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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 address here is only about ways to compute these corrections. Existence of corrections to any order to Bohr-Sommerfeld rules is well known and can be found for example in [8] and [15] Section 4.5.

Our way to get these high-order corrections is inspired by A. Voros's thesis (1977) [13], [14]. 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.

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 [5] 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[1]

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

[1] 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 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 $\sigma_{\rm Weyl}(A)$ the Weyl symbol of the operator A.

The hypothesis:

- We fix some compact interval $I = [E_-, E_+] \subset \mathbb{R},\ E_- < E_+$, 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* $\widehat{H_W} = {\rm Op}_{\rm Weyl}(H_W)$ *is a self-adjoint bounded operator. The* semi-classical spectrum associated to the well W, *denoted by* σ_W, *is defined as follows:*

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

The previous definition is useful 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

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

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 $S_j(E),\ E \in I$.

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 $\gamma_E = H^{-1}(E) \cap \mathcal{A}$.

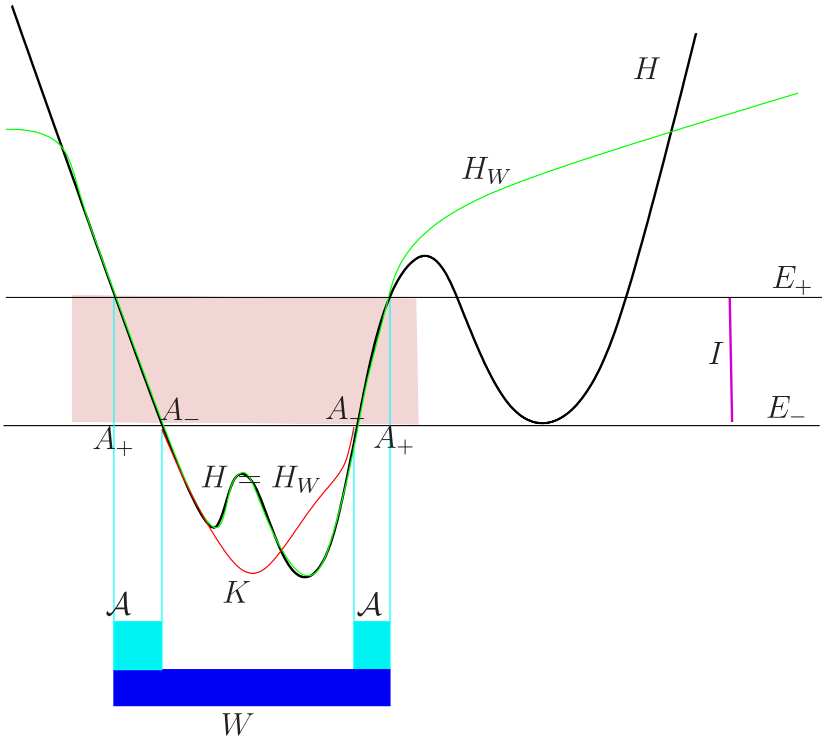

Figure 1. The phase space.

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* [2] *(see also [14]): 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). □

3 Moyal formula

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

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

[2] I learned this formula from Laurent Charles

We have the well-known "Moyal formula" (see [5]):

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

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 (see also [14]):

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 the 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 the 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:

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

2. On the other hand, we compute the Weyl symbol of $f(\widehat{H})$ using Helffer-Sjöstrand's trick (see [5] p. 93):

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

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 putting Equation (1) into (2):

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

The justification of this formal step is done in [5].

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:

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

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 coincides 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 origin. 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 coincide 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 $n = 1, \ldots$.

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

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

A very similar computation can be found in [9] p. 93, formula (0.13).

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

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

Theorem 2 • *If $H = H_0$, we have*

$$S_2 = -\frac{1}{24}\frac{d}{dE}\int_{\gamma_E} \Delta|dt|. \quad (6)$$

• *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 [10, 2] 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 nth eigenvalue in the corresponding well, i.e., the nth 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 avoids 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 interval $I = [E_-, E_+] \subset \mathbb{R},\ E_- < E_+$, 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).

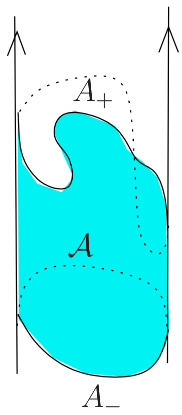

Figure 2. The cylinder.

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.

8.3 Other extensions

It would be nice to extend the previous method to the case of Toeplitz operators on two-dimensional symplectic phase spaces, in the spirit of [3] and [4], and to the case of systems starting from the analysis in [6].

As remarked by Littlejohn, our method does not obviously extend to semi-classical completely integrable systems $\widehat{H_1}, \ldots, \widehat{H_d}$ 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

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

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 [11], [12] and [16].

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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