Regular Bohr-Sommerfeld quantization rules for a h-pseudo-differential operator

The method of positive commutators

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ABSTRACT. We revisit in this Note the well known Bohr-Sommerfeld quantization rule (BS) for a 1-D Pseudo-differential self-adjoint Hamiltonian within the algebraic and microlocal framework of Helffer and Sjöstrand; BS holds precisely when the Gram matrix consisting of scalar products of some WKB solutions with respect to the “flux norm” is not invertible.

RÉSUMÉ. Dans le cadre algébrique et microlocal élaboré par Helffer et Sjöstrand, on propose une ré-écriture de la règle de quantification de Bohr-Sommerfeld (BS) pour un opérateur auto-adjoint h-Pseudo-différentiel 1-D; elle s’exprime par la non-inversibilité de la matrice de Gram d’un couple de solutions WKB dans une base convenable, pour le produit scalaire associé à la “norme de flux”.

KEYWORDS : Semi-classical spectral asymptotics, quantization rules.

MOTS-CLÉS : Analyse spectrale semi-classique, règles de quantification.

1. Introduction

Let $p(x,\xi;h)$ be a smooth real classical Hamiltonian on $T^*\mathbb{R}$; we will assume that p belongs to the space of symbols $S^0(m)$ for some order function m (for example $m(x,\xi) = (1+|\xi|^2)^M$) with

$$S^N(m) = \{p \in C^\infty(T^*\mathbb{R}) : \forall\alpha \in \mathbb{N}^2, \exists C_\alpha > 0,\ |\partial^\alpha p(x,\xi;h)| \leq C_\alpha h^N m(x,\xi)\} \quad (1)$$

This allows to take Weyl quantization $P = p^w(x, h\,D_x; h)$ of p

$$P(x, hD_x; h)u(x;h) = (2\,\pi\,h)^{-1} \int\int e^{\frac{i}{h}\,(x-y)\,\eta}\, p\big(\frac{x+y}{2}, \eta; h\big)\, u(y)\, dy\, d\eta \qquad (2)$$

so that $p^w(x, h\,D_x; h)$ is self-adjoint. We also assume that $p+i$ is elliptic (in the classical sense). We call as usual p_0 the principal symbol, and p_1 the sub-principal symbol; in case of Schrödinger operator $P(x, h\,D_x; h) = (h\,D_x)^2 + V(x),\ p(x,\xi;h) = p_0(x,\xi) = \xi^2 + V(x)$. We make the hypothesis of [7], namely:

Fix some compact interval $I = [E_-, E_+], E_- < E_+$ and assume that there exists a topological ring $\mathcal{A} \subset p_0^{-1}(I)$ such that $\partial\,\mathcal{A} = A_+ \cup A_-$ with $A_\pm$ a connected component of $p_0^{-1}(E_\pm)$. Assume also that p_0 has no critical point in $\mathcal{A}$, and A_- is included in the disk bounded by A_+ (if this is not the case, we can always change p to $-p$). We define the microlocal well W as the disc bounded by par A_+.

For $E \in I$, let $\gamma_E \subset W$ be a periodic orbit in the energy surface $\{p_0(x,\xi) = E\}$ (so that γ_E is an embedded Lagrangian manifold).

Let $K_h^N(E)$ be the microlocal kernel of $P - E$ of order N, i.e. the space of local solutions of $(P-E)u = \mathcal{O}(h^{N+1})$ in the distributional sense, microlocalized on γ_E. This is a smooth complex vector bundle over $\pi_x(\gamma_E)$. Here we address the problem of finding the set of $E = E(h)$ such that $K_h^N(E)$ contains a global section, i.e. of constructing a sequence of quasi-modes (QM) $(u_n(h), E_n(h))$ of a given order N. As usual we denote by $K_h(E)$ the microlocal kernel of $P - E$ mod $\mathcal{O}(h^\infty)$; since the distinction between $K_h^N(E)$ and $K_h(E)$ plays no important role here, we shall content to write $K_h(E)$.

Then if $E_+ < E_0 = \liminf_{|x,\xi|\to\infty} p_0(x,\xi)$, all eigenvalues of P in I are indeed given by *Bohr-Sommerfeld quantization condition* (BS) $\mathcal{S}_h(E_n(h)) = 2\pi n h$, where the *semi-classical action* $\mathcal{S}_h(E)$ has the asymptotics

$$\mathcal{S}_h(E) \sim S_0(E) + hS_1(E) + h^2 S_2(E) + \cdots$$

We determine BS at any accuracy by computing quasi-modes. There are a lot of ways to derive BS: the method of matching of WKB solutions [3], known also as Liouville-Green method [15], which has received many improvements (see [21]), the method of the monodromy operator (see [12] and references therein), the method of quantization deformation based on Functional Calculus and Trace Formulas [14], [7], [6], [11], [1]. Note that the latter one already assumes BS, it only gives a very convenient way to derive it. In the real analytic case, BS rule, and also tunneling expansions, can be obtained using the so-called "exact WKB method" see e.g. [8], [9] when $P = -h^2\Delta + V(x)$ is Schrödinger operator.

Here we present another way to construct quasi-modes of order 2, based on [18], [13]. We stress that our method in the present scalar case, when carried to second order, is a bit more intricated than [14], [7] and its refinements [11]; it is most useful for matrix valued operators with double characteristics such as Bogoliubov-de Gennes Hamiltonian ([10], [4], [5]), or Born-Oppenheimer type Hamiltonians ([2], [16]).

2. The microlocal Wronskian

The best algebraic and microlocal framework for computing 1-D quantization rules in the self-adjoint case, cast in the fundamental works [18], [13], is based on Fredholm theory, and the classical "positive commutator method" using conservation of some quantity called a "quantum flux".

Bohr-Sommerfeld quantization rules result in constructing quasi-modes by WKB approximation along a closed Lagrangian manifold $\Lambda_E \subset \{p_0 = E\}$, i.e. a periodic orbit of Hamilton vector field H_p with energy E. This can be done locally according to the rank of the projection $\Lambda_E \to \mathbb{R}_x$.

Thus the set $K_h(E)$ of asymptotic solutions to $(P - E)\, u = 0$ along Λ_E can be considered as a bundle over $\mathbb{R}$ with a compact base, corresponding to the "classically allowed region" at energy E. The sequence of eigenvalues $E = E_n(h)$ is determined by the condition that the resulting quasi-mode, gluing together asymptotic solutions from different coordinates patches along Λ_E, be single-valued, i.e. $K_h(E)$ have trivial holonomy.

Assuming Λ_E is smoothly embedded in $T^*\mathbb{R}^2$, it can be always be parametrized by a non degenerate phase function. Of particular interest are the critical points of the phase functions, or focal points which are responsible for the change in Maslov index. Recall that $a(E) = (x_E, \xi_E) \in \Lambda_E$ is a focal point if Λ_E "turns vertical" at $a(E)$, i.e. $T_{a(E)}\Lambda_E$ is no longer transverse to the fibers $x = \mathrm{Const.}$ in $T^*\mathbb{R}$.

In any case, however, Λ_E can be parametrized locally either by a phase $S = S(x)$ (spatial representation) or a phase $S = \tilde{S}(\xi)$ (Fourier representation). Choose an orientation on Λ_E and for $a \in \Lambda_E$ (not necessarily a focal point), denote by $\rho = \pm 1$ its oriented segments near a. Let $\chi^a \in C_0^\infty(\mathbb{R}^2)$ be a smooth cut-off equal to 1 near a, and ω_ρ^a a small neighborhood of $\mathrm{supp}[P, \chi^a] \cap \Lambda_E$ near ρ. Here χ^a holds for $\chi^a(x, hD_x)$ as in (2), and we shall equally write $P(x, hD_x)$ (spatial representation) or $P(-hD_\xi, \xi)$ (Fourier representation).

Definition 2.1. *Let P be self-adjoint, and $u^a, v^a \in K_h(E)$ be supported on Λ_E. We call*

$$\mathcal{W}_\rho^a(u^a, \overline{v^a}) = \big(\frac{i}{h}\,[P, \chi^a]_\rho u^a | v^a\big) \tag{3}$$

the microlocal Wronskien *of $(u^a, \overline{v^a})$ in ω_ρ^a. Here $\frac{i}{h}\,[P, \chi^a]_\rho$ denotes the part of the commutateur supported microlocally on ω_ρ^a.*

To understand that terminology, let $P = -h^2\,\Delta + V$, $x_E = 0$, and change χ to Heaviside unit step function $\chi(x)$, depending on x alone. Then in distributional sense, we have $\frac{i}{h}[P, \chi] = -i\, h\, \delta' + 2\,\delta\, hD_x$, where δ denotes the Dirac measure at 0, and δ' its derivative, so that $\big(\frac{i}{h}\,[P, \chi] u | u\big) = -i\, h\,\big(u'(0)\,\overline{u(0)} - u(0)\,\overline{u'(0)}\big)$ is the usual Wronskien of $(u, \overline{u})$.

Proposition 2.1. *Let $u^a, v^a \in K_h(E)$ as above, and denote by $\widehat{u}$ the h-Fourier (unitary) transform of u. Then*

$$\big(\frac{i}{h}\,[P,\chi^a]u^a|v^a\big) = \big(\frac{i}{h}\,[P,\chi^a]\widehat{u}^a|\widehat{v}^a\big) = 0 \tag{4}$$

$$\big(\frac{i}{h}\,[P,\chi^a]_+u^a|v^a\big) = -\big(\frac{i}{h}\,[P,\chi^a]_-u^a|v^a\big) \tag{5}$$

(all equalities being understood mod $\mathcal{O}(h^\infty)$, resp $\mathcal{O}(h^{N+1})$ when considering $u^a, v^a \in K_h^N(E)$). Moreover, $\mathcal{W}^a_\rho(u^a, \overline{v^a})$ doesn't depend mod $\mathcal{O}(h^\infty)$ (resp $\mathcal{O}(h^{N+1})$) of the choice of χ^a as above.

Proof. Since $u^a, v^a \in K_h(E)$ are distributions in L^2, the first equality (4) follows from Plancherel formula and the regularity of microlocal solutions in L^2, $p+i$ being elliptic. If a is not a focal point, u^a, v^a are smooth WKB solutions near a, so we can expand the commutator in $\mathcal{W} = \big(\frac{i}{h}\,[P,\chi^a]u^a|v^a\big)$ and use that P is self-adjoint to show that $\mathcal{W} = \mathcal{O}(h^\infty)$. If a is a focal point, u^a, v^a are smooth WKB solutions in Fourier representation, so again $\mathcal{W} = \mathcal{O}(h^\infty)$. Then (5) follows from Definition 2.1. $\square$

We can find a linear combination of $\mathcal{W}^a_\pm$, (depending on a) which defines a sesquilinear form on $K_h(E)$, so that this Hermitean form makes of $K_h(E)$ a metric bundle, endowed with the gauge group $U(1)$. This linear combinaison is prescribed as the construction of Maslov index : namely we take $\mathcal{W}^a(u^a, \overline{u^a}) = \mathcal{W}^a_+(u^a, \overline{u^a}) - \mathcal{W}^a_-(u^a, \overline{u^a}) > 0$ when the critical point a of π_{Λ_E} is traversed in the $-\xi$ direction to the right of the fiber (or equivalently $\mathcal{W}^a(u^a, \overline{u^a}) = -\mathcal{W}^a_+(u^a, \overline{u^a}) + \mathcal{W}^a_-(u^a, \overline{u^a}) >$ when a is traversed in the $+\xi$ direction to the left of the fiber). Otherwise, just exchange the signs. When γ_E is a convex curve, there are only 2 focal points. In general there may be many focal points a, but each jump of Maslov index is compensated at the next focal point which is traversed to the other side of the fiber (co-cycle property). Maslov index is computed mod 4. Our method consists in constructing Gram matrix of a generating system of $K_h(E)$ in a suitable dual basis; its determinant vanishes precisely at the eigenvalues $E(h)$.

3. QM and BS in the case of a Schrödinger operator

As a warm-up, we derive the well known BS quantization rule using microlocal Wronskians in case of a potential well, i.e. γ_E is convex. Consider the spectrum of Schrödinger operator $P(x, hD_x) = (hD_x)^2 + V(x)$ near the energy level $E_0 < \liminf_{|x|\to\infty} V(x)$, when $\{V \le E\} = [x'_E, x_E]$ and x'_E, x_E are simple turning points, $V(x'_E) = V(x_E) = E$, $V'(x'_E) < 0, V'(x_E) > 0$. It is convenient to start the construction from the focal points a or a'. We set $a' = x'_E$, $a = x_E$, identifying the focal point $a = a_E = (x_E, 0)$ with its projection x_E. We know that microlocal solutions u of $(P-E)u = 0$ near a are of the form

$$u^a(x;h) = \frac{C}{\sqrt{2}}\big(e^{i\,\frac{\pi}{4}}\,(E-V(x))^{-\frac14}\,e^{\frac{i}{h}\,S(a,x)} + e^{-i\,\frac{\pi}{4}}\,(E-V(x))^{-\frac14}\,e^{-\frac{i}{h}\,S(a,x)} + \mathcal{O}(h)\big) \tag{6}$$

where $C \in \mathbb{C}$, $S(y,x) = \int_y^x \xi_+(t)\,dt$, and $\xi_+(t)$ is the positive root of $\xi^2 + V(t) = E$. In the same way, the microlocal solutions of $(P-E)u = 0$ near a' have the form, with $C' \in \mathbb{C}$

$$u^{a'}(x;h) = \frac{C'}{\sqrt{2}}\left(e^{-i\frac{\pi}{4}}\,(E-V(x))^{-\frac{1}{4}}\,e^{\frac{i}{h}S(a',x)} + e^{i\frac{\pi}{4}}\,(E-V(x))^{-\frac{1}{4}}\,e^{-\frac{i}{h}S(a',x)} + \mathcal{O}(h)\right) \tag{7}$$

These expressions result in computing by the method of stationary phase the oscillatory integral that gives the solution of $(P(-hD_\xi,\xi) - E)\,\widehat{u} = 0$ in Fourier representation. The change of phase factor $e^{\pm i\frac{\pi}{4}}$ accounts for Maslov index. For the sake of simplicity, we omit henceforth $\mathcal{O}(h)$ terms, but the computations below extend to all order in h (practically, at least for $N = 2$), thus giving the asymptotics of BS. This will be elaborated in the next Section.

The semi-classical distributions $u^a, u^{a'}$ span the microlocal kernel K_h of $P - E$ in $(x,\xi) \in]a', a[\times\mathbb{R}$; they are normalized using microlocal Wronskians as follows.

Let $\chi^a \in C_0^\infty(\mathbf{R}^2)$ as in the Introduction be a smooth cut-off equal to 1 near a. Without loss of generality, we can take $\chi^a(x,\xi) = \chi_1^a(x)\,\chi_2(\xi)$, so that $\chi_2 \equiv 1$ on small neighborhoods $\omega_\pm^a$, of $\operatorname{supp}(\frac{i}{h}[P,\chi^a]) \cap \{\xi^2 + V = E\}$ in $\pm\xi > 0$. We define $\chi^{a'}$ similarly. By (6) and (7) we have, mod $\mathcal{O}(h)$:

$$\frac{i}{h}[P,\chi^a]u^a = \sqrt{2}\,C\,(\chi_1^a)'(x)\left(e^{i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{\frac{i}{h}S(a,x)} - e^{-i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{-\frac{i}{h}S(a,x)}\right)$$

$$\frac{i}{h}[P,\chi^{a'}]u^{a'} = \sqrt{2}\,C'\,(\chi_1^{a'})'(x)\left(e^{-i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{\frac{i}{h}S(a',x)} - e^{i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{-\frac{i}{h}S(a',x)}\right)$$

Let

$$F_\pm^a(x;h) = \frac{i}{h}[P,\chi^a]_\pm\,u^a(x,h) = \pm\sqrt{2}\,C\,(\chi_1^a)'(x)\,e^{\pm i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{\pm\frac{i}{h}S(a,x)}$$

so that:

$$\begin{aligned}
(u^a|F_+^a - F_-^a) &= |C|^2\left(e^{i\frac{\pi}{4}}\,(E-V)^{-\frac{1}{4}}\,e^{\frac{i}{h}S(a,x)}|(\chi_1^a)'(x)\,e^{i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{\frac{i}{h}S(a,x)}\right)\\
&\quad + |C|^2\left(e^{-i\frac{\pi}{4}}\,(E-V)^{-\frac{1}{4}}\,e^{-\frac{i}{h}S(a,x)}|(\chi_1^a)'(x)\,e^{-i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{-\frac{i}{h}S(a,x)}\right)\\
&\quad = |C|^2\,\Big(\int(\chi_1^a)'(x)\,dx + \int(\chi_1^a)'(x)\,dx\Big) + \mathcal{O}(h) = 2\,|C|^2 + \mathcal{O}(h)
\end{aligned}$$

(the mixed terms such as $\left(e^{i\frac{\pi}{4}}\,(E-V)^{-\frac{1}{4}}\,e^{\frac{i}{h}S(a,x)}|(\chi_1^a)'(x)\,e^{-i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{-\frac{i}{h}S(a,x)}\right)$ are $\mathcal{O}(h^\infty)$ because the phase is non stationary), thus u^a is normalized mod $\mathcal{O}(h)$ if we choose $C = 2^{-1/2}$. In the same way, with

$$F_\pm^{a'}(x;h) = \frac{i}{h}[P,\chi^{a'}]_\pm\,u^{a'}(x,h) = \pm\sqrt{2}\,C'\,(\chi_1^{a'})'(x)\,e^{\mp i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{\pm\frac{i}{h}S(a',x)}$$

we get

$$(u^{a'}|F_+^{a'} - F_-^{a'}) = |C'|^2\,\Big(\int(\chi_1^{a'})'(x)\,dx + \int(\chi_1^{a'})'(x)\,dx\Big) + \mathcal{O}(h) = -2|C'|^2 + \mathcal{O}(h)$$

and we choose again $C' = C$ which normalizes $u^{a'}$ mod $\mathcal{O}(h)$. Normalization carries to higher order, as is shown in the next Section.

So there is a natural duality product between $K_h(E)$ and the span of functions $F_+^a - F_-^a$ and $F_+^{a'} - F_-^{a'}$ in L^2. As in [18], [13] we can show that this space is microlocally transverse to $\mathrm{Im}(P-E)$ on $(x,\xi) \in]a', a[\times\mathbb{R}$, and thus identifies with the microlocal co-kernel $K_h^*(E)$ of $P-E$; in general $\dim K_h(E) = \dim K_h^*(E) = 2$, unless E is an eigenvalue, in which case $\dim K_h = \dim K_h^* = 1$ (showing that $P-E$ is of index 0 when Fredholm.)

Microlocal solutions u^a and $u^{a'}$ extend as smooth solutions on the whole interval $]a', a[$; we denote them by u_1 and u_2. Since there are no other focal points between a and a', they are expressed by the same formulae (which makes the analysis particularly simple) and satisfy :

$$(u_1|F_+^a - F_-^a) = 1, \quad (u_2|F_+^{a'} - F_-^{a'}) = -1$$

Next we compute (still modulo $\mathcal{O}(h)$)

$$\begin{aligned}(u_1|F_+^{a'} - F_-^{a'}) &= \frac{1}{2}\big(e^{i\frac{\pi}{4}}\,(E-V)^{-\frac{1}{4}}\,e^{\frac{i}{h}S(a,x)}|(\chi_1^{a'})'(x)\,e^{-i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{\frac{i}{h}S(a',x)}\big)\\
&+\frac{1}{2}\big(e^{-i\frac{\pi}{4}}\,(E-V)^{-\frac{1}{4}}\,e^{-\frac{i}{h}S(a,x)}|(\chi_1^{a'})'(x)\,e^{i\frac{\pi}{4}}\,(E-V)^{\frac{1}{4}}\,e^{-\frac{i}{h}S(a',x)}\big)\\
&= \frac{i}{2}\,e^{-\frac{i}{h}S(a',a)}\int(\chi_1^{a'})'(x)\,dx - \frac{i}{2}\,e^{\frac{i}{h}S(a',a)}\int(\chi_1^{a'})'(x)\,dx\\
&= -\sin(S(a',a)/h)\end{aligned}$$

(taking again into account that the mixed terms are $\mathcal{O}(h^\infty)$). Similarly $(u_2|F_+^a - F_-^a) = \sin(S(a',a)/h)$. Now we define Gram matrix

$$G^{(a,a')}(E) := \begin{pmatrix} (u_1|F_+^a - F_-^a) & (u_2|F_+^a - F_-^a)\\ (u_1|F_+^{a'} - F_-^{a'}) & (u_2|F_+^{a'} - F_-^{a'})\end{pmatrix} \tag{8}$$

whose determinant $-1+\sin^2(S(a',a)/h) = -\cos^2(S(a',a)/h)$ vanishes precisely on eigenvalues of P in I, so we recover the well known BS quantization condition

$$\oint \xi(x)\,dx = 2\int_{a'}^{a}(E-V(x))^{\frac{1}{2}}\,dx = 2\,\pi\,h\,(k+\frac{1}{2}) + \mathcal{O}(h); \quad k\in\mathbb{Z} \tag{9}$$

and $\det G^{(a,a')}(E)$ is nothing but Jost function which is computed e.g. in [DeDi], [9] by another method.

4. The general case

By the discussion after Proposition 2.1, it clearly suffices to consider the case when γ_E contains only 2 focal points which contribute to Maslov index.

4.1. Well normalized quasi-modes mod $\mathcal{O}(h^2)$

Let $a = (x_E, \xi_E)$ be such a focal point. Following a well known procedure we can trace back to [17], we first seek for asymptotic solutions in Fourier representation near a of the form $\widehat{u}(\xi) = e^{i\psi(\xi)/h}b(\xi;h)$. Here the phase $\psi = \psi_E$ solves Hamilton-Jacobi equation $p_0(-\psi'(\xi),\xi) = E$, and can be normalized by $\psi(\xi_E) = 0$; the amplitude $b(\xi;h) = b_0(\xi) + hb_1(\xi) + \cdots$ has to be found recursively together with $a(x,\xi;h) = a_0(x,\xi) + ha_1(x,\xi) + \cdots$, such that

$$hD_\xi\big(e^{i(x\xi+\psi(\xi))/h}a(x,\xi;h)\big) = e^{i(x\xi+\psi(\xi))/h}b(\xi;h)$$
$$\times\big(p_0(x,\xi) - E + h\widetilde{p}_1(x,\xi) + h^2\widetilde{p}_2(x,\xi) + \mathcal{O}(h^3)\big)$$

p_0 being the principal symbol of P, $\widetilde{p}_1$ its sub-principal symbol for the standard (Feynman) quantization, etc.… Define $\lambda(x,\xi)$ by $p_0(x,\xi) - E = \lambda(x,\xi)(x + \psi'(\xi))$, we get first

$$\lambda(-\psi'(\xi),\xi) = \alpha(\xi) = \partial_x p_0(-\psi'(\xi),\xi)$$

This yields $a_0(x,\xi) = \lambda(x,\xi)b_0(\xi)$ and solving a first order ODE $L(\xi,D_\xi)b_0 = 0$, with $L(\xi,D_\xi) = \alpha(\xi)D_\xi + \big(\frac{1}{2i}\alpha'(\xi) - p_1(\psi'(\xi),\xi)\big)$ we get

$$b_0(\xi) = C_0|\alpha(\xi)|^{-1/2}e^{i\int\frac{p_1}{\alpha}}$$

with an arbitrary constant C_0, we take independent of E. This gives in turn $a_1(x,\xi) = \lambda(x,\xi)b_1(\xi) + \lambda_0(x,\xi)$, with

$$\lambda_0(x,\xi) = \frac{b_0(\xi)\widetilde{p}_1 + i\frac{\partial a_0}{\partial\xi}}{x + \partial_\xi\psi}$$

and $b_1(\xi)$ solution of $L(\xi,D_\xi)b_1 = \widetilde{p}_2 b_0 + i\partial_\xi\lambda_0|_{x=-\psi'(\xi)}$. We eventually get

$$b_0(\xi) + hb_1(\xi) = (C_0 + hC_1 + hD_1(\xi))|\alpha(\xi)|^{-1/2}e^{i\int\frac{p_1}{\alpha}}$$

where we have set

$$D_1(\xi) = \alpha(\xi_E)\int_{\xi_E}^{\xi}\big(i\widetilde{p}_2 b_0 - \partial_\xi\lambda_0|_{x=-\psi'(\xi')}\big)\,|\alpha(\xi')|^{-1/2}e^{-i\int\frac{p_1}{\alpha}}\,d\xi' \tag{10}$$

The integration constants $C_0, C_1, \cdots$ will be determined by normalizing the microlocal Wronskians as follows.

We compute $\mathcal{W}^a_\rho(u^a,\overline{u^a})$ in Fourier representation, with $\widehat{u}(\xi;h) = e^{i\psi(\xi)/h}b(\xi;h)$. Recall $\chi^a \in C_0^\infty(\mathbf{R}^2)$, $\chi^a \equiv 1$ near a_E; without loss of generality, we can take $\chi^a(x,\xi) = \chi_1(x)\chi_2(\xi)$, so that $\chi_2 \equiv 1$ on small neighborhoods $\omega^a_\pm$, of $\mathrm{supp}\frac{i}{h}[P,\chi^a] \cap \gamma_E$ in $\pm(\xi - \xi_E) > 0$. Thus we need only consider the variations of χ_1. Weyl symbol of $\frac{i}{h}[P,\chi^a]$ is given by $c(x,\xi;h) = \big(\partial_\xi p_0(x,\xi) + h\partial_\xi p_1(x,\xi)\big)\chi_1'(x) + \mathcal{O}(h^2)$, so

$$\frac{i}{h}[P,\chi^a]\widehat{u}(\xi) = (2\pi h)^{-1}\int\int e^{i\big(-(\xi-\eta)y+\psi(\eta)\big)/h}c(y,\frac{\xi+\eta}{2};h)(b_0 + hb_1)(\eta)\,dy\,d\eta$$

Evaluating by stationary phase, we find $\frac{i}{h}[P,\chi^a]\widehat{u}(\xi) = e^{i\psi(\xi)/h}d(\xi;h)$, where $d(\xi;h) = d_0 + hd_1 + \mathcal{O}(h^2)$ with $d_0 = c_0b_0$ and d_1 a function of c_0, c_1, b_0, b_1 we have determined so far. It follows

$$\big(\frac{i}{h}[P,\chi^a]_+\widehat{u}|\widehat{u}\big) = \int_{\xi_E}^{\infty} d_0(\xi)\overline{b_0(\xi)}\,d\xi + \mathcal{O}(h)$$

The leading term is simply

$$\int_{\xi_E}^{\infty} |b_0|^2 c_0 \, d\xi = |C_0|^2 \mathrm{sgn}(\alpha(\xi_E)) \int_{\xi_E}^{\infty} \chi_1'(-\psi'(\xi))\psi''(\xi) \, d\xi = |C_0|^2 \mathrm{sgn}(\alpha(\xi_E)) \quad (11)$$

so u^a is normalized mod $\mathcal{O}(h)$, provided $\alpha(\xi_E) > 0$, when $2|C_0|^2 = 1$; we take $C_0 = 1/\sqrt{2}$ as in Schrödinger case. Next step in normalization involves the term $D_1(\xi)$ defined in (10); integrating by parts, we can remove $\chi_1(\xi)$ and its second derivative, so to end up with a simple integral like (11). The computation being rather lengthy, we only state the final result:

Lemma 4.1. *With the hypotheses above, the microlocal Wronskian near a focal point a_E is given by*

$$\mathcal{W}^a(u^a, \overline{u^a}) = \big(\frac{i}{h}([P, \chi^a]_+ - [P, \chi^a]_-)\widehat{u}^a | \widehat{u}^a\big)$$
$$= 2 \, \mathrm{sgn}(\alpha(\xi_E)) \left(|C_0|^2 + h \, (2\mathrm{Re}(\overline{C_0} C_1) + |C_0|^2 \partial_x \big(\frac{p_1}{\partial_x p_0}\big)(\xi_E)) + \mathcal{O}(h^2)\right)$$

The condition that u^a be normalized mod $\mathcal{O}(h^2)$ (once we have chosen C_0 to be real), is then

$$C_1(E) = -\frac{1}{2} \, C_0 \, \partial_x \big(\frac{p_1}{\partial_x p_0}\big)(\xi_E)$$

so that now $\mathcal{W}^a(u^a, \overline{u^a}) = 2\mathrm{sgn}(\alpha(\xi_E)) C_0^2 \big(1 + \mathcal{O}(h^2)\big)$. This procedure carries to any order, we say then that u^a is *well-normalized*. It can be formalized by considering $\{a_E\}$ as a *Poincaré section*, and Poisson operator the operator that assigns to the initial condition C_0 on $\{a_E\}$, in a unique way, the well-normalized (forward) solution u^a to $(P - E)u^a = 0$; see next Section.

The next task consists in extending the solutions away from a_E in the spatial representation. First we expand $u^a(x) = (2\pi h)^{-1/2} \int e^{i\psi(\xi)/h} \, b(\xi; h) \, d\xi$ near a by stationary phase, selecting the 2 critical points $\xi_\rho(x) = \xi_\pm(x)$, that correspond to the phase functions $\varphi_\rho(x) = x\xi_\rho(x) + \psi(\xi_\rho(x))$. So we have

$$u^a(x; h) = u_+^a(x; h) + u_-^a(x; h)$$
$$= \frac{1}{\sqrt{2}} \sum_{\pm} \left(\frac{\partial_\xi \, p_0\big(x, \xi_\pm(x)\big)}{i} \right)^{-\frac{1}{2}} e^{\frac{i}{h} \, S_\pm(x_E, x; h)} \big(1 + \mathcal{O}(h)\big) \quad (12)$$

where

$$S_\pm(x_E, x; h) = \varphi_\pm(x_E, x) + h \int_{\xi_E}^{\xi_\pm(x)} \frac{p_1\big(-\psi'(\zeta), \zeta\big)}{\alpha(\zeta)} \, d\zeta + \sqrt{2} \, h^2 \, \mathrm{Im}\Big(D_1(\xi_\pm(x))\Big) \quad (13)$$

and $\varphi_\pm(x_E, x) = x_E \, \xi_E + \int_{x_E}^{x} \xi_\pm(y) \, dy$. Then we use standard WKB theory with Ansatz $u_\rho^a(x) = a_\rho(x; h) e^{i\varphi_\rho(x)/h}$. Let $\beta_0(x) = \partial_\xi \, p_0\big(x, \varphi'(x)\big) = -\dfrac{\alpha\big(\xi(x)\big)}{\xi'(x)}$, $\beta_1(x) = \partial_\xi \, p_1\big(x, \varphi'(x)\big)$. Omitting the index ρ, we find the usual half-density

$$a_0(x) = \widetilde{C_0} \, |\beta_0(x)|^{-\frac{1}{2}} \, \exp\left(-i \int \frac{p_1\big(x, \varphi'(x)\big)}{\beta_0(x)} \, dx \right)$$

with a new constant $\widetilde{C}_0 \in \mathbf{R}$; the next term is

$$a_1(x) = \big(\widetilde{C_1} + \widetilde{D}_1(x)\big)\, |\beta_0(x)|^{-\frac{1}{2}} \exp\Big(-i \int \frac{p_1\big(x,\varphi'(x)\big)}{\beta_0(x)}\, dx \Big)$$

and $\widetilde{D}_1(x)$ a complex function with

$$\mathrm{Re}\big(\widetilde{D}_1(x)\big) = -\frac{\widetilde{C_0}}{2}\, \frac{\beta_1(x)}{\beta_0(x)} + \mathrm{Const.}$$

and

$$\mathrm{Im}\big(\widetilde{D}_1(x)\big) = \widetilde{C_0}\, \big(\int \frac{\beta_1(x)}{\beta_0^2(x)}\, p_1\big(x,\varphi'(x)\big)\, dx - \int \frac{p_2\big(x,\varphi'(x)\big)}{\beta_0(x)}\, dx \big) \tag{14}$$

4.2. The homology class of the generalized action

Here we identify the various terms in (10) and (14). First on γ_E we have $\psi(\xi) = \displaystyle\int -x\, d\xi + \mathrm{Const.}$, and $\varphi(x) = \displaystyle\int \xi\, dx + \mathrm{Const.}$. By Hamilton equations

$$\dot{\xi}(t) = -\partial_x p_0\big(x(t),\xi(t)\big), \quad \dot{x}(t) = \partial_\xi p_0\big(x(t),\xi(t)\big)$$

so on γ_E we have $\displaystyle\int \frac{p_1}{\alpha}\, d\xi = -\int \frac{p_1}{\partial_\xi p_0}\, dx = -\int_{\gamma_E} p_1\, dt$. The form $p_1\, dt$ is called the subprincipal 1-form. Next we consider $D_1(\xi)$ as the integral over γ_E of the 1-form, defined near a in Fourier representation as

$$\Omega_1 = T_1\, d\xi = \mathrm{sgn}(\alpha(\xi))\, \big(i\, \widetilde{p}_2\, b_0 - \partial_\xi \lambda_0\big)\, |\alpha|^{-1/2}\, e^{-i \int \frac{p_1}{\alpha}}\, d\xi$$

Using WKB constructions, Ω_1 can also be extended in the spatial representation. Since γ_E is Lagrangian, Ω_1 is a closed form that we are going to compute modulo exact forms. Using integration by parts, the integral of $\Omega_1(\xi)$ in Fourier representation simplifies to

$$\sqrt{2}\, \mathrm{Re}\big(D_1(\xi)\big) = -\frac{1}{2}\, \big[\partial_x\big(\frac{p_1}{\partial_x p_0}\big)(-\psi'(\zeta),\zeta)\big]_{\xi_E}^{\xi} \tag{15}$$

$$\sqrt{2}\, \mathrm{Im}\big(D_1(\xi)\big) = \int_{\xi_E}^{\xi} T_1(\zeta)\, d\zeta + \big[\frac{\psi''}{6\,\alpha}\, \frac{\partial^3 p_0}{\partial x^3} + \frac{\alpha'}{4\,\alpha^2}\, \frac{\partial^2 p_0}{\partial x^2}\big]_{\xi_E}^{\xi} \tag{16}$$

$$\begin{aligned} T_1(\zeta) = {} & \frac{1}{\alpha}\left(p_2 - \frac{1}{8}\, \frac{\partial^4 p_0}{\partial x^2 \partial \zeta^2} + \frac{\psi''}{12}\, \frac{\partial^4 p_0}{\partial x^3 \partial \zeta} + \frac{(\psi'')^2}{24}\, \frac{\partial^4 p_0}{\partial x^4}\right) + \frac{1}{8}\, \frac{(\alpha')^2}{\alpha^3}\, \frac{\partial^2 p_0}{\partial x^2} \\ & + \frac{1}{6}\, \psi''\, \frac{\alpha'}{\alpha^2}\, \frac{\partial^3 p_0}{\partial x^3} - \frac{p_1}{\alpha^2}\, \big(\partial_x p_1 - \frac{p_1}{2\,\alpha}\, \frac{\partial^2 p_0}{\partial x^2}\big) \end{aligned} \tag{17}$$

Eq. (15) already shows that $\mathrm{Re}(\Omega_1)$ is exact. We can carry the integration in x-variable between the focal points a_E and a'_E, and in ξ-variable again near a'_E. Now let $\Omega(x,\xi) = f(x,\xi)\, dx + g(x,\xi)\, d\xi$, where $f(x,\xi), g(x,\xi)$ are any smooth functions on $\mathcal{A}$. By Stokes formula

$$\int_{\gamma_E} \Omega(x,\xi) = \int \int_{\{p_0 \le E\}} \big(\partial_x g - \partial_\xi f\big)\, dx \wedge d\xi$$

where, following [CdV], we have extend p_0 inside the disk bounded by A_- so that it coincides with a harmonic oscillator in a neighborhood of the origin ($p_0(0) = 0$, say). Making the symplectic change of coordinates $(x, \xi) \mapsto (t, E)$:

$$\int\int_{\{p_0 \leq E\}} \big(\partial_x g - \partial_\xi f\big)\, dx \wedge d\xi = \int_0^E \int_0^{T(E')} \big(\partial_x g - \partial_\xi f\big)\, dt \wedge dE' \tag{18}$$

where $T(E')$ is the period of the flow of Hamilton vector field H_{p_0} at energy E' ($T(E')$ being a constant near 0). Using these expressions, we recover the well known action integrals (see e.g. [7]):

Lemma 4.2. *Let $\Gamma\, dt$ be the restriction to γ_E of the 1-form*

$$\omega_0(x,\xi) = \left(\frac{\partial^2 p_0}{\partial x^2}\frac{\partial p_0}{\partial \xi} - \frac{\partial^2 p_0}{\partial x\,\partial \xi}\frac{\partial p_0}{\partial\, x}\right) dx + \left(\frac{\partial^2 p_0}{\partial x\,\partial \xi}\frac{\partial p_0}{\partial \xi} - \frac{\partial^2 p_0}{\partial \xi^2}\frac{\partial\, p_0}{\partial x}\right) d\xi$$

We have $\mathrm{Re} \oint_{\gamma_E} \Omega_1 = 0$, *whereas*

$$\mathrm{Im} \oint_{\gamma_E} \Omega_1 = \frac{1}{48}\,\big(\frac{d}{dE}\big)^2 \int_{\gamma_E} \Gamma\, dt - \int_{\gamma_E} p_2\, dt - \frac{1}{2}\frac{d}{dE}\int_{\gamma_E} p_1^2 \tag{19}$$

4.3. BS quantization rule

Recall from (12) the asymptotic solution $u^a(x; h)$ near $a = a_E$. In the last term of (13) we can substitute (16) with T_1 as in (17), that is

$$\sqrt{2}\,\mathrm{Im}\big(D_1(\xi_\pm(x))\big) = \int_{x_E}^x T_1(\xi_\pm(y))\, \xi'_\pm(y)\, dy$$

Similarly, the asymptotic solution near $a' = a'_E$ is given by

$$\begin{aligned} u^{a'}(x;h) &= u_+^{a'}(x;h) + u_-^{a'}(x;h) \\ &= \frac{1}{\sqrt{2}} \sum_\pm \left(\frac{\partial_\xi\, p_0\big(x, \xi_\pm(x)\big)}{-i}\right)^{-\frac{1}{2}} e^{\frac{i}{h} S_\pm(x'_E, x; h)} \big(1 + \mathcal{O}(h)\big) \end{aligned} \tag{20}$$

where as in (12), using (16) and (17)

$$S_\pm(x'_E, x; h) = \varphi_\pm(x'_E, x) - h\int_{x'_E}^x \frac{p_1(y, \xi_\pm(y))}{\partial_\xi p_0(y, \xi_\pm(y))}\, dy + h^2 \int_{x'_E}^x T_1(\xi_\pm(y))\, \xi'_\pm(y)\, dy \tag{21}$$

and similarly for $S_\pm(x_E, x; h)$. The semi-classical distributions $u^a, u^{a'}$ are well normalized as in Lemma 4.1. We compute $F_\pm^a = \dfrac{i}{h}[P, \chi^a]_\pm u_\pm^a$. Still mod $\mathcal{O}(h)$

$$F_\pm^a(x;h) = \pm\,\frac{1}{\sqrt{2}}\, e^{\pm\, i\,\frac{\pi}{4}} \Big(\pm\, \partial_\xi p_0\big(x, \xi_\pm(x)\big)\Big)^{\frac{1}{2}} e^{\frac{i}{h} S_\pm(x_E, x; h)}\, \frac{d\chi_1^a}{dx}(x) \tag{22}$$

and using that the mixed terms $(u_\pm^a | F_\mp^a)$ are $\mathcal{O}(h^\infty)$, we find $(u^a | F_+^a - F_-^a) \equiv 1$ mod $\mathcal{O}(h)$. In the same way, near a' we have $(u^a | F_+^a - F_-^a) \equiv -1$. The normalized microlocal solutions u^a and $u^{a'}$, uniquely extended along γ_E, are now called u_1 and u_2. They verify

$$(u_1 | F_+^{a'} - F_-^{a'}) = \frac{i}{2}\left(e^{\frac{i}{h} A_-(x_E, x'_E; h)} - e^{\frac{i}{h} A_+(x_E, x'_E; h)}\right) \tag{23}$$

$$(u_2|F_+^a - F_-^a) = \frac{i}{2}\Big(e^{-\frac{i}{h}A_-(x_E,x'_E;h)} - e^{-\frac{i}{h}A_+(x_E,x'_E;h)}\Big) \tag{24}$$

where the generalized actions are given by

$$A_\pm(x_E,x'_E;h) = S_\pm(x_E,x;h) - S_\pm(x'_E,x;h) = (x_E - x'_E)\,\xi_E +$$

$$\int_{x_E}^{x'_E} \xi_\pm(y)\,dy - h\int_{x_E}^{x'_E} \frac{p_1\big(y,\xi_\pm(y)\big)}{\partial_\xi p_0\big(y,\xi_\pm(y)\big)}\,dy + h^2\int_{x_E}^{x'_E} T_1\big(\xi_\pm(y)\big)\,\xi'_\pm(y)\,dy$$

We have

$$\int_{x'_E}^{x_E}\big(\xi_+(y) - \xi_-(y)\big)\,dy = \oint_{\gamma_E}\xi(y)\,dy$$

$$\int_{x'_E}^{x_E}\Big(\frac{p_1\big(y,\xi_+(y)\big)}{\partial_\xi p_0\big(y,\xi_+(y)\big)} - \frac{p_1\big(y,\xi_-(y)\big)}{\partial_\xi p_0\big(y,\xi_-(y)\big)}\Big)\,dy = \int_{\gamma_E} p_1\,dt$$

$$\int_{x'_E}^{x_E}\Big(T_1\big(\xi_+(y)\big)\,\xi'_+(y) - T_1\big(\xi_-(y)\big)\,\xi'_-(y)\Big)\,dy = \operatorname{Im}\oint_{\gamma_E}\Omega_1\big(\xi(y)\big)$$

On the other hand, Gram matrix as in (8) has determinant

$$-\cos^2\big(\frac{A_-(x_E,x'_E;h) - A_+(x_E,x'_E;h)}{2h}\big)$$

which vanishes precisely when BS holds. Summing up, we eventually obtain:

Proposition 4.1. *With the notations and hypotheses stated in the Introduction, BS is given in the interval I by $\mathcal{S}_h(E) = 2\,\pi\,n\,h$, $n\in\mathbb{Z}$, where the semi-classical action $\mathcal{S}_h(E) \sim S_0(E) + h\,S_1(E) + h^2\,S_2(E) + \cdots$ consists of :*

(i) *the classical action*

$$S_0(E) = \oint_{\gamma_E}\xi(x)\,dx = \int\int_{\{p_0\le E\}\cap W} d\xi\wedge dx$$

(ii) *Maslov index and the integral of the sub-principal 1-form $p_1\,dt$*

$$S_1(E) = -\pi - \int_{\gamma_E} p_1\big(x(t),\xi(t)\big)\,dt$$

(iii) *the second order term*

$$S_2(E) = \frac{1}{24}\frac{d}{dE}\int_{\gamma_E}\Delta\,dt - \int_{\gamma_E} p_2\,dt - \frac{1}{2}\frac{d}{dE}\int_{\gamma_E} p_1^2\,dt$$

where

$$\Delta(x,\xi) = \frac{\partial^2 p_0}{\partial x^2}\frac{\partial^2 p_0}{\partial \xi^2} - \big(\frac{\partial^2 p_0}{\partial x\,\partial\xi}\big)^2$$

We recall that $S_3(E) = 0$. Note that the signs in front of the first and third term of our formula for $S_2(E)$ differ from those in [7].

5. The discrete spectrum of P in I

Here we recover the fact that BS determines asymptotically all eigenvalues of P in I. We adapt the argument of [19]. It is convenient to think of $\{a_E\}$ and $\{a'_E\}$ as zero-dimensional "Poincaré sections" of γ_E. Let $\mathcal{K}^a(E)$ be the operator (Poisson operator) that assigns to its "initial value" $C_0 \in L^2(\{a_E\}) \approx \mathbb{R}$ the well normalized solution $u(x;h) = \int e^{\frac{i}{h}(x\,\xi+\psi(\xi))}\, b(\xi;h)\, d\xi$ to $(P-E)u = 0$ near $\{a_E\}$. By construction, we have:

$$\pm\mathcal{K}^a(E)^*\, \frac{i}{h}[P,\chi^a]_\pm\, \mathcal{K}^a(E) = \mathrm{Id}_{a_E} = 1 \tag{25}$$

We define objects "connecting" a to a' along γ_E as follows: let $T = T(E) > 0$ such that $\exp TH_{p_0}(a) = a'$. Choose χ^a_f (f for "forward") be a cut-off function supported microlocally near γ_E, equal to 0 along $\exp tH_{p_0}(a)$ for $t \leq \epsilon$, equal to 1 along γ_E for $t \in [2\,\epsilon, T+\epsilon]$, and back to 0 next to a', e.g. for $t \geq T + 2\,\epsilon$. Let similarly χ^a_b (b for "backward") be a cut-off function supported microlocally near γ_E, equal to 1 along $\exp tH_{p_0}(a)$ for $t \in [-\epsilon, T-2\,\epsilon]$, and equal to 0 next to a', e.g. for $t \geq T-\epsilon$. By (25) we have

$$\mathcal{K}^a(E)^*\, \frac{i}{h}[P,\chi^a]_+\, \mathcal{K}^a(E) = \mathcal{K}^a(E)^*\, \frac{i}{h}[P,\chi^a_f]\, \mathcal{K}^a(E) = 1 \tag{26}$$

$$-\mathcal{K}^a(E)^*\, \frac{i}{h}[P,\chi^a]_-\, \mathcal{K}^a(E) = -\mathcal{K}^a(E)^*\, \frac{i}{h}[P,\chi^a_b]\, \mathcal{K}^a(E) = 1 \tag{27}$$

which define a left inverse $R^a_+(E) = \mathcal{K}^a(E)^*\, \frac{i}{h}\,[P,\chi^a_f]$ to $\mathcal{K}^a(E)$ and a right inverse $R^a_-(E) = -\frac{i}{h}[P,\chi^a_b]\,\mathcal{K}^a(E)$ to $\mathcal{K}^a(E)^*$. We define similar objects connecting a' to a, $T' = T'(E) > 0$ such that $\exp T'H_{p_0}(a) = a'$ ($T = T'$ if p_0 is invariant by time reversal), in particular a left inverse $R^{a'}_+(E) = \mathcal{K}^{a'}(E)^*\, \frac{i}{h}\,[P,\chi^{a'}_f]_+$ to $\mathcal{K}^{a'}(E)$ and a right inverse $R^{a'}_-(E) = -\frac{i}{h}\,[P,\chi^{a'}_b]\,\mathcal{K}^{a'}(E)$ to $K^{a'}(E)^*$, with the additional requirement

$$\chi^a_b + \chi^{a'}_b = 1 \tag{28}$$

near γ_E. Define now the pair $R_+(E)u = (R^a_+(E)u, R^{a'}_+(E)u)$, $u \in L^2(\mathbb{R})$ and $R_-(E)$ by $R_-(E)u_- = R^a_-(E)\,u^a_- + R^{a'}_-(E)\,u^{a'}_-$, $u_- = (u^a_-, u^{a'}_-) \in \mathbb{C}^2$, we call Grushin operator $\mathcal{P}(z)$ the operator defined by the linear system

$$\frac{i}{h}\,(P-z)u + R_-(z)u_- = v, \quad R_+(z)\,u = v_+ \tag{29}$$

From [19], we know that the problem (29) is well posed, and

$$\mathcal{P}(z)^{-1} = \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix}$$

with $(P-z)^{-1} = E(z) - E_+(z)\,E_{-+}(z)^{-1}\,E_-(z)$. Actually one can show that the effective Hamiltonian $E_{-+}(z)$ is Gram matrix (8). There follows that the spectrum of P in I is precisely the set of E we have determined by BS quantization rule

6. References

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