A semi-classical inverse problem I: Taylor expansions.

(to the memory of Hans Duistermaat)

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Abstract

In dimension 1, we show that the Taylor expansion of a "generic" potential near a non degenerate critical point can be recovered from the knowledge of the semi-classical spectrum of the associated Schrödinger operator near the corresponding critical value. Contrary to the work of previous authors, **we do not assume that the potential is even.** The classical Birkhoff normal form does not contain enough information to determine the potential, but the quantum Birkhoff normal form does[1].

In a companion paper [5], the first author shows how the potential itself is, without any analyticity assumption and under some mild genericity hypotheses, determined by the semi-classical spectrum.

1 Introduction

In this paper[2], we will only consider a configuration space of dimension 1.

Let us consider a (classical) Hamiltonian

$$H(x,\xi) = \frac{1}{2}\xi^2 + V(x)$$

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[1]This work started from discussions we had during the Hans conference in Utrecht (August 2007). The proofs were completed independently by both authors two months later. We decided then to write a joint paper.

[2]Many thanks to Frédéric Faure for discussions and his computations

with $V(0)=E_0,\ V'(0)=0,\ V''(0)=\pm 1$(3). We have

$$H(x,\xi)\equiv E_0+\Omega_\pm+\sum_{j=3}^{\infty}a_jx^j$$

with $\Omega_\pm=\frac{1}{2}(\xi^2\pm x^2)$. The Hamiltonian H can be quantized as a Schrödinger operator $\hat{H}=-\frac{1}{2}\hbar^2\frac{d^2}{dx^2}+V(x)$ where the Taylor expansion of V at $x=0$ is $E_0+\sum_{j=2}^{\infty}a_jx^j$ with $a_2=\pm\frac{1}{2}$. This operator admits a semi-classical Birkhoff normal form [8] (denoted the QBNF) at the origin of which the Weyl symbol is a formal power series of the form

$$B\equiv\Omega_\pm+\sum_{2j+k\geq 2}b_{j,k}\hbar^{2j}\Omega_\pm^k\ . \tag{1}$$

In this paper, we are interested in the following "inverse spectral problem":

does the QBNF, given in (1), of the Schrödinger operator determine the Taylor series of V?

We cannot hope for a positive answer , because $V(x)$ and $V(-x)$ give the same QBNF. Moreover

Remark 1.1 the classical BNF does not suffice to determine the Taylor expansion of V at x=0

Let $y=f(x)=x+O(x^2)$ be an analytic function whose local inverse near 0 is of the form $x=y+g(y)$ with g an even *function. Then the Hamiltonian $H_f=\frac{1}{2}\left(\xi^2+f(x)^2\right)$ is classically conjugate to Ω_+ near the origin, in particular all its trajectories are of period 2π: it is enough to show that the action integrals $I(E)=\int_{\xi^2+f(x)^2\leq 2E}dxd\xi$ are the same; using the change of variable $x=y+g(y)$, we get $I(E)=\int_{\xi^2+y^2\leq 2E}(1+g'(y))dyd\xi$ and using the fact that g' is* odd *we get the result. A simple example is $V(x)=\frac{1}{2}\left(\sqrt{1+2x}-1\right)^2$. This result is reminiscent of the well known result for Zoll surfaces in Riemannian geometry [2].*

However, an even potential can be determined by the classical BNF, as a consequence of a result of N. Abel [1](4).

Our main result is:

Theorem 1.1 *The coefficients $\pm a_3$ and a_4 are determined from $b_{0,2}$ and $b_{1,0}$ by the formulas:*

$$a_3=\pm\sqrt{b_{1,0}},\ \ a_4=\frac{2}{3}b_{0,2}+\frac{5}{2}b_{1,0}\ .$$

If a_3 **does not vanish,** *all a_j's are determined from the $b_{0,k}$'s and the $b_{1,k}$'s once we have chosen the sign of a_3.*

(3) Assuming that $V''(0)=\pm 1$ does not affect the results below, because $a_2=V''(0)/2$ is known from the first eigenvalue if $a_2>0$ and from the density of states if $a_2<0$

(4) We are grateful to Hans for pointing this out to us

This result is reminiscent of the much more sophisticated results by Zelditch on the Kac problem [9]. If we use a (trivial) particular case of the result of [6], we get

Corollary 1.1 *If we know the asymptotic expansions of the eigenvalues $\lambda_n(\hbar)$ for all n's of a Schrödinger operator near the minimum $x = 0$ of the potential and $V''(0) > 0$, we know the value of $V'''(0)$ and, if $V'''(0) \neq 0$, the Taylor expansion of the potential at that point.*

In fact, we have the more precise result:

Corollary 1.2 *From the knowledge of the N first eigenvalues of $\hat{H}$ modulo $O(\hbar^{2N})$, one can recover the Taylor expansion of V to order $2N$.*

A similar result holds for a local non degenerate maximum of V using the "density of states" techniques. This is the content of Section 10:

Corollary 1.3 *If E_0 is a non degenerate local maximum of V and 0 is the only critical point of V on the set $V = E_0$, the knowledge of the semi-classical spectrum of $\hat{H}$ in some intervall $]E_0, E_1[$ (or $]E_1, E_0[$) determines $V'''(0)$ and, provided that $V'''(0) \neq 0$, the Taylor expansion of V at $x = 0$.*

and also in the case of a local minimum (Section 10.4):

Corollary 1.4 *If E_0 is a non degenerate local minimum of V and 0 is the only critical point of V on the set $V = E_0$, the knowledge of the semi-classical spectrum of $\hat{H}$ in some interval $]E_1, E_2[$, with $E_1 < E_0 < E_2$, determines $V'''(0)$ and, provided that $V'''(0) \neq 0$, the Taylor expansion of V at $x = 0$.*

Knowing the semi-classical spectrum as a function of $\hbar$ seems to be an huge amount of information. As was showed in [3], this is however the case for the effective Hamiltonians driving the propagation of waves inside a stratified medium.

2 A counterexample for a general Hamiltonian

The QBNF of a general Hamiltonian, **independent of** $\hbar$, $H(x,\xi) = \Omega_\pm + O(3)$ is not enough to know the Taylor expansion of H at the singular point. It is enough to consider $H = \frac{1}{2}\left((\xi - 3x^2)^2 + x^2\right)$ which is gauge equivalent to Ω_+ by the gauge transform $u \to ue^{ix^3}$.

3 Review of the Moyal product

The Moyal product is the product rule of symbols of Weyl quantized ΨDO's, it is given by:

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

with

$$\{a,b\}_j := \sum_{p=0}^{j} \left(\begin{array}{c} p \\ j \end{array} \right) (-1)^p \partial_x^p \partial_\xi^{j-p} a \partial_x^{j-p} \partial_\xi^p b \ .$$

We will also use the *Moyal bracket*,

$$[a,b]^\star = a \star b - b \star a \ .$$

We have

$$\frac{i}{\hbar}[a,b]^\star \equiv \sum_{j=0}^{\infty} \frac{1}{2j+1!} \left(\frac{\hbar}{2i}\right)^{2j} \{a,b\}_{2j+1} \ .$$

In particular, $\{a,b\}_1 = a_\xi b_x - a_x b_\xi$ is the Poisson bracket and

$$\{a,b\}_3 = a_{\xi\xi\xi} b_{xxx} - 3a_{\xi\xi x} b_{xx\xi} + 3a_{\xi xx} b_{x\xi\xi} - a_{xxx} b_{\xi\xi\xi} \ .$$

We have:

$$\frac{i}{\hbar}[a,b]^\star \equiv \{a,b\}_1 - \frac{\hbar^2}{24}\{a,b\}_3 + \frac{\hbar^4}{1920}\{a,b\}_5 + \cdots \ .$$

4 The Weyl algebra

The "Weyl algebra" which consists of formal power series in $\hbar$ and (x,ξ)

$$W = \sum_{j=2}^{\infty} W_j$$

where W_j is the space of polynomials in (x,ξ) and $\hbar$ of total degree j and the degree of $x^l \xi^m \hbar^n$ is $l+m+2n$. W is a graded algebra for the Moyal product: we have $W_j \star W_k \subset W_{j+k}$ and hence $\frac{i}{\hbar}[W_j, W_k]^\star \subset W_{j+k-2}$. Moreover, if we define W_j^+ as the subspace of W_j which is generated by monomials of even degree in $\hbar$, we have

$$\frac{i}{\hbar}[W_j^+, W_k^+]^\star \subset W_{j+k-2}^+ \ ;$$

we will define $W^+ = \sum_{j=3}^{\infty} W_j^+$ which is a Lie algebra for the bracket $\frac{\hbar}{i}[.,.]^\star$. W^+ is the (formal) Lie algebra of FIO's which are tangent to the identity at the the origin. The grading is obtained by looking at the action on the (graded) vector space of *symplectic spinors*: if $F \equiv \sum_{j=0}^{\infty} \hbar^j F_j(X)$ with $F \in \mathcal{S}(\mathbb{R})$, we define $f_\hbar(x) = \hbar^{-\frac{1}{2}} F(x/\hbar)$ whose microsupport is the origin. W^+ acts on this space of functions in a graded way as differential operators of infinite degree: if $w \in W$, $w.f = \mathrm{OP}_\hbar(w)(f)$.

5 Moyal versus functional QBNF

There are two different QBNF:

- The first one is a *Weyl symbol* $B \equiv \sum b_{j,k} \hbar^{2j} \Omega^k$ as before,
- The second one is an *operator* which is a formal power series of the harmonic oscillator $\hat{\Omega}$ of the form $\hat{B} \equiv \sum \widehat{b}_{j,k} \hbar^{2j} \hat{\Omega}^k$.

The second one is the Weyl quantization of the first. So they are equivalent. The equivalence can be made explicit in both direction by computing $\mathrm{Op}_{\mathrm{Weyl}}(\Omega^k)$ or the Weyl symbol of $\hat{\Omega}^k$. The functional form is useful in order to compute successive approximations of the eigenvalues, while the Weyl form is easier to compute using the Moyal product.

6 Useful Lemmas

The following result is classical:

Lemma 6.1 *The equation $\{\Omega_\pm, P\}_1 = Q$ where Q is a given homogeneous polynomial of degree N has a solution P, a homogeneous polynomial of degree N,*

- *if N is odd*
- *if $N = 2N'$ is even and $c_\pm(Q) = 0$ where $c_\pm$ is a linear form on the space of homogeneous polynomials of degree N which satisfies $c_\pm(\Omega_\pm^{N'}) = 1$. In particular, given Q, the equation $\{\Omega_\pm, P\}_1 = Q - c_\pm(Q)\Omega_\pm^{N'}$ has a solution.*

Remark 6.1 *In the case Ω_+, $c_+(Q)\Omega_+^{N'}$ is the average of Q under the natural action of S^1 on homogeneous polynomials of degree $2N'$.*

Definition 6.1 *We will denote by $\Sigma_{2N-1}^\pm$ the homogeneous polynomial of degree $2N-1$ which satisfies*

$$\{\Omega_\pm, \Sigma_{2N-1}^\pm\}_1 = x^{2N-1} \ .$$

Lemma 6.2 *We have*

$$\Sigma_{2N-1}^\pm = -\left(\pm x^{2N-2}\xi + \frac{2N-2}{3} x^{2N-4}\xi^3 + \cdots \right) \ .$$

We can also check the:

Lemma 6.3 *The polynomials $x^{2N'}$ are not Poisson brackets of the form $x^{2N'} = \{\Omega_\pm, P\}_1$, i.e. $c_\pm(x^{2N'}) \neq 0$.*

7 The QBNF

In order to reduce to the QBNF, we will use automorphisms of W^+ of the form

$$H \to H_S = \exp(iS/\hbar) \star H \star \exp(-iS/\hbar) = \exp\left(\frac{i}{\hbar} ad(S)^\star\right) H$$

with $S = S_3 + S_4 + \cdots \in W^+$. We get:

$$H_S = H + \frac{i}{\hbar}[S,H]^\star + \cdots + \frac{1}{k!}\left(\frac{i}{\hbar}\right)^k \overbrace{[S,[S,\cdots,[}^{k \text{ brackets}} S,H]^\star]^\star \cdots]^\star + \cdots ,$$

which is a convergent formal power series whose $k-$th term is of degree $\geq k+2$. The brackets will be calculated using the Moyal bracket. We remark that the terms of degree 0 in $\hbar$ give the calculation of the classical BNF (denoted CBNF) where the brackets are now just Poisson brackets.

8 The first terms

Let us consider $V(x) = \frac{1}{2}x^2 + ax^3 + bx^4 + \cdots$ whose QBNF is $\Omega + A\Omega^2 + B\hbar^2 + O(6)$ where $O(6)$ means terms of degree ≥ 6 in the Weyl algebra. Here we assume $\Omega = \frac{1}{2}(\xi^2 + x^2)$. Our first result is:

Theorem 8.1

$$A = -\frac{15}{4}a^2 + \frac{3}{2}b, \ B = a^2 .$$

The calculation: we start with $S = S_3 + S_4$ where $S_3(x,\xi)$(resp. $S_4(x,\xi)$) is a homogeneous polynomial of degree 3(resp. 4). There is no need to put terms in $\hbar^2$ in S_4 because they would be of the form $c\hbar^2$ which is in the center. We have then:

$$\exp(\frac{i}{\hbar}[S,.]^\star)H = \Omega + \frac{i}{\hbar}[S,H]^\star + \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 [S,[S,H]^\star]^\star + 0(6) .$$

By identification of terms of degree 3 and 4 and using the expression of the Moyal bracket $[.,.]^\star$:

$$\frac{i}{\hbar}[f,g]^\star = \{f,g\}_1 - \frac{1}{24}\hbar^2\{f,g\}_3 + \cdots ,$$

we get the system of equations:

$$\begin{cases} (3) & ax^3 + \{S_3,\Omega\}_1 = 0 \\ (4) & bx^4 + \{S_3,ax^3\}_1 + \{S_4,\Omega\}_1 + \frac{1}{2}\{S_3,\{S_3,\Omega\}_1\}_1 - \frac{1}{24}\hbar^2\{S_3,ax^3\}_3 = A\Omega^2 + B\hbar^2 \end{cases}$$

Using Equation (3), Equation (4) splits into 2 equations:

$$\begin{cases} (4') & -\frac{1}{24}\{S_3,ax^3\}_3 = B \\ (4'') & bx^4 + \frac{1}{2}\{S_3,ax^3\}_1 + \{S_4,\Omega\}_1 = A\Omega^2 \end{cases}$$

From Equation (3) and the formula for Σ_{2N-1} given in Lemma 6.1, we get

$$S_3 = -a(x^2\xi + \frac{2}{3}\xi^3) \ . \tag{2}$$

From Equation (4'), we get $B = a^2$. From Equation (4"), we get the value of A.

9 The induction

We carry out the proof in the case of Ω_+ and $E_0 = 0$. The minus case is similar.

Let us start with

$$H' = \Omega_+ + a_3x^3 + \cdots + a_{2N-2}x^{2N-2}$$

and $S' = S_3 + S_4 + \cdots + S_{2N-2}$ with $S_j \in W_j$, so that

$$\exp\left(\frac{i}{\hbar}[S', .]^\star\right) H' = \Omega_+ + B_4 + \cdots + B_{2N-2} + R_{2N-1} + R_{2N} + \cdots (:= B') \ ,$$

with

- $B_{2j} \in W_{2j}^+$ a polynomial in $\hbar^2$ and Ω_+
- For $n = 2N-1$ and $n = 2N$, $R_n \in W_n$.

In other words S' generates the transformation which converts H' into its QBNF mod $O(2N-1)$. The polynomials H' and S' and the partial QBNF B' are known by the induction hypothesis. We are now trying to get $S'' = S_{2N-1} + S_{2N}$ so that $S = S' + S''$ converts $H = H' + ax^{2N-1} + bx^{2N}$ into the QBNF mod $O(2N+1)$. We will only consider the terms of degree 0 and 2 in $\hbar$. So we can split every polynomial P_j in W_j^+ into $P_j = P_j^0 + \hbar^2 P_j^2 + \cdots$ with P_j^2 of degree $j-4$ in (x, ξ).

The equation to solve is:

$$\begin{aligned} \exp\left(\tfrac{i}{\hbar}[S' + S'', .]^\star\right)(H' + ax^{2N-1} + bx^{2N}) = \\ \Omega_+ + B_4 + \cdots + B_{2N-2} + B_{2N} + \quad O(2N+1) \end{aligned} \tag{3}$$

with $B_{2N} = b_{2N}^0\Omega_+^N + b_{2N}^2\hbar^2\Omega_+^{N-2} + \cdots$. We hope to recover a and b from b_{2N}^0 and b_{2N}^2 using what we know already at this step. The left handside of Equation (3) splits into:

$$\exp\left(\frac{i}{\hbar}[S' + S'', .]^\star\right)(ax^{2N-1} + bx^{2N}) = ax^{2N-1} + bx^{2N} + \frac{i}{\hbar}[S_3, ax^{2N-1}]^\star + O(2N+1) \ ,$$

and

$$\exp\left(\frac{i}{\hbar}[S' + S'', .]^\star\right) H' = B' + \frac{i}{\hbar}[S'', \Omega_+ + a_3x^3]^\star +$$

$$+\frac{1}{2}\left(\frac{i}{\hbar}\right)^2 ([S_{2N-1}, [S_3, \Omega_+]^\star]^\star + [S_3, [S_{2N-1}, \Omega_+]^\star]^\star) + 0(2N+1) \ .$$

So that, we get

- **In degree $2N-1$:**

$$ax^{2N-1} + \{S^0_{2N-1}, \Omega_+\}_1 + R^0_{2N-1} = 0$$

$$\{S^2_{2N-1}, \Omega_+\}_1 + R^2_{2N-1} = 0\ .$$

We see that S^2_{2N-1} is known at this step, while S^0_{2N-1} is modulo known terms a solution of

$$\{\Omega_+, S^0_{2N-1}\}_1 = ax^{2N-1}\ .$$

This equation gives, always mod known terms:

$$S^0_{2N-1} = a\Sigma_{2N-1}\ ,$$

with Σ_{2N-1} given by Definition 6.1.

- **In degree $2N$:**

$$bx^{2N} + \frac{i}{\hbar}\left([S_3, ax^{2N-1}]^\star + [S_{2N}, \Omega_+]^\star + [S_{2N-1}, a_3x^3]^\star\right) +$$

$$+\frac{1}{2}\left(\frac{i}{\hbar}\right)^2\left([S_{2N-1}, [S_3, \Omega_+]^\star]^\star + [S_3, [S_{2N-1}, \Omega_+]^\star]^\star\right) + R_{2N} = B_{2N} + O(2N+1)\ .$$

The previous equation gives one equation in $\hbar^0$ and one in $\hbar^2$:

  - **degree $2N$, hbar^0**

$$bx^{2N} + \{S_3, ax^{2N-1}\}_1 + \{S^0_{2N}, \Omega_+\}_1 + \{S^0_{2N-1}, a_3x^3\}_1 +$$

$$+\frac{1}{2}\{S^0_{2N-1}, \{S_3, \Omega_+\}_1\}_1 + \frac{1}{2}\{S_3, \{S^0_{2N-1}, \Omega_+\}_1\}_1 + R^0_{2N} = b^0_{2N}\Omega_+^N$$

  This can be simplified as:

$$\{\Omega_+, S^0_{2N}\}_1 = -b^0_{2N}\Omega_+^N + bx^{2N} + \frac{a}{2}\{S_3, x^{2N-1}\}_1 + \frac{a_3}{2}\{S^0_{2N-1}, x^3\}_1 + R^0_{2N} - \frac{1}{2}\{S_3, R^0_{2N-1}\}_1 \tag{4}$$

  This gives $b^0_{2N} = \beta_N b + \gamma_N a_3 a$ modulo known terms. Moreover, Lemma 6.3 implies $\beta_N \neq 0$.

  - **degree $2N$, hbar^2**

$$-\frac{1}{24}\left(\{S_3, ax^{2N-1}\}_3 + \{S^0_{2N-1}, a_3x^3\}_3\right) + \{S^2_{2N}, \Omega_+\}_1 +$$

$$+\frac{1}{2}\left(\{S^2_{2N-1}, \{S_3, \Omega_+\}_1\}_1 + \{S_3, \{S^2_{2N-1}, \Omega_+\}_1\}_1\right) -$$

$$-\frac{1}{48}\left(\{S^0_{2N-1}, \{S_3, \Omega_+\}_1\}_3 + \{S_3, \{S^0_{2N-1}, \Omega_+\}_1\}_3\right) + R^2_{2N} = b^2_{2N}\Omega_+^{N-2}$$

which can be simplified as:

$$\{\Omega_+, S_{2N}^2\}_1 = -b_{2N}^2\Omega_+^{N-2} - \frac{1}{48}\left(a\{S_3, x^{2N-1}\}_3 + a_3\{S_{2N-1}^0, x^3\}_3\right) + R_{2N}^2\,, \tag{5}$$

modulo known terms. This gives, using Lemma 6.1, $b_{2N}^2 = \delta_N a a_3$ modulo known terms.

From Equation (5) and the expressions for S_3 (Equation (2)) and Σ_{2N-1} (Lemma 6.2), we get:

$$\{\Omega_+, S_{2N}^2\}_1 = a a_3 \frac{(N-1)(2N^2-4N+3)}{3} x^{2N-4} - b_{2N}^2\Omega_+^{N-2} \text{ mod known terms} \tag{6}$$

Because x^{2N-4} is not a Poisson bracket with Ω_+ by Lemma 6.3, we get $\delta_N \neq 0$.

From the fact that β_N and δ_N do not vanish, this concludes the induction $N-1 \to N$.

10 Getting the QBNF from the density of states in case of a local extremum of the potential

10.1 $\hbar$-dependent distributions

Let $T_\hbar$ be an $\hbar$-dependent Schwartz distribution on an open interval J.

Definition 10.1 *The family $T_\hbar$ is*

- regular *at the point $E_0 \in J$ if there exists a sequence of functions T_j which are smooth in some neighbourhood K of E_0 with $j = j_0,\ j_0+1, \cdots$ ($j_0 \in \mathbb{Z}$), so that, for any $f \in C_o^\infty(K)$, we have the asymptotic expansion $T_\hbar(f) \equiv \sum_{j=j_0}^{+\infty} \hbar^j \int_J T_j(x) f(x)dx$.*

- right regular *(resp.* left regular*) at the point $E_0 \in J$ if there exists $E_1 > E_0$ (resp. $E_1 < E_0$) and a sequence of functions T_j which are smooth in some neighbourhood of E_0 with $j = j_0,\ j_0+1, \cdots$ ($j_0 \in \mathbb{Z}$), so that, for any $f \in C_o^\infty(]E_0, E_1[)$, we have the asymptotic expansion $T_\hbar(f) \equiv \sum_{j=j_0}^{+\infty} \hbar^j \int_J T_j(x) f(x)dx$.*

We will use the following notations:

Definition 10.2 *If $T_\hbar$ is a family of distributions on J and $E_0 \in J$, $T_\hbar^+$ (resp. $T_\hbar^-$), the* right (resp left) singular part of *$T_\hbar$ is the equivalence class of $T_\hbar$ modulo families of distributions which are right-(resp. left-)regular at the point E_0.*

10.2 Density of states

Consider a smooth potential $V : I \to \mathbb{R}$ where I is an open interval with $0 \in I$ and $\liminf_{x\to\partial I} V(x) = E_\infty > -\infty$ and let $\hat{H}$ be the Schrödinger operator with potential V.

Definition 10.3 *The* density of states *is the* $\hbar-$*dependent Schwartz distribution* $T_\hbar$ *on* $]-\infty, E_\infty[$ *defined by*

$$D_\hbar(f) := \mathrm{Trace} f(\hat{H}) \ .$$

Lemma 10.1 *If* J *is an open subset of* $]-\infty, E_\infty[$ *which contains no critical values of* V*, the density of states is regular at every point of* J*.*

Proof.–

Let us denote by $H = \frac{1}{2}\xi^2 + V(x)$ the symbol of the Schrödinger operator $\hat{H}$. The operator $f(\hat{H})$ is a pseudo-differential operator whose symbol $f^\star(H)$ is given (see [4]) by:

$$f^\star(H) = f(H) + \sum_{j\geq 1,\ l\geq 1} \hbar^{2j} P_{j,l}(x,\xi) f^{(l)}(H) \ ,$$

where the $P_{j,l}$'s are smooth functions locally computable from the symbol H. It is now enough to check that $f \to (2\pi\hbar)^{-1} \int\int P_{j,l}(x,\xi) f^{(l)}(H) dx d\xi$ is regular at each point of J using the fact that H has no critical value in J.

□

10.3 Singularity of the density of states near a local maximum of the potential

Let us assume that $V(0) = E_0 < E_\infty,\ V'(0) = 0$ and $V''(0) < 0$. Assume also that 0 is the unique critical point of V whose critical value is E_0.

We have the:

Theorem 10.1 *If the QBNF of* $\hat{H}$ *is*

$$B \equiv \Omega_- + \sum_{2j+k\geq 2} b_{j,k} \hbar^{2j} \Omega_-^k \ ,$$

the density of states is right and left singular at the point E_0 *and one can recover the full QBNF (the coefficients* $b_{j,k}$*) from the right (resp. left) singular part* $D_\hbar^+$ *(resp.* $D_\hbar^-$*)of the density of states* $D_\hbar$ *at* E_0*.*

In what follows, it is more convenient to use $\Omega_- = x\xi$.

10.3.1 The singularity of the density of states and the QBNF

Lemma 10.2 *If B is the QBNF of $\hat{H}$, the singular part of the density of states is the same as that of the family of distributions*

$$G_\hbar : f \to \frac{1}{2\pi\hbar}\int\int_D f^\star(B)dxd\xi \ ,$$

where $f^\star(B)$ is the Weyl symbol of $f(\hat{B})$ and D is the square $\max(|x|,|\xi|) \leq 1$.

Proof.–

Let $\Pi = \mathrm{Op}_{\mathrm{Weyl}}(\omega)$ be a compactly supported ΨDO whose Weyl symbol ω is $\equiv 1$ near $(0,0)$. We have

$$D_\hbar(f) = (2\pi\hbar)^{-1}\left(\int\int \omega \star f^\star(H)dxd\xi + \int\int(1-\omega)\star f^\star(H)dxd\xi\right) \ .$$

Using (the proof of) Lemma 10.1, the second term is a regular distribution. The first term can be transformed using the QBNF: there exists an FIO U, microlocally unitary, which transforms $\hat{H}$ into its QBNF and hence for every function f, we have:

$$U^\star f(\hat{B})U = f(\hat{H})$$

microlocally near the origin. In this way, we get

$$\mathrm{Trace}(\Pi \circ f(\hat{H})) \equiv \mathrm{Trace}(\Pi U^\star f(\hat{B})U) \ .$$

Introducing $\Pi_1 := U\Pi U^\star$ (a ΨDO whose Weyl symbol is $\equiv 1$ near the origin) and using the commutativity of the trace, we have:

$$\mathrm{Trace}(\Pi \circ f(\hat{H})) \equiv \mathrm{Trace}(\Pi_1 \circ f(\hat{B}))) \ .$$

It remains to check that, if $\Pi_1 = \mathrm{Op}_{\mathrm{Weyl}}(\omega_1)$, $f \to \int\int_{(I\times\mathbb{R})\setminus D} \omega_1 \star f^\star(B)dxd\xi$ is regular.

□

10.3.2 Computing some singularities

Lemma 10.3 *Let us consider the family of distributions*

$$K_\hbar(f) = \int\int_D f\left(\sum_{j=0}^{\infty}\hbar^{2j}b_j(x\xi)\right)dxd\xi$$

on $]E_0, E_1[$ *(we consider only the case* $E_1 > E_0$*, the other case is similar), where the* b_j*'s are smooth on* $[E_0, E_1]$ *and* $b_0(u) \equiv E_0 + \sum_{j=1}^{\infty} \beta_j u^j$ *with* $\beta_1 > 0$*. Then* $K_\hbar(f)$ *admits an asymptotic expansion in powers of* $\hbar$*:*

$$K_\hbar(f) \equiv \sum_{j=0}^{\infty} K_j(f)\hbar^{2j}$$

and the right singularities of $K_0, \cdots, K_N$ *at the point* E_0 *determine the Taylor expansions of* $b_0, \cdots, b_N$ *at the origin.*

Proof.–

Let us Taylor expand the integrand as:

$$\begin{aligned} f\left(\sum_{j=0}^{\infty} \hbar^{2j} b_j(x\xi)\right) &\equiv f(b_0(x\xi)) + f'(b_0(x\xi))\left(\sum_{j=1}^{\infty} \hbar^{2j} b_j(x\xi)\right) \\ &+ \sum_{k=2}^{\infty} \frac{1}{k!} f^{(k)}(b_0(x\xi))\left(\sum_{j=1}^{\infty} \hbar^{2j} b_j(x\xi)\right)^k . \end{aligned},$$

$$\equiv f(b_0(x\xi)) + \sum_{j=1}^{\infty} \hbar^{2j}\left(f'(b_0(x\xi))b_j(x\xi) + \sum_l f^{(l)}(b_0(x\xi))R_{j,l}(x\xi)\right),$$

where the functions $R_{j,l}$ depend only on $b_1, \cdots, b_{j-1}$.

We have to prove the following 2 facts:

1. The right singularity of

$$\int\int_D f(b_0(x\xi))dxd\xi$$

determines the Taylor expansion of b_0 at the origin.

2. The right singularity of

$$\int\int_D f'(b_0(x\xi))b_j(x\xi)dxd\xi$$

determines the Taylor expansion of b_j at the origin, assuming the Taylor expansion of b_0 is known.

Both are easy consequences of the following elementary calculus result:

$$\int\int_D f'(b_0(x\xi))b_j(x\xi)dxd\xi \equiv \int_{E_0}^{E_1} f'(t)b_j(c_0(t))c_0'(t)|\log(t-E_0)|dt$$

(modulo smooth distributions) where c_0 is the inverse function of b_0.

□

10.3.3 End of the proof of Theorem 10.1

We have

$$f^{\star}(B)(z_0) = \sum_{j=0}^{\infty} \frac{1}{2j!} \left(f^{(2j)}(B(z_0))(B - B(z_0))^{\star 2j} \right)(z_0) \ .$$

It is enough to check the:

Lemma 10.4 *If*

$$f^{\star}(B) \equiv f(B) + \sum_{j=1}^{\infty} \hbar^{2j} \sum_{l} f^{(2l)}(B) R_{j,l} \ ,$$

the $R_{j,l}$'s depend only on $b_0, \cdots, b_{j-1}$.

Proof.–

The $\star-$powers of $B - B(z_0)$ evaluated at z_0 start with terms in $\hbar^2$ and the b_l's, for $l \geq j$ have already an $\hbar^{2j}$ in front of them!

□

So everything works as if $f^{\star}(B) = f(B)$ and we are reduced to Lemma 10.3.

10.4 The case of a local minimum

The same strategy applies, but now the density of states is right AND left regular, with a jump singularity at the point E_0.

We get:

Theorem 10.2 *If the QBNF of $\hat{H}$ is*

$$B \equiv \Omega_+ + \sum_{2j+k \geq 2} b_{j,k} \hbar^{2j} \Omega_+^k \ ,$$

the density of states is singular at the point E_0 and one can recover the full QBNF (the coefficients $b_{j,k}$) from the singular part of the density of states $D_\hbar$ at E_0.

The proof is very similar to the case of a local maximum. We have now a "Heaviside singularity", meaning that the density of states is right AND left regular, but the functions T_j defined by

$$D_\hbar(f) = \sum_{j=-1}^{\infty} \int f T_j \hbar^j$$

and their derivatives have jumps at the point E_0. We have only to look at the singularities of $T : f \to \int f(\Omega_+) dx d\xi$. We have $T(f) = 2\pi \int_0^{+\infty} f(u) du$, so $T = 2\pi Y$ where Y is the Heaviside function.

11 Open problems

- **Is the result still true if $a_3 = 0$?** This is the case modulo some global assumption on V (see [5]). In fact in [5], it is shown that, modulo some genericity assumptions, the potential itself is determined from its semi-classical spectrum.
- **Is the result still valid in any dimension?** We think that the answer is no, at least it does not work with the same arguments; let us assume that the quadratic part of the Hamiltonian is $H_2 = \omega_1\Omega_1 + \omega_2\Omega_2$ with Ω_1 (resp. Ω_2) harmonic oscillators in x_1 (resp. x_2).
  - Non resonant case: ω_1 and ω_2 are independent over $\mathbb{Z}$. In degree 4, the QBNF has 4 unknown coefficients, an homogeneous polynomial of degree 2 in (Ω_1, Ω_2) and the coefficient of $\hbar^2$. On the other hand, $V_3(x_1, x_2) + V_4(x_1, x_2)$ has $9(> 4)$ coefficients. However, it is possible that higher terms in the QBNF give other information's...
  - Resonant case: $\omega_1 = \omega_2$. In degree 4, the classical BNF has already 9 coefficients (it is a polynomial of degree 4 on $\mathbb{R}^4$ invariant by the circle action generated by the flow of $\Omega_1 + \Omega_2$), this seems promising. However, we have to take into account an $O(2)$ action by isometries in $\mathbb{R}^2$: on one hand, we can only expect to determine the potential up to this action; on the other hand, the QBNF is determined only up to action by $SU(2)$.

12 Homogeneity properties of the QBNF

We have the following:

Theorem 12.1 *The $b_{j,k}$'s (coefficients of $\hbar^{2j}\Omega^k$ in the QBNF) satisfy the following homogeneity properties:*

$$b_{j,k}(ta_3, t^2a_4, \cdots, t^n a_{n+2}, \cdots) = t^{2(2j+k)-2} b_{j,k}(a_3, a_4, \cdots) \ .$$

Proof.–

Let us consider

$$\hat{H}_t = \frac{1}{2}\left(-\hbar^2 \frac{d^2}{dx^2} + x^2\right) + ta_3x^3 + \cdots + t^{n-2}a_n x^n + \cdots \ ,$$

and make the change of variable $tx = y$, $\hbar_1 = t^2\hbar$. We get a new operator

$$t^{-2}\left[\frac{1}{2}\left(-\hbar_1^2 \frac{d^2}{dy^2} + y^2\right) + a_3y^3 + \cdots + a_n y^n + \cdots\right] \ .$$

The spectrum of the second one is then t^{-2}times that of the first one. This implies the property.

$\square$

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