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WKB for semiclassical operators: How to fly over caustics (and more)

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Abstract. The method initiated by Wentzel, Kramers, and Brillouin to find approximate solutions to the Schrödinger equation lies at the origin of the spectacular development of microlocal and semiclassical analysis. When used naively, the approach appears to break down at caustics, but Maslov showed how a simple generalization could overcome this difficulty. In this paper, after a partial historical review, we take advantage of more recent advances in microlocal analysis to present a unified treatment of this generalized Maslov–WKB method, using the microlocal sheaf-theoretic approach of the author (2000). This framework provides a rigorous proof of the Bohr–Sommerfeld–Einstein–Brillouin–Keller quantization conditions for the eigenvalues of general semiclassical operators (pseudodifferential and Berezin–Toeplitz) in one degree of freedom. We also review some applications and extensions.

1. EBK and WKB

In 1926, almost simultaneously, three papers appeared to propose an approximate solution to the newly published Schrödinger equation [64]:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2} + V\Psi = E\Psi, \tag{1.1}$$

where m is the particle mass, $V\colon x \mapsto V(x)$ the potential, $\Psi\colon x \mapsto \Psi(x)$ the wavefunction, and E the energy eigenvalue. The three authors are Wentzel [73] (received on June 18, 1926), Brillouin [4, 5] (received on July 1, 1926 and October 13, 1926), Kramers [48] (received on September 9, 1926).

This approximate solution, now called the WKB ansatz, has the form

$$\Psi(x) = a_\hbar(x)e^{\frac{i}{\hbar}\varphi(x)}, \tag{1.2}$$

where the reduced Planck constant $\hbar$ is treated as a small real parameter, and the function $a_\hbar(x)$ admits an asymptotic expansion in non-negative integral powers of $\hbar$:

$$a_\hbar(x) = a_0(x) + \hbar a_1(x) + \hbar^2 a_2(x) + \cdots$$

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in some adequate topology. The fact that the small parameter appears in front of the derivative in (1.1) makes the limit $\hbar \to 0$ *singular*, in the sense that the "kinetic" term $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2}$ should *not* be considered smaller than the "potential" term $V\Psi$. The WKB ansatz (1.2) reflects this by the highly oscillatory behavior of the phase (the function φ is real-valued).

Both historically and scientifically, it would have been interesting to be there, back in 1926, to interview these three scientists and understand how the very same idea came up to their minds at the same time. Investigating this nowadays would require the competence of a historian, which I do not possess; the only thing I can say is that Brillouin's papers mention Wentzel, and Kramers' paper, which, by the way, was written in Utrecht,[1] does mention Brillouin and Wentzel's work, which makes the usual ordering of the three initials difficult to justify.[2] I have no clue as to whether this was reciprocal.

On the other hand, this idea did not come from nowhere, not at all. Already in 1899, there were several papers by Horn [44, 45] treating the same differential equation with the same ansatz, and he himself based his work on previous studies by Sturm and others. Historical papers usually also mention the work of Jeffreys [46], which interestingly was published just a few months before the famous Schrödinger papers. So, it is actually difficult to claim that the WKB ansatz was really novel in 1926. On the contrary, one should not be surprised that, as soon as Schrödinger published his equation, many researchers tried to find a way to solve it and came up with this ansatz.

What is really interesting in the WKB approach is that these authors were the first — to my knowledge — to realize that the asymptotic expansion of Horn and others actually enlightens the relationship between the old classical mechanics of Hamilton and the new quantum mechanics of Schrödinger. In particular, the phase φ must satisfy the now called Hamilton–Jacobi equation

$$H\left(x, \frac{\partial \varphi}{\partial x}\right) = E,$$

where H is Hamilton's function[3]

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

Even more fascinating, they show how this ansatz gives a very simple justification of the EBK quantization rule of the old quantum theory.

This rule, a generalization of the Bohr–Sommerfeld quantization formula, claims that in order for the energy E to be a correct eigenvalue of the Schrödinger operator, it should satisfy the following geometrical equation:

$$\frac{1}{2\pi\hbar}\oint_{\gamma_E} \xi \, \mathrm{d}x = n \in \mathbb{Z},$$

[1] Where Duistermaat, another name in this story, spent most of his career.

[2] The WKB ordering reflects the publication dates if one omits the CRAS note [4]. French researchers often use BKW because it is alphabetical — or for a less honorable reason.

[3] From now on, I incorporate the mass m into the new semiclassical parameter $\frac{\hbar}{m}$.

where γ_E denotes a closed classical orbit in phase space with energy E, and ξ is the classical momentum (denoted by p in the physics literature) conjugate to the position coordinate x (often denoted by q). The integer n is called the quantum number.

Like WKB, EBK is another concatenation of three authors' initials: Einstein, Brillouin (the same Brillouin), and Keller. But this time, contrary to WKB, the historical progression is clear. To make it simple, one can say that Einstein [29] proposed the quantization rule based on geometric considerations (and of course on earlier works, in particular by Bohr, Ehrenfest, Epstein, Schwarzschild, Sommerfeld), then Brillouin showed the connection with Schrödinger's new quantum mechanics (this is the same paper as the one cited for WKB!), and finally Keller [47] explained that, in order to be more accurate, the rules require a correction (now also called the Maslov correction)

$$\frac{1}{2\pi\hbar}\oint_{\gamma_E}\xi\,\mathrm{d}x = n + \frac{\mu}{4}, \quad n \in \mathbb{Z},$$

where μ is called the (Keller–)Maslov index; it is defined from topological properties of the loop γ_E and accounts for phase shifts at caustics or turning points. This remarkably simple rule, (partly) justified by the WKB ansatz, bridges classical mechanics and quantum mechanics by imposing discrete energy levels based on classical trajectories and corrected by topological information.

2. From WKB to microlocal analysis

This is not the end of the story. In fact, I would rather say that the WKB ansatz was the starting point of a new and fascinating mathematical development of intimidating breadth: microlocal analysis.

Indeed, mathematicians had decades of headaches trying to properly justify the WKB approach. The first problem comes from turning points (see Olver's treatise [58]), which can be interpreted as *caustics*. These are points where the approximation ceases to be uniform and in fact blows up. For the one-dimensional Schrödinger equation, these turning points correspond, on the Hamiltonian side, to a position x where the momentum ξ of the particle vanishes. Thus, the energy level set has there a vertical tangent, and hence the phase function φ has an infinite derivative, which forbids the Hamilton–Jacobi equation to be solved by smooth functions.

At this point, it is difficult not to notice that the EBK quantization rule, by contrast, has no singular behavior whatsoever at turning points. So is EBK better than WKB, or more general? This is really tempting to say so, because in fact not only does EBK have no singularity, but it can also be generalized to any kind of Hamiltonian function, not specifically the one obtained from Schrödinger operators, which indicates that it could be used to solve eigenvalue problems arising from more general partial differential equations. The extension of the WKB method to a large class of operators was done thirty years later by Lax [49], but he was still constrained by the caustic issue. It seems that Maslov [56]

was the first to substantially extend the WKB ansatz to a form that would swallow caustics using partial Fourier transforms. Then, Hörmander [39–43], also inspired by Sato's microfunctions [63], wrapped up the whole thing into a formidable theory now called (homogeneous) microlocal analysis. Unfortunately, Hörmander neither wanted to motivate his theory by quantum mechanics nor to apply it to this field. He was interested in the regularity theory of distributional solutions to general partial differential equations and did not use any small parameter $\hbar$. Duistermaat [23] was the first to incorporate the semiclassical parameter $\hbar$ back again in order to use microlocal analysis towards recovering Maslov's results. This was the birth of semiclassical analysis. In doing so, Duistermaat relied on the theory of Fourier integral operators, recently developed by Hörmander and himself [24] (following a thread of ideas including in particular the work of Egorov [28]), in order to generalize the notion of WKB solutions, now called semiclassical lagrangian distributions. Formally (that is, ignoring the problem of convergence of integrals), a lagrangian distribution is simply a linear superposition of standard WKB ansätze, as follows:

$$\Psi(x) = \frac{1}{(2\pi\hbar)^{\frac{n}{2}}} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}\varphi(x,\theta)} a_\hbar(x,\theta)\, \mathrm{d}\theta. \tag{2.1}$$

3. The lagrangian manifold viewpoint

Consider the phase space $\mathbb{R}^{2n}$ equipped with the canonical symplectic form $\omega = \mathrm{d}\xi \wedge \mathrm{d}x = \sum_{j=1}^n \mathrm{d}\xi_j \wedge \mathrm{d}x_j$. A lagrangian[4] (sub)manifold is a submanifold of $\mathbb{R}^{2n}$ of dimension n on which the symplectic form vanishes. For instance, the "horizontal fiber" $\{\xi = \text{const}\}$ is a lagrangian submanifold (of some importance, as we shall see later). Of course, the same notion extends to any symplectic manifold. What do lagrangian manifolds have to do with the Schrödinger equation? Well, Alan Weinstein had this now famous sentence: "everything is a lagrangian manifold" [72]. I am not going to fully justify this, but let me explain why any WKB solution — even in the generalized Maslov sense (2.1) — of the Schrödinger equation is associated to a lagrangian manifold.

Recall that the phase φ is a solution to the Hamilton–Jacobi equation

$$H\left(x, \frac{\partial\varphi}{\partial x}\right) = E.$$

So we have a natural subset of the energy level set, defined by the set Λ_φ of all pairs $(x, \frac{\partial\varphi}{\partial x})$, which is the graph of the differential of φ. I claim that this graph is a lagrangian submanifold. Indeed, if you restrict the symplectic form $\mathrm{d}\xi \wedge \mathrm{d}x$ to this graph, you obtain

$$\mathrm{d}\xi \wedge \mathrm{d}x_{\restriction \Lambda_\varphi} = \mathrm{d}(\xi \mathrm{d}x)_{\restriction \Lambda_\varphi} = \mathrm{d}(\mathrm{d}\varphi) = 0. \tag{3.1}$$

[4] I follow here Weinstein's use [71] of the fully adjectival form "lagrangian"— that is, without capital "L"; I also second Weinstein in ending the word with "ian" instead of "ean"; after all, Joseph Louis de Lagrange was born Giuseppe Luigi Lagrangia.

(The Liouville 1-form $\alpha = \xi\,\mathrm{d}x$ has this remarkable "tautological" property that, when restricted to a section of the cotangent bundle — i.e., a 1-form —, it produces back the 1-form itself, here $\mathrm{d}\varphi$.)

In the case of the generalized WKB ansatz, as in equation (2.1), and under generic conditions on φ, we can see by the stationary phase lemma that the integral localizes on the critical points of the map

$$\theta \mapsto \varphi(x,\theta),$$

that is, on the set

$$C_\varphi = \left\{(x,\theta) \;\middle|\; \frac{\partial\varphi}{\partial\theta}(x,\theta) = 0\right\}.$$

At these localized points, the asymptotic expansion of $\Psi(x)$ becomes a usual WKB ansatz. Hence, one can show that if it is a solution to the Schrödinger equation, we must have the Hamilton–Jacobi equation

$$H\left(x, \frac{\partial\varphi}{\partial x}(x,\theta)\right) = E, \quad \text{where } (x,\theta) \in C_\varphi.$$

And again, one can check that the image of C_φ under the map

$$(x,\theta) \mapsto \left(x, \frac{\partial\varphi}{\partial x}(x,\theta)\right)$$

is a lagrangian submanifold. Remarkably, one can prove conversely that a (non-empty) class of lagrangian distributions which are locally of form (2.1) can be associated to *any* lagrangian submanifold; this is one of the main achievements of Maslov, extended to a great generality by Hörmander (but for homogeneous lagrangian submanifolds) and then Duistermaat; for a thorough explanation, I recommend Duistermaat's paper [23]. It follows that, in order to find a good phase for a (generalized) WKB solution to the Schrödinger equation (or to any good semiclassical equation, see below), it is simply enough to find an arbitrary lagrangian submanifold contained in the required energy level set $H(x,\xi) = E$.

One of the (many) magical aspects of lagrangian manifolds is that such a lagrangian is automatically *invariant* by the Hamiltonian flow of H. Indeed, if v is tangent to Λ, then

$$\omega(\mathcal{X}_H, v) = -\mathrm{d}H \cdot v = 0,$$

the first equality defining the Hamiltonian vector field $\mathcal{X}_H$ and the second one expressing that v is tangent to the level set of H. Therefore, $\mathcal{X}_H$ is symplectically orthogonal to Λ. But since Λ is lagrangian, its symplectic orthogonal is itself, and hence $\mathcal{X}_H$ is tangent to Λ![5]

We now see that solving the Schrödinger equation by means of the WKB ansatz, at first order $\mathcal{O}(\hbar)$, amounts to finding an *invariant lagrangian submanifold* of the phase space.

[5]More details concerning the geometry of the WKB approximation can be found in the nice book [3].

(By invariant we shall always mean invariant under the Hamiltonian flow of the classical Hamiltonian H.)

The reader may wonder why we introduce general lagrangian manifolds here, while in this paper we are mostly interested in the one-dimensional case: the phase space is $\mathbb{R}^2$, or a two-dimensional surface, and a lagrangian manifold is just a curve in that space. Well, one reason is that the first part of the WKB papers, which deals with approximate solutions to the Schrödinger equation, actually works in any dimension and hence defines general lagrangian submanifolds, which provides a nice geometric interpretation of the wave function Ψ. However, the second part, which aims at justifying the Bohr–Sommerfeld quantization condition, is much more delicate and only works in dimension 1, or for separable or completely integrable systems. But, and this is our second reason, it turns out that our main tool for a rigorous justification of the Bohr–Sommerfeld condition, even in dimension 1, will be Fourier integral operators, which themselves are actually WKB functions defined in a higher-dimensional space.

4. Semiclassical operators and microlocal solutions

Microlocal analysis was first developed for (semiclassical) pseudodifferential operators, which is a large class of linear operators containing all differential operators with smooth coefficients (and hence the Schrödinger operator).[6] It was then realized that the whole theory can also be applied to a very different class of operators, the so-called Berezin–Toeplitz operators (see, for instance, [53]). These are not differential operators. Instead, for each fixed value of $\hbar$, they act on a finite-dimensional Hilbert space, the dimension of which grows to infinity as $\hbar \to 0$. In this paper, following an idea of [54, Appendix A], we will call *semiclassical operators* operators that are either semiclassical pseudodifferential operators or Berezin–Toeplitz operators. In both cases, we shall denote by $\mathcal{H}$ the natural Hilbert space on which they act (this space depends on $\hbar$ in the Berezin–Toeplitz case), and by M the phase space (so $\mathcal{H} = L^2(\mathbb{R}^n)$ and $M = \mathbb{R}^{2n}$ in the pseudodifferential case).

In the Berezin–Toeplitz case, the admissible values of $\hbar$ are quantized: typically, $\hbar = \frac{1}{k}$ with $k \in \mathbb{N}^*$. However, I wrote this text with a bias toward pseudodifferential operators; hence, for notational simplicity, we shall say "$\hbar \in]0, 1]$" when we actually mean "$\hbar$ admissible and inside $]0, 1]$". We shall also denote by (x, ξ) a point in phase space, even though for a general symplectic manifold there might not be such global coordinates. In the Berezin–Toeplitz quantization scheme, the WKB phase $e^{\frac{i}{\hbar}\varphi(x)}$ must be replaced

[6] Technically, one requires a moderate growth of the coefficients; for a Schrödinger operator, this means that V must be smooth and behave at most polynomially at infinity. In current microlocal terminology, the symbols of our operators must belong to an appropriate *class*, which we shall implicitly assume throughout this article. See, for instance, [74] for details.

by a holomorphic section of a prequantum line bundle, which is flat on some lagrangian manifold Λ, see [7]. (This also covers the "generalized WKB ansatz" (2.1).)

Let P be a semiclassical operator with symbol $H(x,\xi)$. We say that $\psi \in \mathcal{H}$ is a WKB solution of order N to the equation $(P-E)\psi = 0$ if ψ is a lagrangian distribution whose associated lagrangian submanifold is contained in the energy level set $H = E$, and such that ψ is a quasimode of order N, that is,

$$(P-E)\psi = \mathcal{O}(\hbar^N). \tag{4.1}$$

For instance, when $P = \frac{\hbar}{i}\frac{\partial}{\partial x}$, which is arguably the simplest semiclassical operator, then $\psi(x) = Ce^{\frac{i}{\hbar}Ex}$, $x \in \mathbb{R}$, is a *plane wave* and a lagrangian distribution associated with the lagrangian manifold $\{(x,\xi); \xi = E\}$, and is a WKB solution to (4.1) at any order.

For a lagrangian distribution, the quasimode condition (4.1) with $N = 1$ is automatic. However, for larger N, one has to solve transport equations beyond the Hamilton–Jacobi equation in order to obtain higher-order solutions. In this paper, I do not describe the transport equations, because they will be hidden in the more general theory of semiclassical Fourier integral operators.

In which sense, or in which topology, do we want equation (4.1) to hold? It will be convenient to use the notion of a *microlocal solution*, which asserts that equation (4.1) holds microlocally near a point (x,ξ) in phase space if and only if it holds in the $\mathcal{H}$ norm after microlocal projection in a neighborhood of that point. And, by microlocal projection, we mean a semiclassical operator whose symbol is 1 in a small neighborhood of (x,ξ) and 0 outside some compact set. An element $u_\hbar \in \mathcal{H}$ is said to be *microlocally supported*[7] in some set $\Sigma \subset M$ if it is microlocally $\mathcal{O}(\hbar^\infty)$ outside of Σ. The microlocal support is also called the semiclassical wavefront set. See, for instance, [54, Definitions A.1 and A.4].

Using semiclassical partitions of unity, one can show that the set of microlocal solutions has a nice sheaf structure. This means that if you have two solutions defined on two different small open sets with a non-empty intersection, and which coincide on the intersection, then they can be glued to produce a solution on the union of the open sets. As we shall see, one can always choose the second solution such that the coincidence on this intersection holds. In other words, any *local section* of the sheaf over the first open set extends to a section over the union of both open sets. However, even if we have a family of open sets covering a compact invariant lagrangian submanifold, if that manifold is not simply connected, a *global* section of the sheaf might not always exist. If it does exist (which in general will impose some conditions on E), then the solution actually extends to a true global solution in L^2 of equation (4.1). Therefore, this proves (at least for self-adjoint operators) that the energy E is $\hbar^N$-close to the spectrum of the operator P. These ideas were implemented by Colin de Verdière in the pioneering article [9].

Let us now see how it works more precisely in the one-dimensional case.

[7] Some authors use the term "microsupported".

5. The Bohr–Sommerfeld cocycle

Let P be a self-adjoint semiclassical operator with discrete spectrum in a spectral window $[E_1, E_2]$ (for instance, the Schrödinger operator with a confining potential, or any Berezin–Toeplitz operator on a compact Kähler manifold).

We shall assume from now on that P has only one degree of freedom: the phase space has dimension 2, and that the interval $[E_1, E_2]$ is contained in the set of regular values of the principal symbol H of P. Moreover, we assume that $H^{-1}([E_1, E_2])$ is compact. We wish here not only to use the WKB ansatz to obtain approximate solutions to $(P - E)\psi = 0$, but actually to show that *all* solutions are indeed obtained in this way, and in turn to obtain a very precise description of the spectrum of P in $[E_1, E_2]$.

For Schrödinger operators, specific proofs can be found in the literature, see, for instance, the interesting lecture by Voros [70]. But for a statement of this generality, a full microlocal approach is more appropriate. To my knowledge, the papers [12, 34, 62] were among the first ones to employ deep microlocal analysis to derive the Bohr–Sommerfeld rules. Here, my plan is to be "even more microlocal", in the sense that we start to describe the problem locally near a point in phase space, and try to pass from local to global. The strategy follows [66, 68], but I shall give more details here.

Given an arbitrary function $\hbar \mapsto E(\hbar)$, let us denote by $\mathcal{D} = \mathcal{D}_{(P,E)}$ the sheaf of microlocal solutions of $P - E(\hbar)$. In other words, the set $\mathcal{D}(\Omega)$ of sections of $\mathcal{D}$ over an open subset $\Omega \subset M$ is the space of microlocal solutions $\psi_\hbar$ to the equation $(P - E(\hbar))\psi_\hbar = \mathcal{O}(\hbar^\infty)$ on Ω.

First note that, by standard semiclassical ellipticity, if $E(\hbar) \to E_0$, then $\mathcal{D}$ is supported in the energy level set $H = E_0$. Since the phase space has dimension 2, this level set is generically just a curve and hence a lagrangian submanifold by itself. The key result, which says that $\mathcal{D}$ is locally given by WKB solutions near any regular point of H, is the following.

Proposition 5.1 ([66]). *Near any regular point m of H, the space of microlocal solutions to $(P - E)\psi = 0$ is one-dimensional, more precisely,*

- *There exist a fixed*[8] *neighborhood Ω of m, and for any $E \in H(\Omega)$, a WKB solution (i.e., a lagrangian distribution) $\Psi_\hbar = \Psi_{\hbar,E}$, depending smoothly on E, with $\|\Psi_\hbar\| = 1$, such that*
$$(P - E)\Psi_\hbar = \mathcal{O}(\hbar^\infty) \quad \text{on } \Omega.$$
- *If $\psi = \psi_\hbar$ satisfies $(P - E)\psi_\hbar = \mathcal{O}(\hbar^\infty)$ near m and $\|\psi_\hbar\| = 1$, then there exist a WKB solution $\Psi_\hbar$ and a constant phase $C = C(E, \hbar) \in U(1)$, such that*
$$\psi_\hbar - C(\hbar)\Psi_\hbar = \mathcal{O}(\hbar^\infty) \quad \text{on } \Omega.$$

In both items, the remainder $\mathcal{O}(\hbar^\infty)$ is locally uniform in E.

[8] That is, independent of $\hbar$.

When we say that a WKB solution depends smoothly on E, we mean that, in (2.1), both the phase φ and the amplitude $a_\hbar$ depend smoothly on E, uniformly with respect to $\hbar$. This statement can be seen as a semiclassical variant of [24]; it relies on the theory of Fourier integral operators (FIO).

FIOs are perhaps the most powerful tool in microlocal analysis. One of their celebrated uses is to quantize canonical transformations of phase space as unitary operators. If U is such an FIO quantizing the canonical transformation (i.e., symplectic diffeomorphism) χ, then for any semiclassical operator P with symbol $H(x,\xi)$, the conjugated operator

$$U^{-1}PU$$

is again a semiclassical operator, and its symbol is $H\circ\chi+\mathcal{O}(\hbar)$ (this statement is called the Egorov theorem). See, for instance, [7, Proposition 4.3] or [74, Theorem 11.5].

Remarkably, we have here another illustration of Weinstein's "symplectic creed" [72], because FIOs are also lagrangian distributions! (More precisely, the graph of χ in the product space $\mathbb{R}^{2n}\times\mathbb{R}^{2n}$ is automatically a lagrangian submanifold,[9] and by definition an FIO is an operator whose Schwartz kernel is a lagrangian distribution associated with this graph.)

Proof Proposition 5.1. Since m is regular, i.e., $\mathrm{d}H(m)\neq 0$, there exist local canonical coordinates (x,ξ) near m such that $H(x,\xi)-H(m)=\xi$ when $(x,\xi)\in\mathbb{R}^2$ stay in some neighborhood $\widetilde{\Omega}$ of the origin. (This is the statement of Darboux–Carathéodory's theorem.) Let U be an FIO associated with this change of variables. Let $E_0=H(m)$. We obtain, microlocally near m,

$$U^{-1}(P-E_0)U=\frac{\hbar}{i}\frac{\partial}{\partial x}+\mathcal{O}(\hbar).$$

By a standard procedure (*this is where the WKB transport equations are hidden*; see [67, Section 3.2] or the foundational paper [24, Proposition 6.1.4] — in the homogeneous case), one can multiply U by a suitable unitary semiclassical operator V such that, with $\widetilde{U}:=UV$,

$$\widetilde{U}^{-1}(P-E_0)\widetilde{U}=\frac{\hbar}{i}\frac{\partial}{\partial x}+\mathcal{O}(\hbar^\infty).$$

Working in coordinates, one can show that Proposition 5.1 holds for the operator $\frac{\hbar}{i}\frac{\partial}{\partial x}-E$; indeed, its solutions are plane waves $\psi(x)=Ce^{\frac{i}{\hbar}Ex}$. This proves the proposition with

$$\Psi_\hbar=C\widetilde{U}e^{\frac{i}{\hbar}(E-E_0)x}.$$

[9] This holds if the product $\mathbb{R}^{2n}\times\mathbb{R}^{2n}$, sometimes denoted by $\mathbb{R}^{2n}\times\overline{\mathbb{R}^{2n}}$, is equipped with the direct sum symplectic form $\omega\oplus(-\omega)$.

Since $E \in H(\Omega)$, there exists $(x_0, \xi_0) \in \widetilde{\Omega}$ such that $\xi_0 = E - E_0$; hence the microsupport of $e^{\frac{i}{\hbar}(E-E_0)x}$ intersects $\widetilde{\Omega}$, and we can normalize it by a uniform constant. The fact that, for any fixed E, such a $\Psi_\hbar$ is indeed a generalized WKB ansatz associated with the lagrangian manifold $\{H = E\}$ follows from the fact that the Schwartz kernel of U is a lagrangian distribution. By a stationary phase argument, one shows that the application of the semiclassical operator V does not modify this (this is called the semiclassical FIO calculus, see, for instance, [31, Section 9.7] or [7, Proposition 2.7]). ∎

Remark 5.2. In Proposition 5.1, the energy parameter E is purely decorative. Indeed, if P depends on an additional parameter λ, then the parametric version of the proposition holds. Therefore, one can set $P_E := P - E$ and describe solutions to $P_E \Psi_\hbar = \mathcal{O}(\hbar^\infty)$ by viewing E as a parameter. This remark becomes far-reaching for spectral problems where the "spectral" parameter does not appear in a linear fashion.

This proposition allows us to understand in a simple way the sheaf $\mathcal{D}$ of microlocal solutions to the equation $(P - E)\psi = \mathcal{O}(\hbar^\infty)$, when the energy E is a regular value of H: this sheaf is then simply a *flat bundle*, meaning that for each point $m = (x_0, \xi_0)$ of the level set $H(x, \xi) = E$, there exists a neighborhood U of m in which any two microlocal solutions must differ by a multiplicative constant.

Thus, at least theoretically, it is easy to determine when the sheaf has a *global* section (i.e., a microlocal solution in a full neighborhood of the energy level set $H = E$): this happens when the flat bundle is trivial, or equivalently when its first Čech cohomology group $\check{H}^1(\mathcal{D})$ vanishes (modulo $\mathcal{O}(\hbar^\infty)$).

How to compute this cohomology? When E is a regular value of H, we know that the level set $H = E$ is a finite union of closed smooth (embedded) curves $\mathcal{C}_k = \mathcal{C}_k(E)$, $k = 1, \dots, d$. Let us consider a fixed j and denote by $\mathcal{D}_k$ the restriction of $\mathcal{D}$ to a small tubular neighborhood of $\mathcal{C}_k$. The curve $\mathcal{C}_k$ is diffeomorphic to a circle and has a natural orientation given by the Hamiltonian vector field X_H, which does not vanish on it by hypothesis. Let Ω_j, $j = 1, \dots, N_k$, be an open cover of $\mathcal{C}_k$ by small balls, on each of which Proposition 5.1 holds, and whose centers $z_j \in \mathcal{C}_k$ are ordered along the orientation of $\mathcal{C}_k$. For each j, the proposition gives a WKB function $\Psi_\hbar^j$ generating $\mathcal{D}(\Omega_j)$. By restricting to $\Omega_j \cap \Omega_{j+1}$ (indices are written modulo N_k), the uniqueness part of the proposition yields a constant phase $C_j = C_j(E, \hbar) \in U(1)$ such that

$$\Psi_\hbar^{(j+1)} = C_j \Psi_\hbar^{(j)} + \mathcal{O}(\hbar^\infty) \quad \text{on } \Omega_j \cap \Omega_{j+1}. \tag{5.1}$$

Definition 5.3. The assignment $\Omega_j \cap \Omega_{j+1} \mapsto C_j$ is called the *Bohr–Sommerfeld cocycle* of the curve $\mathcal{C}_k$.

(It is indeed a cocycle in the sense of Čech cohomology.)

Proposition 5.4. *There exists a microlocal solution of* $(P - E)$ *on a neighborhood of* $\mathcal{C}_k$ *if and only if the pair* $(E, \hbar)$ *satisfies the equation*

$$C_1(E, \hbar) \cdots C_{N_k}(E, \hbar) = 1 + \mathcal{O}(\hbar^\infty). \tag{5.2}$$

Proof. The solution exists if and only if the Bohr–Sommerfeld cocycle is a coboundary, i.e., there exist constants $d_j = d_j(E,\hbar) \in \mathbb{C}^*$, $j = 1,\dots,N_k$, such that

$$C_j = d_{j+1}^{-1} d_j + \mathcal{O}(\hbar^\infty). \tag{5.3}$$

Indeed, in this case, we see from (5.1) that the local sections $d_j \Psi_\hbar^{(j)}$ actually coincide (modulo $\mathcal{O}(\hbar^\infty)$) on the intersections $\Omega_j \cap \Omega_{j+1}$. Therefore, they can be glued together by a microlocal partition of unity to form a solution on a full neighborhood of $\mathcal{C}_k$.

Conversely, if such a global section $\Psi_\hbar$ exists, by Proposition 5.1 we have constants d_j such that $\Psi_\hbar = d_j \Psi_\hbar^{(j)} + \mathcal{O}(\hbar^\infty)$ on each Ω_j. In view of (5.1), it follows that (5.3) holds.

It remains to show why the coboundary equation (5.3) is equivalent to (5.2). Since indices j are taken modulo N_k, it is clear that (5.3) implies (5.2). Conversely, if (5.2) holds, we let $d_1 = 1$, $d_j = (C_1 \cdots C_{j-1})^{-1}$ for $j = 2,\dots,C_k$, which gives

$$d_1^{-1} d_{N_k} = (C_1 \cdots C_{N_k - 1})^{-1} = C_{N_k} + \mathcal{O}(\hbar^\infty),$$

which proves (5.3) for $j = N_k$ (other j's are automatic.) ∎

Equation (5.2) will be called the Bohr–Sommerfeld condition of the curve $\mathcal{C}_k$. Since the curves for different k are disjoint, we obtain the following assertion.

Proposition 5.5. *There exists a non-trivial section of $\mathcal{D}$, i.e., a microlocal solution on a neighborhood of $H = E$, if and only if at least one of the Bohr–Sommerfeld conditions associated with the curves $\mathcal{C}_1,\dots,\mathcal{C}_d$ is satisfied.*

At this point, it is not clear how to relate this Bohr–Sommerfeld condition to the EBK prediction. This is given by the following proposition.

Proposition 5.6. *The semiclassical action $A_k(E,\hbar) := \log(C_1 \cdots C_{N_k})$ admits an asymptotic expansion of the form*

$$A_k(E,\hbar) = \frac{1}{\hbar} A_{k,0}(E) + A_{k,1}(E) + \hbar A_{k,2} + \hbar^2 A_{k,3} + \cdots \tag{5.4}$$

with smooth coefficients $A_{k,j}$. Moreover, we have

$$A_{k,0} = \int_{\mathcal{C}_k} \alpha, \tag{5.5}$$

where α is the Liouville 1-form.

Proof. We use the same quantum Darboux–Carathéodory normal form as in the proof of Proposition 5.1, this time repeated on each Ω_j. Thus, we may obtain the Bohr–Sommerfeld cocycle (C_j) by choosing $\Psi_\hbar^{(j)} := \widetilde{U}_j e^{\frac{i}{\hbar}(E - H(m))x}$. (If we viewed E as a parameter, see Remark 5.2, we could simply take $\Psi_\hbar^{(j)} := \widetilde{U}_j 1$.)

From (5.1), we obtain, microlocally on $\Omega_j \cap \Omega_{j+1}$,

$$C_j = e^{-\frac{i}{\hbar}(E - H(m))x} U_j^{-1} U_{j+1} e^{\frac{i}{\hbar}(E - H(m))x} + \mathcal{O}(\hbar^\infty).$$

Since C_j is constant, it can be evaluated on any point in $\Omega_j \cap \Omega_{j+1}$. Since the Schwartz kernels of U_j and U_{j+1} are lagrangian distributions, i.e., take form (2.1), with an amplitude $a_\hbar$ admitting an asymptotic expansion in integral powers of $\hbar$, we obtain that, for each fixed E, C_j must have an asymptotic expansion of the form

$$C_j \sim e^{\frac{i}{\hbar}S_0}(a_0 + \hbar a_1 + \hbar^2 a_2 + \cdots), \tag{5.6}$$

and all coefficients depend smoothly on E. Since $|C_j| = 1 + \mathcal{O}(\hbar^\infty)$, we must have $|a_0| = 1$. Hence we may also write

$$C_j \sim e^{\frac{i}{\hbar}\sum_{j\geq 0}\hbar^j S_j}$$

(as Brillouin [5] suggested), which gives (5.4).

In order to compute $A_{k,0}$, recall that $\Psi_\hbar^{(j)}$ is a WKB solution associated to the curve $\mathcal{C}_k \subset \{H = E\}$. Hence, near any point m in the lagrangian manifold $\mathcal{C}_k$, we have a phase function φ_j as in (2.1); using (3.1), this phase, viewed as a function on $\mathcal{C}_k$, satisfies $\mathrm{d}\varphi_j = \alpha$, where $\alpha = \xi\,\mathrm{d}x$ is the Liouville 1-form. Evaluating (5.1) on a point m of $\Omega_j \cap \Omega_{j+1}$, we deduce that the coefficient $S_0 = S_0^{(j)}$ of (5.6) takes the form

$$S_0^{(j)} = \varphi_{j+1}(m) - \varphi_j(m)$$

but since $\mathrm{d}(\varphi_{j+1} - \varphi_j) = 0$, the function $\varphi_{j+1} - \varphi_j$ is constant, and the set of all of these constants, i.e., $(S_0^{(j)})_{j=1,\ldots,N_k}$ is exactly the Čech cocycle associated with the closed 1-form α on $\mathcal{C}_k$. (See, for instance, [3, Appendix C].) Thus, $\sum_{j=1}^{N_k} S_0^{(j)} = \int_{\mathcal{C}_k}\alpha$, which gives (5.5). ∎

Actually, it is also possible to describe the second term $A_{k,1}$; in the pseudodifferential case, if P has no subprincipal symbol, $A_{k,1} = \mu\frac{\pi}{2}$, where μ is the (Keller–Leray–)Maslov index of $\mathcal{C}_k$ which, in $\mathbb{R}^2$, is always equal to 2. In the Berezin–Toeplitz case, see [7]. In the special case of the Schrödinger operator, an iterative scheme to obtain $A_{k,j}$ for all j is known [2, 14].

6. Quasimodes and eigenvalues

Let us now upgrade the microlocal result of Proposition 5.1 to a concrete statement about honest eigenvalues and eigenfunctions, in order to fully justify the EBK rule.

First of all, as expected, the generalized WKB construction will give us good quasimodes, i.e., solutions $(\Psi_\hbar, E(\hbar))$ to

$$\|(P - E(\hbar))\Psi_\hbar\|_{\mathcal{H}} = \mathcal{O}(\hbar^\infty).$$

But we have much more: exact eigenfunctions must be $\mathcal{O}(\hbar^\infty)$-close to these quasimodes, and hence the whole spectrum in $[E_1, E_2]$ is $\mathcal{O}(\hbar^\infty)$-close (in every possible sense, including multiplicity) to the set of E's for which the microlocal WKB construction was valid.

Most treatments of the Bohr–Sommerfeld rule in the literature make the simplifying assumption that energy level sets are connected;[10] this is quite understandable, since the presentation becomes much simpler, and adding connected components is "well known to the experts". From the point of view of symplectic geometry, this makes no difference indeed, since each component can be treated separately.[11] The microlocal treatment is equally similar. However, proving that WKB solutions exhaust the spectrum (which is the goal of this section) requires an additional argument, which we present here. One way to achieve this (and again, this is known to experts, I do not claim much originality) is to use the fact that quasimodes associated to different components are mutually orthogonal modulo $\mathcal{O}(\hbar^\infty)$ [7, Proposition 2.6].

One of the first mathematical accounts of the Bohr–Sommerfeld rule is due to Helffer and Robert [34]; interestingly, motivated by quantum tunneling, they did consider multiple components, but with a symmetry assumption implying that all periods of the Hamiltonian flow on $H^{-1}(E)$ are equal, allowing them to apply an idea of Colin de Verdière [11].

Theorem 6.1 (Bohr–Sommerfeld eigenvalues). *Let P be a self-adjoint semiclassical operator with one degree of freedom and spectrum $\sigma(P)$. Consider a spectral window $I = [E_1, E_2]$ which contains only regular values of the principal symbol H of P. Assume moreover that $H^{-1}(I + [-\varepsilon, \varepsilon])$ is compact in the phase space M, for some $\varepsilon > 0$. Then $\sigma(P) \cap I$ is discrete and is described as follows:*

(1) *There exists an integer $d \geq 0$ such that for each $E \in I$, the energy level set $H^{-1}(E)$ is the disjoint union of d smooth curves $\mathcal{C}_1(E), \ldots, \mathcal{C}_d(E)$.*

(2) *There exist smooth functions $E \mapsto A_{k,j}(E)$, for $k = 1, \ldots, d$ and $j \in \mathbb{N}$, and smooth functions $I \times]0,1] \ni (E, \hbar) \mapsto A_k(E;\hbar)$ admitting the asymptotic expansion*

$$A_k(E;\hbar) \sim \frac{1}{\hbar} \sum_{j=0}^{\infty} \hbar^j A_{k,j}(E)$$

in the smooth topology, such that $\sigma(P) \cap I$ coincides modulo $\mathcal{O}(\hbar^\infty)$, and including multiplicities, with the disjoint union $\bigsqcup_{k=1}^{d} \sigma_k(\hbar)$, which we denote by

$$\sigma(P) \cap I = \bigsqcup_{k=1}^{d} \sigma_k(\hbar) + \mathcal{O}(\hbar^\infty) \tag{6.1}$$

with

$$\sigma_k(\hbar) := A_k(\cdot;\hbar)^{-1}(2\pi\mathbb{Z}). \tag{6.2}$$

[10] A notable exception is the recent paper [21].

[11] Actually, there is a topological subtlety, which is never discussed to my knowledge, concerning a distinction between the global fibration by H and the semiglobal one — i.e., in a neighborhood of a connected component: if $H^{-1}(E)$ is assumed to be compact, then it is a union of circles, and near any circle $\mathcal{C}$, the action-angle theorem asserts in particular that neighboring fibers are also compact and connected … which means: *in a saturated neighborhood of* $\mathcal{C}$; but this does *not* imply that neighboring global fibers of $H : M \to \mathbb{R}$ are compact.

Precisely, for each eigenvalue $E = E(\hbar)$ of P, for any the spectral multiplicity of the interval $B = [E - \hbar^N, E + \hbar^N]$ is, for $\hbar$ small enough, equal to the number of non-empty sets $\sigma_k \cap B$.

(3) *$A_{k,0}(E) = \int_{\mathcal{C}_k(E)} \alpha$, where α is the Liouville 1-form, and the map $E \to A_{k,0}(E)$ is a diffeomorphism from I to its image.*

(4) *In particular, if $d = 1$, then the spectrum in I is simple for $\hbar$ small enough, and gaps are of order $\mathcal{O}(\hbar)$.*

(5) *If P has no subprincipal symbol, then $A_{k,1}$ is the Keller–Maslov index of $\mathcal{C}_k$.*

Remark 6.2. We will be sloppy here on two technical points:

(1) The precise definition of "two subsets of $\mathbb{R}$ depending on $\hbar$ which coincide modulo $\mathcal{O}(\hbar^\infty)$ including multiplicity", see [30, Definition 1.5]. This notion is natural but some care has to be taken at the "boundary" of the sets. See Step 4 of the proof below.

(2) The precise definition of the Keller–Maslov index, both in the pseudodifferential [23] (see also [31, Section 5.13]) and the Berezin–Toeplitz cases [7].

Proof. Step 1. *Discrete spectrum.* This step is only necessary in the pseudodifferential case, where the phase space M is not compact, and it is now standard. Let a smooth function f be equal to 1 on I and compactly supported in $I + [-\varepsilon, \varepsilon]$. Then $1_I f = 1_I$ and hence by functional calculus $1_I(P) = 1_I(P) f(P)$. The symbol $f(H(x, \xi))$ and all its derivatives vanish outside the compact set $H^{-1}(I + [-\varepsilon, \varepsilon])$, so by pseudodifferential functional calculus, $f(P)$ is compact (see [22, Theorems 8.7 and 9.4], and also [31, Section 13.6]). Thus, $1_I(P)$ is compact as well, which implies that its range is finite dimensional.

Step 2. *Quasimodes.* Let us fix $k \in \{1, \dots, d\}$. We define the map A_k to be the semiclassical action of Proposition 5.6.

Thus, the map $E \to A_{k,0}(E)$ is the action integral on the energy set $H = E$; a classical computation shows that its derivative is the map $E \mapsto \tau_k(E)$, where $\tau_k(E)$ is the period of the Hamiltonian flow of H on $\mathcal{C}_k(E)$. Since E is a regular value, the Hamiltonian vector field cannot vanish on the level set, and hence $\tau_k(E) \neq 0$. This shows that $A_{k,0}$ is a diffeomorphism, and hence that the map $\hbar A_k(\cdot; \hbar)$ is invertible for $\hbar$ small enough. This also implies that the inverse $G_k(\hbar) := [\hbar A_k(\cdot; \hbar)]^{-1}$ admits an asymptotic expansion in powers of $\hbar$. Hence, for convenience, we may define this inverse modulo $\mathcal{O}(\hbar^\infty)$ for all $\hbar \in]0, 1]$ by a Borel summation, which we call $G_k(\hbar)$ again.

It now follows from (6.2) that

$$E(\hbar) \in \sigma_k(\hbar) \;\Leftrightarrow\; E(\hbar) = G_k(\hbar)(2\pi\hbar n) \quad \text{for some } n \in \mathbb{Z}. \tag{6.3}$$

(The integer n being of course subjected to the fact that $2\pi n$ must belong to the range of $A_k(\cdot, \hbar)$.)

For such a family $\{E(\hbar); \hbar \in J\}$, where $J \subset]0,1]$ accumulates at zero, we may apply Proposition 5.4 and obtain a microlocal solution to $(P-E)\Psi_\hbar = \mathcal{O}(\hbar^\infty)$ in a neighborhood of $\mathcal{C}_k$. By a microlocal cutoff outside of $\mathcal{C}_k$ and vanishing on the other $\mathcal{C}_{k'}$'s, $k' \neq k$, we obtain a normalized quasimode $\Psi_\hbar^{(k)}$:

$$\|(P-E)\Psi_\hbar^{(k)}\|_{\mathcal{H}} = \mathcal{O}(\hbar^\infty).$$

By the spectral theorem, there must be an element $\lambda(\hbar) \in \sigma(P)$ such that $|\lambda(\hbar) - E(\hbar)| = \mathcal{O}(\hbar^\infty)$. This shows

$$\sigma_k \subset \sigma(P) + \mathcal{O}(\hbar^\infty).$$

Step 3. *Microsupport.* Let $\psi = \psi_\hbar \in \mathcal{H}$ be an eigenfunction of P for the eigenvalue $E = E(\hbar) \in I$. Assume that $E(\hbar) \to E_0$, at least for some subsequence of values of $\hbar$. By semiclassical ellipticity, the microsupport of ψ is contained in $H^{-1}(E_0)$, and is not empty if we normalize $\|\psi\| = 1$. This microsupport is invariant by the Hamiltonian flow of H (this follows, for instance, from Proposition 5.1). Hence it is a finite union of curves $\mathcal{C}_k(E_0)$. Let W_k be a saturated neighborhood of $\mathcal{C}_k(E_0)$: for E close to E_0, the whole curve $\mathcal{C}_E$ is contained in W_k.

Now, the microlocal restriction of ψ on W_k is a section of the sheaf $\mathcal{D}$ for all E near E_0, and hence by Proposition 5.4 the corresponding Bohr–Sommerfeld conditions must be satisfied: thus $E \in \sigma_k(\hbar)$. This shows

$$\sigma(P) \subset \sigma_k + \mathcal{O}(\hbar^\infty).$$

Step 4. *Multiplicities.* For simplicity, we did not state explicitly the result about multiplicities within the theorem, see Remark 6.2. Here is a more precise statement, which we could not find in the literature (although it is not very far from the method employed in [35]), except very recently in the Berezin–Toeplitz case [21]. While the idea is simple (the multiplicity of E should be exactly the number of k for which $E \in \sigma_k$), the correct statement is more involved due to boundary effects (eigenvalues may surreptitiously enter or leave any given set when $\hbar$ varies arbitrarily little, and this may not be detected because of the $\mathcal{O}(\hbar^\infty)$ error).

Let us prove the following assertion.

Claim. *For each eigenvalue $E = E(\hbar) \in I$ of P, let $N \geq 2$, let $B = B(\hbar)$ be the ball around $E(\hbar)$, of radius $\hbar^N$. Let $N' > N$ and let $\widetilde{B}$ be a slightly smaller ball, of radius $\hbar^N - \hbar^{N'}$. Then, when $\hbar$ is small enough,*

(1) *the spectral multiplicity of B is at least equal to the number of k's such that σ_k intersects $\widetilde{B}$;*

(2) *the spectral multiplicity of $\widetilde{B}$ is at most equal to the number of k's such that σ_k intersects B.*

Here, we used the terminology "spectral multiplicity of B" to denote the rank of the spectral projector of P onto B. First, remark that in each σ_k, the discussion is simple:

if two energies $E_1(\hbar)$ and $E_2(\hbar)$ are separated by some Ch^N, $N \geq 1$, then they must correspond to different integers n_1 and n_2 in (6.3): hence $|n_1(\hbar) - n_2(\hbar)| \geq 1$, and hence

$$|E_1(\hbar) - E_2(\hbar)| \geq c\hbar$$

for some $c > 0$.

Let $B = B(\hbar)$ be a ball around some energy $E(\hbar) \in I$, of radius $\hbar^N$ with $N \geq 2$, and let $\widetilde{B}$ be a slightly smaller ball as in the statement, so that $\widetilde{B} + \mathcal{O}(\hbar^\infty) \subset B$. By the above argument, for $\hbar$ small enough, each set $\sigma_k + \mathcal{O}(\hbar^\infty)$ can contain at most one element of $\widetilde{B}$. If this happens for two different integers $k \neq \ell$, then the corresponding WKB quasimodes are microsupported on different curves and hence their scalar product is $\mathcal{O}(\hbar^\infty)$. Therefore, they cannot be collinear for $\hbar$ small enough, which means, using the variational characterization of the spectrum, that the spectral multiplicity of B is at least equal to the number of k's such that σ_k intersects $\widetilde{B}$.

Conversely, as in the previous step, any eigenfunction in the range of $1_{\widetilde{B}}(P)$ must be supported on some union of $\mathcal{C}_k$'s and hence is microlocally equal to a linear combination of the corresponding WKB quasimodes. Since we have an orthonormal basis of eigenfunctions, and since, again, the WKB quasimodes are mutually almost orthogonal, we deduce that the spectral multiplicity cannot exceed this number of k's. ∎

We see from the proof that one actually has a precise description of eigenfunctions and quasimodes.

Theorem 6.3 (Bohr–Sommerfeld eigenfunctions). *With the same hypothesis as Theorem 6.1,*

(1) *Any quasimode of P (and hence, any eigenfunction) is equal, modulo $\mathcal{O}(\hbar^\infty)$, to a linear combination of the WKB solutions.*

(2) *Each of these WKB solutions, with approximate eigenvalue $E = E(\hbar)$, must correspond to a component $\mathcal{C}_k$ such that σ_k intersects an $\mathcal{O}(\hbar^\infty)$ ball around E.*

(3) *For each k, to any solution $E(\hbar)$ of the Bohr–Sommerfeld condition (5.2) on the curve $\mathcal{C}_k$, one can associate (for $\hbar$ small enough) a unique eigenvalue of P, for which the corresponding WKB ansatz is a quasimode.*

7. Caustics?

Comparing with most texts on WKB (quasi)modes, like [32], it is perhaps surprising that no discussion of turning points or introduction of the Airy function has been necessary here. Actually, in our treatment, caustics have been superbly ignored. What has become of them?

As we saw in the preceding sections, WKB solutions live intrinsically on the curves $\mathcal{C}_k$, which are smooth lagrangian submanifolds of the phase space M. In the usual pseudodifferential setting, a problem occurs due to the fact that we ultimately need eigenfunctions

that depend on the position variable only, x; and in general the curves $\mathcal{C}_k$ cannot be globally parameterized by x.

Definition 7.1. Let $\Lambda \subset \mathbb{R}^{2n}$ be a lagrangian manifold. A point $(x,\xi) \in \Lambda$ is called *caustic* if the map $(x,\xi) \to x$ restricted to Λ is *not* a local diffeomorphism.

Thus, if $n = 1$, any closed smooth curve $\mathcal{C}$ in $\mathbb{R}^2$ must have at least two caustics, corresponding to the extrema of x on the curve. The *Maslov index* of $\mathcal{C}$ is the intersection number of the curve with the vertical fibration: i.e., the number of times the tangent to the curve crosses the vertical direction, counted algebraically: $+1$ if the oriented curve stays locally on the left of the vertical tangent. For a circle in $\mathbb{R}^2$ oriented counter-clockwise, the Maslov index is 2. By homotopy invariance, the Maslov index of any smooth loop in $\mathbb{R}^2$ is ± 2.

Remark 7.2. In the Berezin–Toeplitz category, the caustic issue does not exist, because elements of the Hilbert space $\mathcal{H}$ are directly defined on the phase space M. As a matter of fact, we could have avoided caustics altogether by transforming pseudodifferential operators into Berezin–Toeplitz operators (in the non-compact phase space $\mathbb{C}^n$) using the FBI transform. This is not our method here, but it can be done efficiently, see [26, 60].

Symplectically, due to the Darboux–Carathéodory theorem, any regular point of $H^{-1}(E)$ plays the same role, be it in $\mathbb{R}^{2n}$ or in a compact Kähler manifold, be it caustic or not. Since our method is to quantize the Darboux–Carathéodory charts, the microlocal description completely flies over the caustics. But, looking carefully, they are still there: they influence the dimension of the θ variable in the generalized WKB ansatz (2.1) used for the kernel of the Fourier integral operator quantizing the Darboux–Carathéodory chart. By stationary phase, this dimension shows up in the asymptotic expansion of the transition constant between two WKB solutions, which is our Bohr–Sommerfeld cocycle (5.6), see the proof of Proposition 5.6. Then, in the final result, Theorem 6.1, the only remaining footprint of the caustic analysis is the Maslov index, causing the famous $\frac{1}{2}$-shift in the quantum numbers.

8. Applications

The description of Theorem 6.1 is so precise that almost any asymptotic statement about eigenvalues of P in $I = [E_1, E_2]$ should directly follow from it. Here are some examples, certainly known to experts, but which we could not find explicitly in the literature. The hypotheses are the same as those of the theorem.

Corollary 8.1 (Density of the spectrum). *Given any $E_0 \in I$, there exists a family of eigenvalues $E(\hbar) \in \sigma(P)$ such that $E(\hbar) \to E_0$, and more precisely $E(\hbar) - E_0 = \mathcal{O}(\hbar)$.*

Proof. Let us apply formula (6.2). Let $c(\hbar) = \hbar A_k(E_0;\hbar)$. We have

$$c(\hbar) = c_0 + \mathcal{O}(\hbar), \quad c_0 = A_{k,0}(E_0),$$

and $G_k(\hbar)(c(\hbar)) = E_0 + \mathcal{O}(\hbar^\infty)$. Let $n(\hbar) = \lfloor \frac{c(\hbar)}{2\pi\hbar} \rfloor \in \mathbb{Z}$, so that

$$|2\pi n(\hbar)\hbar - c(\hbar)| \leq 2\pi\hbar.$$

Since $G_k(\hbar)$ is locally Lipschitz, uniformly in $\hbar$, we obtain

$$G_k(\hbar)(2\pi n(\hbar)\hbar) - G_k(\hbar)(c(\hbar)) = \mathcal{O}(\hbar),$$

and by (6.2) we obtain $E(\hbar) \in \sigma(P)$ with

$$G_k(\hbar)(2\pi n(\hbar)\hbar) = E(\hbar) + \mathcal{O}(\hbar^\infty),$$

which gives the result. ∎

In the above result, we notice that the quantum number $n(\hbar)$ which labels the eigenvalues is allowed to depend on $\hbar$, and the distance $|E(\hbar) - E_0|$ cannot in general be better than $\mathcal{O}(\hbar)$. A different question is to try to investigate the behavior, as $\hbar$ varies, of an eigenvalue with a given, fixed, n. This is what concerns the following statement.

Corollary 8.2 ($\hbar$-behavior of individual eigenvalues). *All eigenvalues of P in I "depend smoothly on $\hbar$ modulo $\mathcal{O}(\hbar^\infty)$" in the following sense: for any $\varepsilon > 0$ and any $N \geq 2$, there exists $\hbar_1 > 0$ such that the following holds. Let $\hbar_0 \in]0, \hbar_1]$, and consider an eigenvalue $E(\hbar_0) \in \sigma(P) \cap [E_1, E_2]$. There exist a family of eigenvalues $\{E(\hbar), \hbar \in]0, 1]\}$ and a smooth map $\hbar \mapsto \lambda(\hbar)$ such that, as long as $\lambda(\hbar) \in I$,*

$$|E(\hbar) - \lambda(\hbar)| \leq \varepsilon\hbar^N.$$

In the pseudodifferential case, this family always leaves the interval I for $\hbar$ small enough.

Proof. We use the bijection given by (6.1). This defines, for $\hbar = \hbar_0$, an integer $k \in \{1, \ldots, d\}$, labeling a connected component of the energy level set, and another integer $n \in \mathbb{Z}$ (the quantum number) labeling the approximate eigenvalue $A_k(\cdot; \hbar_0)^{-1}(2\pi n)$. We let

$$\lambda(\hbar) := G_k(\hbar)(2\pi\hbar n)$$

as in (6.3), and the result follows. In other words, we just reformulate (6.1) as

$$\sigma(P) \cap I = \bigsqcup_{\substack{k=1,\ldots,d,\, n\in\mathbb{Z},\\ 2\pi\hbar n \in \mathrm{Dom}(G_k(\hbar))}} G_k(\hbar)(2\pi\hbar n) + \mathcal{O}(\hbar^\infty)$$

which expresses the spectrum as a union of $\hbar$-smooth branches indexed by (k, n).

Note that $G_k(\hbar) = G_{k,0} + \mathcal{O}(\hbar)$, and $G_{k,0}$ is the reciprocal of the action variable $E \mapsto A_{k,0}(E)$. In the pseudodifferential case, the action is the area below $\mathcal{C}_k$ and hence cannot vanish unless E is a critical value. This means that $G_{k,0}(0)$ cannot belong to I, which forces the eigenvalue to exit this interval. ∎

Note that the *drifting* of eigenvalues, forcing them to exit any interval of regular values, was described for general quantum integrable systems in [17].

From this corollary, all eigenvalues belong to smooth branches. In general, the branches associated to different connected components may intersect. Whether the exact eigenvalues follow the branches as $\hbar$ moves continuously (in the pseudodifferential setting), or instead "hop" to another branch, creating *avoided crossing* seems to be an open question for general pseudodifferential operators. Of course, for one-dimensional Schrödinger operators, because of the simplicity of the spectrum, we know that all crossings must be avoided.

Corollary 8.3 (Poor man's tunnel effect). *Assume that two connected components $\mathcal{C}_k$, $\mathcal{C}_\ell$ are "quantum symmetric" (for instance, they are exchanged by an affine symplectic map and P is invariant under the corresponding metaplectic transformation, or P is a Schrödinger operator with symmetric potential wells). Then we have doublets of eigenvalues $E_k(\hbar)$ and $E_\ell(\hbar)$ such that*

(1) $E_k(\hbar) = E_\ell(\hbar) + \mathcal{O}(\hbar^\infty)$;

(2) *the spectral multiplicity of any ball of radius $\hbar^N$, $N \geq 2$, around $E_k(\hbar)$ (or $E_\ell(\hbar)$) is at least 2. It is exactly 2 if $d = 2$.*

Proof. The symmetry ensures that the Bohr–Sommerfeld cocycles are the same for both connected components. The result then follows directly from Theorem 6.1. ∎

See [25] for a thorough discussion of tunneling for one-dimensional pseudodifferential operators in relation to the Bohr–Sommerfeld rules.

Let us now count eigenvalues. The usual Weyl law (see, for instance, [22, Theorem 10.1]) gives the number of eigenvalues (with multiplicities) in I:

$$\mathcal{N}(P, I; \hbar) = \frac{1}{2\pi\hbar}\mathrm{Vol}(H^{-1}(I)) + \mathcal{O}(1),$$

where Vol is the symplectic volume. So

$$\mathrm{Vol}(H^{-1}(I)) = \int_{H^{-1}(I)} |\omega|$$

which by Stokes is (recall that $\mathrm{d}\alpha = \omega$)

$$\begin{aligned}\Big|\int_{H(x,\xi)=E_2} \alpha - \int_{H(x,\xi)=E_2} \alpha\Big| &= \sum_{k=1}^{d} \Big|\oint_{\mathcal{C}_k(E_2)} \alpha - \oint_{\mathcal{C}_k(E_1)} \alpha\Big| \\ &= \sum_{k=1}^{d} |A_{k,0}(E_2) - A_{k,0}(E_1)|.\end{aligned}$$

Using Theorem 6.1, we can not only go one step further in the approximation, but also, surprisingly (maybe), obtain an exact expression, without remainder.

Corollary 8.4 (Exact Weyl law). *Assume P has no subprincipal symbol. Let $\widetilde{E}_j(\hbar) \in I$, where $\hbar \in]0,1]$ or $\hbar$ belongs to some subset accumulating at 0, be such that*

(1) $\widetilde{E}_j(\hbar) \to E_j$ *as* $h \to 0$;

(2) $\operatorname{dist}(\widetilde{E}_j, \sigma(P)) \geq \varepsilon\hbar$ *for some* $\varepsilon > 0$.

Then, for $\hbar$ small enough, the number of eigenvalues of P in $\tilde{I} := [\widetilde{E}_1(\hbar), \widetilde{E}_2(\hbar)]$ is exactly

$$\mathcal{N}(P, \tilde{I}; \hbar) = \sum_{k=1}^{d} \Big\lfloor \frac{1}{2\pi} A_{k,0}(\widetilde{E}_2) + \frac{1}{2} \Big\rfloor - \Big\lfloor \frac{1}{2\pi} A_{k,0}(\widetilde{E}_1) + \frac{1}{2} \Big\rfloor. \tag{8.1}$$

Moreover, for the fixed interval I, this gives

$$\mathcal{N}(P, I; \hbar) = \frac{1}{2\pi\hbar} \operatorname{Vol}(H^{-1}(I)) + \frac{1}{2\pi}(\tau_k(E_2) - \tau_k(E_1)) + \delta(\hbar) + \mathcal{O}(\hbar),$$

where $\tau_k(E)$ is the period of the Hamiltonian flow of H on $\mathcal{C}_k(E)$, and $|\delta(\hbar)| < 1$.

Proof. We use decomposition (6.1) and count the number of elements $N_k(\hbar)$ of each set $\sigma_k(\hbar)$.

By (6.2), $N_k(\hbar) = \#(A_k(\cdot\,;\hbar)^{-1}(2\pi\mathbb{Z}))$; in other words, it is the number of integers $n \in \mathbb{Z}$ such that $A_k(E;\hbar) = 2\pi n$ for some $E \in I$. Since $A_{k,0}$ is a local diffeomorphism, A_k is, for $\hbar$ small enough, a monotonous bijection from I into its image, so $N_k(\hbar)$ is the number of integers in the interval $[\beta_1, \beta_2]$, where

$$\beta_j := \beta_j(\hbar) = \frac{A_k(\widetilde{E}_j(\hbar);\hbar)}{2\pi}, \quad j = 1, 2.$$

By assumption, β_j's stay away from integers by a distance at least $\widetilde{\varepsilon}$, for some $\widetilde{\varepsilon} > 0$ depending on ε. So they cannot be integers, and

$$N_k(\hbar) = \lfloor \beta_2(\hbar) \rfloor - \lfloor \beta_1(\hbar) \rfloor.$$

We have

$$\beta_j(\hbar) = \frac{1}{2\pi\hbar} A_{k,0}(\widetilde{E}_j) + \frac{1}{2\pi} A_{k,1}(\widetilde{E}_j) + \mathcal{O}(\hbar),$$

and if P has no subprincipal symbol, we have $A_{k,1}(E) = \pi$. What is more, when $\hbar$ is small enough so that the remainder $\mathcal{O}(\hbar)$ is less than $\frac{\widetilde{\varepsilon}}{2}$, the sum $\frac{1}{2\pi\hbar} A_{k,0}(E_j) + \frac{1}{2\pi} A_{k,1}(E_j)$ cannot be an integer either. This gives

$$N_k(\hbar) = \Big\lfloor \frac{1}{2\pi\hbar} A_{k,0}(\widetilde{E}_2) + \frac{1}{2} \Big\rfloor - \Big\lfloor \frac{1}{2\pi\hbar} A_{k,0}(\widetilde{E}_1) + \frac{1}{2} \Big\rfloor.$$

Summing over k, we obtain the correct number modulo $\mathcal{O}(\hbar^\infty)$. But since we are after an integer number, we can disregard the $\mathcal{O}(\hbar^\infty)$ remainder for $\hbar$ small enough, which proves (8.1).

Finally, we can write

$$N_k(\hbar) = \frac{1}{2\pi\hbar} A_{k,0}(\widetilde{E}_2) - \frac{1}{2\pi\hbar} A_{k,0}(\widetilde{E}_1) + \delta,$$

where $|\delta| < 1$. Choosing $\widetilde{E}_j$ such that $E_j - \widetilde{E}_j = \mathcal{O}(\hbar)$, and Taylor expanding at order 2, we obtain

$$N_k(\hbar) = \frac{1}{2\pi\hbar}(A_{k,0}(E_2) - A_{k,0}(E_1)) + \frac{1}{2\pi}(\tau_k(E_2) - \tau_k(E_1)) + \delta + \mathcal{O}(\hbar)$$

which yields the result. ∎

Of course, in the statement of this corollary, we may replace the interval I by any closed subinterval.

The assumption on the vanishing subprincipal symbol was not crucial; we obtain a general formula by using the correct value for $A_{k,1}$, which is the sum of the Maslov index and the integral over $\mathcal{C}_k$ of the subprincipal symbol, see [66].

It also follows from Theorem 6.1 that the moving endpoints $\widetilde{E}_j(\hbar)$ in the statement of this corollary always exist. Actually, in the pseudodifferential case, one can even choose $\widetilde{E}_j(\hbar) = E_j$, provided that we select a subsequence of $\hbar$'s; this is due to the drifting phenomenon of Corollary 8.2.

Inverse problems. Theorem 6.1 is also key in solving inverse problems. Let me just mention the Schrödinger case, where we wish to recover the potential V from the spectrum [15], and the general pseudodifferential or the Berezin–Toeplitz case, where we recover the principal symbol modulo symplectomorphisms [52, 69]. In both cases, the Bohr–Sommerfeld rules are crucial.

9. Beyond EBK

What is nice about the sheaf approach that we have presented here is the ease of generalization. Let us end this paper by exploring some extensions to the WKB/EKB methods.

Smaller errors. While an error term of size $\mathcal{O}(\hbar^\infty)$ is extremely accurate, it is still insufficient for some important applications like quantum tunnel effects. A better accuracy, namely $\mathcal{O}(e^{-\frac{c}{\hbar}})$, can be reached under analyticity assumptions. One needs for this Sjöstrand's microlocal theory [65], which was recently proven to extend to Berezin–Toeplitz operators [8, 18, 20, 61]. The application to exponentially precise Bohr–Sommerfeld rules was recently obtained by Duraffour [26], based on ideas from [36], in the pseudodifferential case, and Deleporte–Le Floch [21] in the Berezin–Toeplitz case.

Integrable systems. As was already noted by Brillouin [5], the equations for the semiclassical action $e^{\frac{i}{\hbar}S_\hbar(x)}$ can be solved by quadrature in the one-dimensional case, or if

the variables are separated. In fact, one can go even further. A quantum completely integrable system, with a phase space of dimension $2n$, is a set of n pairwise commuting self-adjoint semiclassical operators $(P_1, \dots, P_n)$. The corresponding classical symbols $(H_1, \dots, H_n)$ form a Liouville integrable system. Since the Darboux–Carathéodory theorem extends to such integrable systems, it can be shown that the whole microlocal strategy holds, see [66, 67]. This establishes both WKB solutions which are joint quasimodes of the system, and Bohr–Sommerfeld rules for the joint spectrum. To my knowledge, the first mathematical treatment of these joint Bohr–Sommerfeld rules can be found in [1, 6, 12]. A review of these results is presented in [68].

Singularities. While the Darboux–Carathéodory theorem applies only to *regular* points, the microlocal sheaf strategy can, surprisingly, be extended to energy level sets containing *singular points*. For instance, a local extremum of the potential V. The easiest case concerns elliptic singularities, for which the Hamiltonian is a microlocal perturbation of the Harmonic oscillator; see [10, 19, 33, 50]. The most spectacular application concerns hyperbolic points (for instance, a local maximum of V). It has been worked out by Colin de Verdière–Parisse [16] for the pseudodifferential case, and Le Floch [51] in the Berezin–Toeplitz case. The main idea is to extend Proposition 5.1 to a neighborhood of the critical point. One can show that, this time, the space of microlocal solutions has dimension not one but *two*. Of course, the level sets are not circles anymore, but immersed curves with transversal intersections. The number of branches (4) at each crossing fits nicely with the dimension 2 of the microlocal solutions, and produces new *singular* Bohr–Sommerfeld conditions by expressing the vanishing of some determinant related to the topology of the critical fiber [16]. The analogous question for degenerate singularities, for instance, a quartic oscillator $\xi^2 + x^4 + \mathcal{O}(x^5)$, is still quite open; see [13, 55].

Non-self-adjoint operators. Given the heavy use of real symplectic geometry that the microlocal method requires, it seems hazardous to extend it to non-self-adjoint operators, i.e., semiclassical operators whose symbols are not necessarily real-valued. Nevertheless, it turned out that this can be achieved, and symplectic normal forms in the complexified phase space remain very effective. For small non-self-adjoint perturbations of self-adjoint pseudodifferential operators, Bohr–Sommerfeld rules with $\mathcal{O}(\hbar^\infty)$ remainder have been obtained by Rouby [60], following the pioneering works of Melin–Sjöstrand [57] and Hitrik [37]. The extension to more general one-dimensional operators is currently an active area of research, see, for instance, [21, 27, 38, 59].

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