $\hat{H}$. Then the partition function

$$Z(t) = \sum_{n=1}^{\infty} e^{-t\lambda_n}$$

admits, as $t \to 0^+$, the following asymptotic expansion

$$Z(t) = \frac{1}{\sqrt{4\pi t}} \left(a_0 + a_1 t + \cdots + a_j t^j + \cdots \right) + O(t^\infty)$$

where the a_j's are of the following form

$$a_j = \int_0^1 A_j \left(q(x), q'(x), \cdots, q^{(l)}(x), \cdots \right) |dx|$$

where the A_j's are polynomials. The a_j's are called the Korteweg-de Vries invariants because they are independent of u if $q_u(x) = Q(x, u)$ is a solution of the Korteweg-de Vries equation. See [7], [8] and [11].

Let us translate the previous objects in the semi-classical context: we have $Z(h^2) = \mathrm{Tr}\left(\exp(-h^2\hat{H})\right)$ and $h^2\hat{H}$ is the semi-classical operator of order 0 whose Weyl symbol is $\xi^2 + h^2 q(x)$. If we put $f(E) = e^{-E}$, the partition function is exactly a trace of the form used in our method except that $E \to e^{-E}$ is not compactly supported. Nevertheless, the similarity between both situations is rather clear.

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