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Bohr–Sommerfeld Quantization Condition Derived by a Microlocal WKB Method

Setsuro Fujiié[1] and Maher Zerzeri[2]

[1] *Mathematical Institute of Tohoku University, Aoba, Aramaki-aza, Aoba-Ku, Sendai 980-8578, Japan*
[2] *Département de Mathématiques, Université Paris Nord, Paris, France*

Abstract. It is useful to consider the WKB method on the phase space via the global FBI transformation. It enables us to avoid the difficulty arising from caustics. As an application, the Bohr–Sommerfeld quantization condition is obtained.

1. Introduction

The purpose of this paper is to explain in an elementary way the microlocal WKB method via FBI transformation used for the study of semiclassical distribution of eigenvalues or resonaces. In order to make the calculation explicit (especially the Maslov index) and clarify its utility, we study the simplest case, that is, the one-dimensional Schrödinger equation with a simple-well potential and show the derivation of the well-known Bohr–Sommerfeld quatization rule of eigenvelues. Gérard and Sjöstrand studied in [2] a more general multi-dementional case for the semiclassical quantization condition of resonances created by a hyperbolic closed trajectory.

Let us consider the eigenvalue problem

$$Pu = Eu, \tag{1.1}$$

where

$$P = -h^2 \frac{d^2}{dx^2} + V(x)$$

is the one-dimensional Schrödinger operator with potential $V(x)$. We assume $V(x)$ is a real-valued analytic function on $\mathbb{R}$ and the classically allowed region $\{x \in \mathbb{R}; V(x) \leq E_0\}$ is a connected interval $[\alpha, \beta]$ $(-\infty < \alpha < \beta < +\infty)$. We assume moreover that $V'(\alpha) < 0, V'(\beta) > 0$. For $E \in (E_0 - \epsilon, E_0 + \epsilon)$

with sufficiently small ϵ, the classically allowed region is still connected interval $[\alpha(E), \beta(E)]$.

It is well known that the eigenvalues near E_0 satisfy the so-called *Bohr–Sommerfeld quantization condition* in the semiclassical limit $h \to 0$

$$C(E) = (2n+1)\pi h + O(h^2), \quad n \in \mathbb{N} = \{0, 1, 2, ...\}, \tag{1.2}$$

where the function $C(E)$ is the *action integral* defined by

$$C(E) = 2 \int_{\alpha(E)}^{\beta(E)} \sqrt{E - V(x)} dx. \tag{1.3}$$

In the case of the harmonic oscillator $V(x) = x^2$, this function can be calculated and one has $C(E) = \pi E$. The eigenvalues are known to be $\{(2n+1)h\}_{n=0}^{\infty}$, and the Bohr–Sommerfeld quantization condition (1.2) holds exactly without remainder term.

The quantization condition (1.2) is usually derived by the WKB method applied on the configuration space $\mathbb{R}_x$, or rigorously by the so-called complex WKB method or exact WKB method on $\mathbb{C}_x$. WKB solutions are defined on the regions bounded by the turning points $\alpha(E)$ and $\beta(E)$ (i.e. the classically allowed region $(\alpha(E), \beta(E))$ and the classically forbidden regions $(-\infty, \alpha(E))$, $(\beta(E), +\infty)$), and the connection formulae between these solutions at the turning points give the global behavior of the solution and in particular the quantization condition of eigenvalues.

The microlocal method we shall study, on the other hand, is also a WKB method but applied on the phase space $\mathbb{R}^2_{x,\xi} = T^*\mathbb{R}$. This makes us free from turning point and avoid the connection problem.

Let $p(x, \xi) = \xi^2 + V(x)$ be the semiclassical symbol of P and

$$H_p = \frac{\partial p}{\partial \xi}\frac{\partial}{\partial x} - \frac{\partial p}{\partial x}\frac{\partial}{\partial \xi} = 2\xi\frac{\partial}{\partial x} - V'(x)\frac{\partial}{\partial \xi}$$

the Hamilton vector field. The Hamilton flow $\exp tH_p$ is invariant on the energy surface $p^{-1}(E) = \{(x, \xi) \in \mathbb{R}^2; p(x, \xi) = E\}$ for each fixed energy E. Put

$$K(E) = \{(x, \xi) \in p^{-1}(E); \exp tH_p \not\to \infty \quad \text{as} \quad |t| \to \infty\}.$$

This is called the *trapped set*. In our setting, it is a simple closed curve with period $T = T(E)$

$$\{\gamma(t)\}_{t=0}^{T} = \{(x(t), \xi(t))\}_{t=0}^{T}, \quad \gamma(0) = \gamma(T)$$

subject to the Hamilton equation

$$\begin{cases} \dot{x}(t) = 2\xi(t) \\ \dot{\xi}(t) = -V'(x(t)), \end{cases} \quad p(x(0),\ \xi(0)) = E,$$

which in fact coincides with the energy surface $p^{-1}(E)$. The period $T(E)$ can be written as

$$T(E) = 2\int_{\alpha(E)}^{\beta(E)} \frac{dx}{\dot{x}} = \int_{\alpha(E)}^{\beta(E)} \frac{dx}{\sqrt{E - V(x)}} = C'(E).$$

The action integral $C(E)$ is then the volume of the domain in the phase space bounded by the curve γ, or equivalently the integral of the canonical 1 form ξdx over the curve $\gamma(E)$,

$$C(E) = \int_{\gamma(E)} \xi dx. \tag{1.4}$$

Our method is based on the fact that the eigenfunction corresponding to an eigenvalue E is localized on the trapped set $K(E) = \gamma$ in the semiclassical limit. Microlocal semiclassical behavior of a function $u(x,h)$ will be measured via the so-called *global FBI transformation* T. T is a unitary operator from L^2 on the configuration space $\mathbb{R}$ into L^2 on the phase space $\mathbb{R}^2_{x,\xi}$, and an L^2-normalized function u is said to be localized on a set if Tu is exponentially small on the complement.

The microlocal WKB method consists in reducing the original equation (1.1) on the configuration space to an equation on the phase space conjugating by T, and constructing a WKB solution along γ. Roughly speaking, the condition that the WKB solution is single-valued along γ gives the quantization condition in the semiclassical limit.

An advantage of this method is that we do not encounter the connection problem at the turning points. In other words, the Maslov index 1, which appears on the right hand side of (1.2), is derived in a geometrical way by our method while it comes from the Airy-type connection formula at each turning point by the usual WKB method.

2. Global FBI Transformation

In this section, we define the global FBI transformation and review some elements of the microlocal and semiclassical analysis. Here the dimension is arbitrary and will be denoted by n. For proofs and more details, see [1].

For $u(y,h) \in \mathcal{S}'(\mathbb{R}^n)$, and $z = x - i\xi \in \mathbb{C}^n$, we define the *global FBI transform* (or Bargman transform) by

$$(Tu)(z;h) = \langle u, e^{-(z-\cdot)^2/2h} \rangle = \int_{\mathbb{R}^n} e^{-(z-y)^2/2h} u(y) dy$$
$$= e^{\xi^2/2h} \int_{\mathbb{R}^n} e^{i(x-y)\cdot\xi/h - (x-y)^2/2h} u(y,h) dy,$$

We denote the integral of the last expression by

$$(\tilde{T}(x,\xi;h)u) = c_{n,h} \int_{\mathbb{R}^n} e^{i(x-y)\cdot\xi/h - (x-y)^2/2h} u(y,h) dy,$$

where $c_{n,h} = 2^{-n/2}(\pi h)^{-3n/4}$ is a normalization constant in the sense of Proposition 2.1, (2).

The following properties can easily be checked.

Proposition 2.1.
(1) *For $u \in \mathcal{S}'$, $(Tu)(z;h)$ is an entire function with respect to z.*
(2) *$\tilde{T}$ is unitary from $L^2(\mathbb{R}^n)$ to $L^2(\mathbb{R}^{2n})$, that is,*

$$\|\tilde{T}u\|_{L^2(\mathbb{R}^{2n}_{x,\xi})} = \|u\|_{L^2(\mathbb{R}^n_x)}.$$

(3) *The image of $L^2(\mathbb{R}^n)$ by $\tilde{T}$ is $e^{-\xi^2/2h}\mathcal{H}(\mathbb{C}^n_z) \cap L^2(\mathbb{R}^{2n}_{(x,\xi)})$ and the adjoint is given by*

$$(\tilde{T}^* v)(x;h) = c_{n,h} \int\int e^{i(x-y)\cdot\xi/h-(x-y)^2/2h} v(y,\xi)dyd\xi.$$

Next we see the action of the global FBI transformation on pseudo-differential operators. Let P be the pseudo-differential operator whose semiclassical Weyl symbol is $p(x,\xi)$:

$$Pu = \frac{1}{(2\pi h)^n} \int\int_{\mathbb{R}^{2n}} e^{i(x-y)\cdot\xi/h} p\left(\frac{x+y}{2}, \xi\right) u(y)dyd\xi.$$

Then we have the following formula:

Proposition 2.2. *Let $p(x,\xi)$ be a symbol defined on $\mathbb{R}^2_{x,\xi}$ and $q(z,\zeta)$ be the symbol on the I-Lagrangian manifold*

$$\Lambda = \{(z,\zeta) \in \mathbb{C}^{2n};\ \mathrm{Re}\,\zeta = -\mathrm{Im}\ z,\ \mathrm{Im}\ \zeta = 0\}$$

defined by

$$q(z,\zeta) = p(z + i\zeta, \zeta).$$

Then one can naturally define the pseudo-differential operator Q whose semiclassical Weyl symbol is q and one has

$$T \circ P = Q \circ T.$$

Finally we define the *microsupport* of a distribution u and review some properties concerning the microsupport when u satisfies an analytic differential equation.

Definition 2.3. *For $u \in \mathcal{S}'(\mathbb{R}^n)$ (h-dependent) and $(x_0,\xi_0) \in \mathbb{R}^{2n}$, one says that u is microlocally exponentially small near (x_0,ξ_0) if and only if there exists $\delta > 0$ such that*

$$\tilde{T}u(x,\xi;h) = O(e^{-\delta/h})$$

uniformly for (x,ξ) in a neighborhood of (x_0,ξ_0) and sufficiently small $h > 0$. The complement of such points (x_0,ξ_0) is called the microsupport of u and denoted by $MS(u)$.

The microsupport $MS(u)$ coincides with the analytic wave front set $WF_a(u)$ defined by Hörmander [3] when u is independent of h, more precisely,

$$MS(u) = WF_a(u) \cup [\operatorname{Supp} u \times \{0\}].$$

The following propositions are analogies of the h-independent case.

Proposition 2.4. *If $Pu = 0$ and u is locally normalized by L^2 norm, then $MS(u) \subset Char(P)$ where $Char(P) = \{(x, \xi); p(x, \xi) = 0\}$ and p is the principal symbol of P.*

Proposition 2.5. *Assume $Pu = 0$ and u is locally normalized by L^2 norm. Then $MS(u)$ is invariant under the flow of H_p.*

As one of the most important properties of the h-dependent case, we have the following proposition which says that the microsupport of a WKB solution is included in the Lagrangian manifold defined by the phase function:

Proposition 2.6. *If $u(x; h) = a(x, h) \exp(i\phi(x)/h)$ and u is locally normalized by L^2 norm, where a is an analytic symbol, then $MS(u) \subset \{(x, \xi); \xi = \partial_x \phi(x)\}$.*

3. Derivation of the Bohr–Sommerfeld Quantization Condition

In this section, we derive the Bohr–Sommerfeld quantization condition (1.2) by the microlocal WKB method applied on the phase space via the global FBI transformation.

Let $p(x, \xi) = \xi^2 + V(x)$ be the semiclassical Weyl symbol of the Schrödinger operator. By the change of the dependent variable $v(z, h) = Tu$, the equation (1.1) is reduced to the equation

$$Qv = Ev, \tag{3.1}$$

where Q is the pseudo-differential operator whose semiclassical Weyl symbol is

$$q(z, \zeta) = p(z + i\zeta, \zeta)$$

(see Proposition 2.2). This can be written as $q = p \circ \kappa^{-1}$ with the canonical transformation

$$\kappa : (x, \xi) \mapsto (z, \zeta) = (x - i\xi, \xi).$$

The new symbol $q(z, \zeta)$ is defined on $\Lambda = \{(z, \zeta) \in \mathbb{C}^{2n}; \operatorname{Re} \zeta = -\operatorname{Im} z, \operatorname{Im} \zeta = 0\}$. It is important to notice that the projection π of Λ on $\mathbb{C}_z$ is bijective while the projection of the phase space $\mathbb{R}^2_{x,\xi}$ on the configuration space $\mathbb{R}_x$ is not injective.

The Hamiltonian flow $(z(t), \zeta(t))$ of q defined on Λ by the Hamilton equation

$$\begin{cases} \dot{z} = \partial_\zeta q(z, \zeta), \\ \dot{\zeta} = -\partial_z q(z, \zeta) \end{cases} \tag{3.2}$$

is the image by κ of the Hamiltonian flow $(x(t), \xi(t))$ of p:

$$(z(t), \zeta(t)) = \kappa(x(t), \xi(t)).$$

It is a curve on the energy surface $q^{-1}(E) = \{(z, \zeta) \in \Lambda; q(z, \zeta) = E\}$ for a fixed energy E.

By the simple well assumtion on the potential $V(x)$ (see Introduction), the Hamiltonian flow of p on $p^{-1}(E)$, $E \in (E_0 - \epsilon, E_0 + \epsilon)$ is a simple periodic curve $\gamma(E)$, and so is the Hamiltonian flow $\kappa \circ \gamma(E)$ of q on $q^{-1}(E)$. The action $C(E) = \int \xi dx$ (see (1.3) and (1.4)) and the period $T(E)$ are also invariant by κ:

$$C(E) = \int_{\pi \circ \kappa \circ \gamma(E)} \zeta dz, \quad T(E) = C'(E) = \int_{\alpha(E)}^{\beta(E)} \frac{dx}{\sqrt{E - V(x)}}.$$

Now we study the eigenvalue problem (1.1), that is, look for energies E near E_0 with which there exists a non-trivial solution $u \in L^2(\mathbb{R})$. Conjugating the equation with the global FBI transformation T, we see by Proposition 2.1 that E is an eigenvalue if and only if

(Q_1) There exists a non-trivial solution $v(z; E, h)$ of (2.1) satisfying

$$v(z; E, h) \in \mathcal{H}(\mathbb{C}_z) \cap e^{\xi^2/2h} L^2(\mathbb{R}^2_{x,\xi}).$$

The equation (3.1) has, in general, singular points. For example, in the case of harmonic oscillator, since $p(x, \xi) = \xi^2 + x^2$ and $q(z, \zeta) = p(z + i\zeta, \zeta) = z^2 + 2iz\zeta$, the reduced operator Q on $\mathbb{C}_z$ is

$$Q = 2izhD_z + z^2 + h.$$

For this operator, the origin $z = 0$ is a regular singular point. Hence in general the solution v of (3.1) is ramified around this point.

On the other hand, we also know by any one of Propositions 1.4, 1.5, 1.6 that the microsupport of u is included in $\gamma(E)$, that is $v = Tu$ is localized on $\gamma(E)$ in the semiclassical limit if E is an eigenvalue. From this point of view, it is natural to modify the condition (Q_1) as follows:

(Q_2) There exists a non-trivial solution $v(z; E, h)$ of (3.1) which is single-valued on $\pi \circ \kappa \circ \gamma(E)$.

The condition (Q_2) can be studied by the WKB method. Put

$$v(z; E, h) = a(z; E, h) e^{i\psi(z;E)/h}, \quad a(z; E, h) \sim \sum_{j-0}^{n} a_j(z; E) h^j. \tag{3.3}$$

We then obtain the eikonal and the transport equations for the phase ψ and each term a_j of the symbol a respectively. In particular the eikonal equation and the first transport equation are as follows:

$$q(z; \psi') = E, \tag{3.4}$$

$$\partial_\zeta q(z, \psi') \frac{da_0}{dz} + \frac{1}{2}\{\partial_\zeta^2 q(z, \psi')\psi'' + \partial_z \partial_\zeta q(z, \psi')\} a_0 = 0, \tag{3.5}$$

where $' = d/dz$. Note that

$$\frac{d}{dz}\{\partial_\zeta q(z, \psi'(z))\} = \partial_\zeta^2 q(z, \psi')\psi'' + \partial_z \partial_\zeta q(z, \psi').$$

So the first transport equation (3.5) can be solved explicitly and one gets

$$a_0(z) = \text{const.}\{\partial_\zeta q(z, \psi')\}^{-1/2}. \tag{3.6}$$

Now to understand the condition (Q_2), we continue the WKB solution (3.3) along the closed trajectory $\pi \circ \kappa \circ \gamma(E)$.

First we have

$$\begin{aligned}(Q_2) &\iff a(z(t), h)\exp(i\psi(z(t))/h)|_{t=0}^{T} = 0,\\ &\iff \frac{a(z(T), h)}{a(z(0), h)} \exp\{i(\psi(z(T)) - \psi(z(0)))/h\} = 1.\end{aligned}$$

On $\kappa \circ \gamma(E)$, we have $\zeta = \psi'(z)$ by the eikonal equation (3.4), and hence

$$\psi(z(T)) - \psi(z(0)) = \int_{z(0)}^{z(T)} \psi' dz = \int_\gamma \zeta dz = C(E).$$

Thus we obtain

$$(Q_2) \iff C(E) - ih \log M(E, h) = 2n\pi h \quad (n \in \mathbb{Z}),$$

where

$$M(E, h) = \frac{a(z(T), h)}{a(z(0), h)}.$$

Next we replace a by its principal term a_0:

$$M(E, h) = \frac{a_0(z(T))}{a_0(z(0))}(1 + O(h)).$$

The solution a_0 of the first transport equation (3.5) is given by (3.6), and if moreover $z = z(t)$ is on $\pi \circ \kappa \circ \gamma(E)$, then $\partial_\zeta q(z, \psi') = \dot{z}$ by (3.2). The complex number can be identified with a tangent vector of γ, and by the simple-well assumption, we have

$$\dot{z}(T) = e^{-2\pi i}\dot{z}(0), \quad \text{i.e.} \quad \left\{\frac{\dot{z}(T)}{\dot{z}(0)}\right\}^{-1/2} = e^{-\pi i}.$$

Hence we have

$$M(E, h) = e^{-\pi i}(1 + O(h)).$$

Thus we obtain the Bohr–Sommerfeld condition from the condition (Q_2).

The number $e^{-\pi i}$ of $M(E, h)$ corresponds to the Maslov index counted at the turning points $\alpha(E)$ and $\beta(E)$. It is interesting to see that the Maslov index is counted in a continuous way all along the closed curve γ.

References

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