

The Maslov-WKB Method for the (an-)Harmonic Oscillator

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In his book "Théorie des Perturbations et Méthodes Asymptotiques" V.P. MASLOV has given an ingenious approximation method which overcomes certain well known difficulties in the classical WKB approach. One of these difficulties is connected with the singularities of the amplitudes of the wave function which appear at turning points of a classical motion. Another arises from the fact that the relative phases of the different contributions to the WKB wave function are obtained from a priori knowledge about its behaviour outside the domain of the classical motion and are therefore not intrinsic. Both these problems are solved in a most natural way in MASLOV's approach. Unfortunately, his book is not easy to read and often it is difficult to decide whether the assertions are really proved.

This paper is an attempt to present MASLOV's method at an elementary level, thus making his beautiful ideas available to a larger audience. We restrict ourselves to the easiest possible case, the harmonic oscillator in one dimension. This we hope will make the exposition more transparent. It turns out that the necessary techniques to prove the assertions in this easy example are already prototypes for the proofs in the general case. Therefore our limitation to a particular example is only a matter of convenience and not really a simplification of the main problems which occur in the most general situation.

Since it is our goal to explore the limit $\hbar \rightarrow 0$ in quantum mechanics, we begin with a short study of the classical system for our model Hamiltonian

$$H(x, p) = p^2 + x^2$$

before turning to the investigation of the time independent Schrödinger equation. We fix once and for all an energy $E > 0$ *. The Hamiltonian equations are then

$$\begin{aligned} \left(\frac{dp}{dt}\right)(t) &= -2x(t) = -\frac{\partial H}{\partial x}(x(t), p(t)), \\ \left(\frac{dx}{dt}\right)(t) &= 2p(t) = \frac{\partial H}{\partial p}(x(t), p(t)), \end{aligned} \tag{1}$$

$$p(t)^2 + x(t)^2 = E.$$

* This means that our estimates will *not* be independent of E . We shall omit the subscript E for E -dependent objects.

We fix the initial conditions

$$p(0) = E^{\frac{1}{2}}, \quad x(0) = 0,$$

so that the solution of (1) is

$$\begin{aligned} p(t) &= E^{\frac{1}{2}} \cos(2t), \\ x(t) &= E^{\frac{1}{2}} \sin(2t). \end{aligned} \tag{2}$$

(Note that one cycle has period π .) The trajectory of $(p, x)(t)$ in the phase space \mathbb{R}^2 is the Lagrangian manifold*

$$\Gamma = \{(p, x)(t) | t \in \mathbb{R}\}.$$

This set is independent of the particular initial conditions since it also has the form

$$\{(p, x) \in \mathbb{R}^2 | H(x, p) = E\};$$

in our case this is a circle of radius \sqrt{E} centered at the origin.

An important object in the transition to quantum mechanics is the action \hat{S} and its time independent part S . The function $\hat{S}(x, t)$ is defined as a solution of the equation

$$H\left(x, \frac{\partial \hat{S}}{\partial x}\right) + \frac{\partial \hat{S}}{\partial t} = 0.$$

Since H is independent of t , one makes the substitution

$$\hat{S}(x, t) = S_E(x) - Et,$$

so that the new equation for $S = S_E$ reads

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

For our particular H , this equation has the solutions

$$S_{\pm}(x) = \text{const.} \pm \int_0^x (E - \xi^2)^{\frac{1}{2}} d\xi$$

in the region $|x| < E^{\frac{1}{2}}$. A better understanding of S can be gained by considering it as a function on Γ .

Let

$$\sigma(t) = \int_0^{x(t)} p dx, \quad 0 \leq t < \pi,$$

(defined as an integral on Γ , that is along the trajectory of the physical motion). Then

$$S_{\pm}(x) = \hat{S}_{\pm} + \sigma(t_{\pm}(x)),$$

* In several dimensions, a manifold Γ is called Lagrangian if $dp \wedge dx = 0$ on Γ .

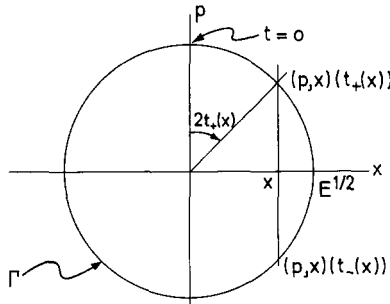


Figure 1

where $t_{\pm}(x)$ are the two solutions* of $x(t) = x$, $0 \leq t < \pi$, indicated in Figure 1. We shall henceforth identify $(p, x)(t)$ with the time value t , so that t can be viewed as a point on Γ . We shall see below that the advantages (and, unfortunately, also the notational difficulties) of MASLOV's approach originate from considering Γ , and not x , as the basic space. For this reason we shall use the notation σ and not S .

Before we proceed it will be convenient to review the usual WKB method. The time-independent Schrödinger equation canonically associated with the Hamiltonian H and the energy E is

$$(H(x, -i\hbar\partial_x) - E)\varphi_{\hbar}(x) = 0, \tag{3}$$

considered as an equation in $L_2(\mathbb{R})$. The symbol ∂_x stands for d/dx . The WKB method consists of the following approximation procedure**. We write

$$\varphi_{\hbar}(x) \sim e^{\frac{i}{\hbar}s(x)}(f(x) + \hbar f_1(x) + \dots)$$

and "solve" equation (3) by perturbation expansion up to order \hbar^2 . The "solution" $\exp i\left(\frac{s(x)}{\hbar}\right)f(x)$ will be denoted by $\varphi_{\hbar}^{(2)}(x)$. By direct computation, the equations for s and f are seen to be

$$H\left(x, \frac{ds}{dx}\right) = E \tag{4}$$

and

$$2\left(\frac{ds}{dx}\right)\left(\frac{df}{dx}\right) + \left(\frac{d^2s}{dx^2}\right)f = 0.$$

Obviously s is the action, and f turns out to be

$$f(x) = \text{const.} \left|\frac{ds}{dx}\right|^{-\frac{1}{2}}(x) = \text{const.} \left|\frac{dx}{dt}\right|^{-\frac{1}{2}}(x).$$

This result has the well-known interpretation that

$$\int_{x_0}^{x_0+\Delta} |\varphi_{\hbar}^{(2)}(x)|^2 dx$$

* The important point is that the number of solutions is finite.

** See Appendix A 5 for a derivation in the anharmonic case.

is proportional to the probability of finding the classical particle in the interval $[x_0, x_0 + \Delta]$, for in fact

$$\int_{x_0}^{x_0 + \Delta} \left| \frac{dx}{dt}(x) \right|^{-1} dx$$

is proportional to the time the classical particle needs to cross this interval.

Equation (4) has the two independent solutions S_{\pm} , so that a more general solution of (3) in the WKB approximation is a linear combination

$$\begin{aligned} \varphi_h^{(2)}(x) = & \frac{A_+}{(E - x^2)^{\frac{1}{4}}} e^{\frac{i}{h}(\mathring{S}_+ + \int_0^x (E - \xi^2)^{1/2} d\xi)} \\ & + \frac{A_-}{(E - x^2)^{\frac{1}{4}}} e^{\frac{i}{h}(\mathring{S}_- - \int_0^x (E - \xi^2)^{1/2} d\xi)} \end{aligned}$$

In the usual WKB approach one then shows the following result:

If h is such that

$$\pi E = \oint p dx = 2\pi h(n + \frac{1}{2}),$$

for some $n=0, 1, 2, \dots$, then the requirement that $\varphi_h^{(2)}(x)$ should fall off exponentially for $x^2 > E$ can be fulfilled by choosing

$$\mathring{S}_+ = \mathring{S}_- + h\frac{\pi}{2} \quad \text{and} \quad A_+ = A_-.$$

What can be said about the function $\varphi_h^{(2)}$ which is obtained in this fashion? By construction, it is locally an approximate solution of (3) for $x^2 < E$. However, it does not (a priori) approximate the function φ_h in L_2 as $h \rightarrow 0$ and it is in fact not even in the domain of $H(x, -ih\partial_x)$ *. Therefore while $\varphi_h^{(2)}$ is an approximate solution, it is not known whether it is an approximation to the true eigenfunction. This situation is drastically improved in MASLOV's approach, where one constructs a function ϕ_h which is an approximate solution of (3) in the L_2 sense (Theorem 5 below). This will allow an inversion of $H(x, -ih\partial_x) - E$ and a proof that ϕ_h approximates the true eigenfunction φ_h in the L_2 sense as $h \rightarrow 0$ (Theorem 7).

We now show where the drawbacks in the usual WKB method originate and how they are ingeniously overcome by MASLOV's method. The main observation is that there is no reason to treat the variables x and p on a different footing. In fact, the quantization $H(ih\partial_p, p)$ of $H(x, p)$ is as natural as the one we have considered so far. Let us therefore denote the previously obtained solution $\varphi_h^{(2)}$ by $\varphi_{x,h}$. By p -quantization we find

$$\varphi_{p,h}(p) = \sum_{\pm} A_{\pm} e^{\frac{i}{h} s_{p \pm}(p)} f_p(p),$$

with

$$H\left(\frac{ds_p}{dp}, p\right) = E,$$

$$2\left(\frac{ds_p}{dp}\right)\left(\frac{df_p}{dp}\right) + \left(\frac{d^2s_p}{dp^2}\right)f_p = 0.$$

* Because of the pole at $x = \pm\sqrt{E}$.

The entire discussion continues as before for $\varphi_{x,h}$, leaving however a solution which is irregular at the points $|p| = \sqrt{E}$.

It is now important that a connection between $\varphi_{p,h}$ and $\varphi_{x,h}$ can be established through the canonical transformation

$$T: x \rightarrow p, p \rightarrow -x$$

and its quantum mechanical counterpart, the unitary map

$$U^*: L_2(\mathbb{R}, dp) \rightarrow L_2(\mathbb{R}, dx)$$

given by the h -dependent Fourier transform $\tilde{\cdot}$:

$$\tilde{F}(x) = (2\pi h)^{-\frac{1}{2}} \int e^{\frac{i}{h} px} F(p) dp.$$

In fact, if Q is the “correctly” defined quantization operation (the first variable of H going into multiplication, the second variable into $-ih$ times differentiation), then

$$U(QH)U^* = Q(TH). \tag{5}$$

To see this, let

$$H(x, p) = \sum c_{mn} x^m p^n; *$$

then $(TH)(x, p) = H(p, -x)$. Moreover

$$QH = \sum c_{mn} x^m (-ih\partial_x)^n = H(x, -ih\partial_x)$$

and

$$Q(TH) = \sum c_{mn} (+ih\partial_p)^m p^n = H(ih\partial_p, p).$$

We note that $H(x, p)$ must be considered as a non-commutative function of its symbols x, p . Now as operators on L_2 ,

$$\begin{aligned} U(-ih\partial_x)U^* &= p, \\ UxU^* &= ih\partial_p, \end{aligned}$$

by a well known property of the Fourier transform. The assertion now follows from the fact that U is unitary.

The connection (5) immediately provides us with the (obvious) fact that the exact solution of problem (3) is covariant under the canonical transformation T :

$$(H(x, -ih\partial_x) - E)\varphi_h = 0$$

is equivalent to

$$(H(ih\partial_p, p) - E)\tilde{\varphi}_h^{-1} = 0.$$

We may therefore expect, after an appropriate choice of phases, that

$$\varphi_{x,h} \sim \tilde{\varphi}_{p,h}$$

* For more general H , the assertion follows if one defines

$$(H(x, -ih\partial_x)f)(x) = (2\pi h)^{-1} \int e^{\frac{i}{h} px} H(x, p) e^{-\frac{i}{h} py} f(y) dp dy$$

and

$$(H(ih\partial_p, p)g)(p) = (2\pi h)^{-1} \int e^{-\frac{i}{h} px} e^{\frac{i}{h} xq} H(x, q)g(q) dx dq.$$

that is,

$$U(\text{“WKB”}) = (\text{“WKB”})T$$

since the constituents of $\varphi_h^{(2)}$, namely the functions s_X, s_P and f_X, f_P are related through T . As we expect $\varphi_h \sim \varphi_h^{(2)}$ for $h \rightarrow 0$, and since φ_h is covariant, the Fourier transform should act in this limit only by canonically transforming s and f . This makes the ensuing lemma intuitively obvious, the tool for the proof being the stationary phase method.

In analogy with $\varphi_{X,h}$ and $\varphi_{P,h}$ we define two functions on Γ :

$$\begin{aligned} u_{X,h}(t) &= e^{\frac{i}{h} \int_0^t p dx} g(t) \left| \frac{dx}{dt} \right|^{-\frac{1}{2}}(t) e_{t_0}(t), \\ u_{P,h}(t) &= e^{-\frac{i}{h} \int_0^t x dp} g(t) \left| \frac{dp}{dt} \right|^{-\frac{1}{2}}(t) e_{t_0}(t), \end{aligned} \tag{6}$$

where $e_{t_0} \in C_0^\infty$ has support in a small neighborhood of $t=t_0$, $e_{t_0}(t_0)=1$, and $\text{supp } e_{t_0}$ is such that the maps

$$t \rightarrow x(t), \quad t \rightarrow p(t)$$

have unique inverses (denoted by $t_X(x)$ and $t_P(p)$, respectively).

These maps depend on t_0 ; moreover such an e_{t_0} can be found for all $t_0 \in \Gamma \setminus \Sigma$, where

$$\Sigma = \left\{ t \in \Gamma, t = 0 \pmod{\left(\frac{\pi}{4}\right)} \right\}.$$

By definition Σ is the union of the critical points for the WKB method in either the x or the p coordinate. We define the $\hat{}$ operation by*

$$\hat{u}_{P,h}(p) = \begin{cases} u_{P,h}(t_P(p)) & \text{if } p \in \{p | \exists t \in \text{supp } e_{t_0} \text{ with } p(t) = p\}^{**} \\ 0 & \text{otherwise} \end{cases}.$$

This definition simply interprets $u_{P,h}$ as a function of p .

Note that the amplitudes of $u_{X,h}$ and $u_{P,h}$ are chosen to be identical, and to equal $g(t)$ when considered on Γ .

Lemma 1. *With the above definitions, we have for fixed $t_0 \in \Gamma \setminus \Sigma$*

$$u_{X,h}(t_0) - \hat{u}_{P,h}(x(t_0)) e^{\frac{i\pi}{4} \text{sign}\left(\frac{dx}{dp}\right)(t_0)} = O(h).$$

Proof. By definition,

$$\begin{aligned} \hat{u}_{P,h}(x) &= (2\pi h)^{-\frac{1}{2}} \int_{p(\text{supp } e_{t_0})} dp e^{\frac{i}{h} p x} u_{P,h}^\wedge(p) \\ &= (2\pi h)^{-\frac{1}{2}} \int_{p(\text{supp } e_{t_0})} dp e^{\frac{i}{h} p x} \left(e^{-\frac{i}{h} \int_0^\tau x dp} e_{t_0}(\tau) g(\tau) \left| \frac{dp}{dt} \right|^{-\frac{1}{2}}(\tau) \right)_{\tau=t_P(p)}. \end{aligned}$$

* This definition will be slightly generalized below (see (12)).

** We write this set as $p(\text{supp } e_{t_0})$.

We now apply the stationary phase method (cf. Lemma A2 in the Appendix). The phase in the integral is

$$\rho_x(p) = \frac{1}{h} \left(px - \int_0^{t_P(p)} x dp \right).$$

Its derivative is

$$\partial_p \rho_x(p) = \frac{1}{h} (x - x(t_P(p))),$$

which for $x = x(t_0)$ has a unique zero* at $p_0 = p(t_0)$, since $x(t_0) = x(t_P(p(t_0)))$. The second derivative at this point is

$$\partial_p^2 \rho_{x(t_0)}(p_0) = -\frac{1}{h} \frac{dx}{dp}(t_0) \neq 0 \tag{7}$$

since $t \notin \Sigma$. Furthermore, we have

$$\rho_{x(t_0)}(p_0) = \frac{1}{h} \left(p(t_0)x(t_0) - \int_0^{t_0} x dp \right) = \frac{1}{h} \int_0^{t_0} p dx. \tag{8}$$

Therefore, by Lemma A2,

$$u_{p,h} \tilde{\wedge}(x(t_0)) = (2\pi h)^{-\frac{1}{2}} e^{-\frac{i\pi}{4} \text{sign} \frac{dx}{dp}(t_0)} (2\pi)^{\frac{1}{2}} \left| \frac{1}{h} \partial_p^2 \rho_{x(t_0)}(p_0) \right|^{-\frac{1}{2}} \cdot e^{\frac{i}{h} \rho_{x(t_0)}(p_0)} e_{t_0}(t_0) \left| \frac{dp}{dt} \right|^{-\frac{1}{2}}(t_0) g(t_0) + O(h),$$

so that the assertion follows from (7) and (8).

The proof of this lemma shows that on functions of the type (6) the Fourier transform is a *local*, linear operation up to terms of order $O(h)$; namely $u_{p,h} \tilde{\wedge}(x(t_0))$ depends only on $u_{p,h}(t_0)$ and its derivatives. In particular, if $g_1(t) \in C^\infty$, then

$$(u_{p,h} g_1) \tilde{\wedge}(x(t)) = (u_{p,h} \tilde{\wedge}(x(t))) g_1(t) + O(h).$$

We now return to the main problem and define two WKB-like functions with adjusted phases on the simply connected covering of Γ (i.e. for $t \in \mathbb{R}$). We shall later combine these two functions into an approximation of the eigenfunction φ_h . First define

$$\begin{aligned} \psi_{X,h}(t) &= \pi^{-\frac{1}{2}} \left| \frac{dx}{dt} \right|^{-\frac{1}{2}}(t) e^{\frac{i}{h} \int_0^t p dx} e^{iI_X(t)}, \\ \psi_{P,h}(t) &= \pi^{-\frac{1}{2}} \left| \frac{dp}{dt} \right|^{-\frac{1}{2}}(t) e^{-\frac{i}{h} \int_0^t x dp} e^{iI_P(t)}, \end{aligned}$$

where

$$\begin{aligned} I_X(t) &= -m \frac{\pi}{2} \quad \text{for } t \in \left(m \frac{\pi}{2} - \frac{\pi}{4}, m \frac{\pi}{2} + \frac{\pi}{4} \right], \\ I_P(t) &= -m \frac{\pi}{2} + \frac{\pi}{4} \quad \text{for } t \in \left(m \frac{\pi}{2}, (m+1) \frac{\pi}{2} \right] \\ &= I_X \left(t - \frac{\pi}{4} \right) + \frac{\pi}{4}. \end{aligned}$$

* That is, the phase is stationary on the classical trajectory.

Note that I_X and I_P are chosen to be constant in regions where respectively x and p are regular.

Theorem 2. For any $t_0 \not\equiv 0 \pmod{\frac{\pi}{4}}$, we have

$$\psi_{X,h}(t_0) - (\psi_{P,h} e_{t_0})^\wedge(x(t_0)) = O(h), \tag{9}$$

while for $x^2 < E$,

$$\sum_{t: x(t)=x} \psi_{X,h}(t) - \psi_{P,h}^\wedge(x) = O(h). \tag{10}$$

Proof. This is almost obvious from Lemma 1. We have $g(t) = 1$. To determine the phases, note that

$$\left(-\frac{dx}{dp}\right)(t) > 0 \quad \text{for } t \pmod{\frac{\pi}{2}} \in \left(0, \frac{\pi}{4}\right),$$

$$\left(-\frac{dx}{dp}\right)(t) < 0 \quad \text{for } t \pmod{\frac{\pi}{2}} \in \left(\frac{\pi}{4}, \frac{\pi}{2}\right),$$

(see Figure 1 or Equation (2)). Thus for $t \pmod{\frac{\pi}{2}} \in \left(0, \frac{\pi}{4}\right)$ the function $(\psi_{P,h} e_t)^\wedge(x(t))$ picks up a phase $\exp i\left(\frac{\pi}{4}\right)$, which is reflected by the choice $I_X(t) = I_P(t) + \frac{\pi}{4}$ in this region. Similarly for $t \pmod{\frac{\pi}{2}} \in \left(\frac{\pi}{4}, \frac{\pi}{2}\right)$, $(\psi_{P,h} e_t)^\wedge(x(t))$ picks up a phase $\exp i\left(\frac{\pi}{4}\right)$, which is compensated by the choice $I_X(t) = I_P(t) - \frac{\pi}{4}$. This completes the proof of (9). Equation (10) is obtained from (9) by writing

$$\begin{aligned} \sum_{t: x(t)=x} \psi_{X,h}(t) - \psi_{P,h}^\wedge(x) &= \sum_{t: x(t)=x} \{\psi_{X,h}(t) - (\psi_{P,h} e_t)^\wedge(x)\} - (\psi_{P,h} (1 - \sum_{t: x(t)=x} e_t))^\wedge(x) \\ &= O(h) + O(h^N) \end{aligned}$$

and using Corollary A1, because the expression

$$\left(1 - \sum_{t: x(t)=x} e_t\right)^\wedge$$

has support away from $\{p(t) | x(t) = x\} = \{p | x(p) = x\}$.

It should be obvious to the reader that the choice of I_X and I_P is dictated only by the topology and structure of Γ . For this reason, MASLOV was able to give a canonical definition of corresponding “indices” (I_X, I_P) on Lagrangian manifolds of arbitrary dimension. A Lagrangian manifold furthermore has the important property (in arbitrary dimensions) that in any small open set one can obtain regular local coordinates by choosing for each degree of freedom either x or p as coordinate.

We now turn to the construction of the approximation Φ_h to φ_h . We are interested in functions of the variable x in order to apply the operator $H(x, -ih\partial_x)$, and we want to combine the good properties of $\psi_{X,h}$ and $\psi_{P,h}$ into one. The idea is to choose $\psi_{P,h}$ as the approximation at those points where $\psi_{X,h}$ is singular, and vice versa. This choice is made possible by forming a partition of the identity

on the manifold $\Gamma, e_X + e_P = 1$, so that $\psi_{X,h}e_X$ has its support only where $\psi_{X,h}$ is regular and $\psi_{P,h}e_P$ has its support only where $\psi_{P,h}$ is regular. By Theorem 2, at points where both $\psi_{X,h}$ and $\psi_{P,h}$ are regular, the particular choice of e_X and e_P makes no difference in the limit $h \rightarrow 0$. To obtain a function of x , we choose in the term $\psi_{X,h}e_X$ all values of t for which $x(t) = x$ and we apply a Fourier transformation to $\psi_{P,h}e_P$ considered as a function of p . We now formalize this construction.

Let e_X, e_P be a real C^∞ partition of unity on Γ , namely

$$e_X, e_P \in C^\infty, \quad e_X(t) + e_P(t) = 1 \quad \text{for } t \in [0, \pi).$$

In particular we shall require e_X and e_P to vanish in a neighborhood of the singular points of $\psi_{X,h}$ and $\psi_{P,h}$ respectively (i.e. in a neighborhood of $t = \frac{\pi}{4}, \frac{3\pi}{4}$ and $t = 0, \frac{\pi}{2}, \pi$ respectively).

Let

$$\bar{e}_X(t) = e_X(t \pmod{\pi}), \quad \bar{e}_P(t) = e_P(t \pmod{\pi}),$$

be the periodic extensions of e_X and e_P . We now define the approximation $\Phi_h(x)$ by taking the mean over an infinite number of periods of the classical physical motion. The treatment of $\psi_{X,h}$ and $\psi_{P,h}$ becomes asymmetrical at this point because we want to arrive at a function of the variable x . Specifically, we put

$$\Phi_h(x) = \lim_{M \rightarrow \infty} \frac{1}{M} \left\{ \left(\sum_{\substack{t \in [-M\frac{\pi}{2}, M\frac{\pi}{2}] \\ x(t) = x}} \psi_{X,h}(t) \bar{e}_X(t) + (\psi_{P,h} \bar{e}_P|_{|t| \leq M\frac{\pi}{2}})^\wedge(x) \right) \right\}, \quad (11)$$

where

$$(\psi_{P,h} \bar{e}_P|_{|t| \leq M\frac{\pi}{2}})^\wedge(p) = \sum_{\substack{t \in [-M\frac{\pi}{2}, M\frac{\pi}{2}] \\ p(t) = p}} \psi_{P,h}(t) \bar{e}_P(t). \quad (12)$$

Lemma 3. *If $-\pi + \frac{1}{h} \oint p dx \not\equiv 0 \pmod{2\pi}$ then $\Phi_h(x) = 0$.*

Remarks. (1) Note that

$$-\pi + \frac{1}{h} \oint p dx = I_X(\pi) - I_X(0) + \frac{1}{h} \int_{t=0}^{t=\pi} p dx = I_P(\pi) - I_P(0) - \frac{1}{h} \int_0^\pi x dp$$

is the phase difference between $\psi_{X,h}(\pi)$ and $\psi_{X,h}(0)$ or between $\psi_{P,h}(\pi)$ and $\psi_{P,h}(0)$.

(2) If $-\pi + \frac{1}{h} \oint p dx \equiv 0 \pmod{2\pi}$ then the expression on the right hand side of (11) is independent of M and one can take $M = 1$.

(3) In the case of the harmonic oscillator we have

$$\oint p dx = \pi E.$$

The requirement

$$-\pi + \frac{1}{h} \oint p dx \equiv 0 \pmod{2\pi}$$

is equivalent to

$$E = 2h(n + \frac{1}{2}), \quad n = 0, 1, 2, \dots \tag{13}$$

This is the famous BOHR-SOMMERFELD quantization condition. Lemma 3 asserts that the natural definition of Φ_h leads to non-zero functions only if condition (13) is fulfilled. In other words, the quasi-classical approximation is only interesting if the problem has been pre-quantized.

Proof of Lemma 3. Suppose

$$-\pi + \frac{1}{h} \int_0^\pi p dx \not\equiv 0 \pmod{2\pi}.$$

Then by definition we must have

$$\psi_{X,h}(\pi) = \psi_{X,h}(0) e^{i\alpha}$$

for some $\alpha \not\equiv 0 \pmod{2\pi}$, and hence also

$$\psi_{X,h}(t + \pi) = \psi_{X,h}(t) e^{i\alpha}.$$

Therefore we find that

$$\begin{aligned} \lim_{M \rightarrow \infty} \frac{1}{M} \left| \sum_{\substack{t \in [-\frac{M\pi}{2}, \frac{M\pi}{2}] \\ x(t) = x}} \psi_{X,h}(t) \bar{e}_X(t) \right| \\ \leq 2 \max_{t \in [0, \pi]} |\psi_{X,h}(t) e_X(t)| \lim_{M \rightarrow \infty} \frac{1}{M} \left| \sum_{n=-M}^M e^{i\alpha n} \right| = 0, \end{aligned}$$

because

$$\lim_{M \rightarrow \infty} \frac{1}{M} \sum_{n=-M}^M e^{i\alpha n} = e^{i\alpha} \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{n=-M}^M e^{i\alpha n}$$

and because the equation

$$z = e^{i\alpha} z, \quad z \in \mathbb{C}$$

has only the solution $z = 0$ if $\alpha \not\equiv 0 \pmod{2\pi}$. We apply the same argument to $\psi_{P,h} \bar{e}_P$ before performing the Fourier transformation. The Fourier transform and $\lim_{M \rightarrow \infty}$ can be exchanged because of the uniformity of the bounds in question. This completes the proof of Lemma 3.

Lemma 4. $\Phi_h(x)$ is independent of e_X, e_P up to terms of order $O(h)$.

Proof. For $x^2 < E$ this is evident from Theorem 2. For $x^2 \geq E$, consider two partitions e_X, e_P and e'_X, e'_P . Then

$$\Phi_h^{e_X, e_P}(x) - \Phi_h^{e'_X, e'_P}(x) = (\psi_{P,h}(e_P - e'_P))^\wedge(x),$$

and the right hand side here is $O(h^N)$, $N = 1, 2, \dots$, since $e_P - e'_P$ has support in the complement of a neighborhood of $t = \frac{\pi}{4}, \frac{3\pi}{4} \leftrightarrow x^2 = E$ (Corollary A 1.).

We note that $\Phi_h(x)$ is smooth at $x^2 = E$ because it is either identically zero or else equals (in a neighborhood of $x^2 = E$) the function $(\psi_{P,h} e_P)^\wedge$, which in turn

is the Fourier transform of a C^∞ function with compact support. Therefore, the MASLOV-WKB method has improved the behaviour of the approximation at $x^2 = E$ by comparison with the usual WKB method. But even more, one has the following important

Theorem 5. *With the above definitions*

$$\|(H(x, -ih\partial_x) - E)\Phi_h\|_{L_2} = O(h^2).$$

Proof. Fix $h > 0$. If $h \neq \frac{E}{2(n+\frac{1}{2})}$, then $\Phi_h = 0$ and the assertion is trivially correct. We let $h = \frac{E}{2(n+\frac{1}{2})}$ in the sequel, so that Φ_h can be different from zero. Since Φ_h is smooth at $x^2 = E$ (see above), we may estimate $\int |(H - E)\Phi_h|^2$ for $x^2 < E$ and $x^2 > E$ separately. We start with the case $x^2 < E$ (the classical region).

Let

$$\sigma^\vee(x) = \sigma(t(x)) = \int_0^x (E - \xi^2)^{\frac{1}{2}} d\xi, \quad f_X(x) = (E - x^2)^{-\frac{1}{2}}.$$

$$H_h = H(x, -ih\partial_x) - E \quad \text{and} \quad \tilde{H}_h = e^{-\frac{i}{h}\sigma^\vee} H_h e^{\frac{i}{h}\sigma^\vee}.$$

A simple computation shows that

$$H'_h = H(x, -ih\partial_x + (\partial_x \sigma^\vee)(x)) - E = H(x, -ih\partial_x + p(x)) - E,$$

since $\partial_x \sigma^\vee = p$. By the WKB construction

$$H_h e^{\frac{i}{h}\sigma^\vee} f_X = h^2 g_{X,h},$$

where $g_{X,h}(x)$ is uniformly bounded in h and in x , away from $x = \pm\sqrt{E}$.

To discuss the action of H_h on Φ_h it is advantageous first to fix a t such that $t \rightarrow x(t)$ and $t \rightarrow p(t)$ have locally unique inverses $t_X(x)$ and $t_P(p)$ respectively.

Given x , we have then a contribution $e^{\frac{i}{h}\sigma^\vee(t)} f_X(x) e^{iI_X(t)} e_X(t)|_{t=t_X(x)}$ to Φ_h from $\psi_{X,h} e_X$. Acting with H_h on this, the result is

$$(e^{iI_X(t)} e^{\frac{i}{h}\sigma^\vee(t)})_{t=t_X(x)} \{h^2 g_{X,h}(x) e_X(t_X(x)) + [H'_h, e_X(t_X(\cdot))](x) f_X(x)\},$$

where $[,]$ denotes the commutator, and where we have used the fact that $I_X(t)$ is constant in a region in which $t \rightarrow x(t)$ is one-to-one.

By virtue of the canonical construction, the treatment in the p coordinate is similar. Let

$$\tilde{H}_h = H(ih\partial_p, p) - E,$$

$$\tilde{\sigma}^\wedge(p) = \tilde{\sigma}(t(p)) = - \int_{\sqrt{E}}^p (E - \xi^2)^{\frac{1}{2}} d\xi, \quad f_P(p) = (E - p^2)^{-\frac{1}{2}}.$$

Then

$$\begin{aligned} \tilde{H}'_h &= e^{-\frac{i}{h}\tilde{\sigma}^\wedge} \tilde{H}_h e^{+\frac{i}{h}\tilde{\sigma}^\wedge} \\ &= H(ih\partial_p - (\partial_p \tilde{\sigma}^\wedge), p) - E \\ &= H(ih\partial_p + x(p), p) - E. \end{aligned}$$

The argument above shows that

$$\begin{aligned} & (\tilde{H}_h(e^{iI_P(t)} e^{\frac{i}{h}\tilde{\sigma}(t)} e_P(t) f_P(p))_{t=t_P(\cdot)}) \sim (x) \\ & = h^2 (e^{iI_P(t)} e^{\frac{i}{h}\tilde{\sigma}(t)} e_P(t) g_{P,h}(p))_{t=t_P(\cdot)} \sim (x) \\ & + (e^{iI_P(t)} e^{\frac{i}{h}\tilde{\sigma}(t)} [\tilde{H}'_h, e_P(t_P(\cdot))] f_P(p))_{t=t_P(\cdot)} \sim (x). \end{aligned}$$

The first term has an L_2 norm which is $O(h^2)$ because the Fourier transform is a unitary operation. The second term is $O(h)$, and not $O(h^2)$, but the following procedure shows that the sum of the two terms containing the commutators $[H'_h, e_X]$ and $[\tilde{H}'_h, e_P]$ is $O(h^2)$! Consider e_P as a function of p . By the Leibnitz rule

$$\begin{aligned} [\tilde{H}'_h, e_P] f_P &= ih(\partial_p e_P) \cdot \left(\frac{\partial H}{\partial x}\right) (ih\partial_p + x(p), p) f_P + O(h^2) \\ &= ih(\partial_p e_P) \cdot \left(\frac{-dp}{dt}\right) f_P + O(h^2), \end{aligned}$$

where the last equality follows from the equations of motion. Therefore the term coming from $[\tilde{H}'_h, e_P]$ equals

$$ih \left(e^{iI_X} e^{\frac{i}{h}\sigma} (\partial_p e_P)(x) \left(\frac{-dp}{dt}\right) f_X + O(h) \right) + O(h^2).$$

The terms which are $O(h^2)$ have finite L_2 norms, since they are Fourier transforms of C_0^∞ functions. Also,

$$\begin{aligned} [H'_h, e_X] f_X &= -ih(\partial_x e_X) \left(\frac{\partial H}{\partial p}\right) (x, -ih\partial_x + p(x)) f_X + O(h^2) \\ &= -ih(\partial_x e_X) \left(\frac{\partial x}{\partial t}\right) f_X + O(h^2). \end{aligned}$$

Therefore the two commutator terms sum to

$$-ih \left(\left(\frac{de_X}{dt} \cdot \frac{dt}{dx}\right) \left(\frac{dx}{dt}\right) - \left(\frac{de_P}{dt} \cdot \frac{dt}{dp}\right) \left(\frac{-dp}{dt}\right) \right) f_X e^{iI_X} e^{\frac{i}{h}\sigma} + O(h^2),$$

which is $O(h^2)$ since $\partial_t(e_X + e_P) = 0$ by construction.

Now $H_h \Phi_h(x)$ for $x = x(t)$, and t as above is a sum of terms of the form just described. This verifies that $H_h \Phi_h(x) = O(h^2)$ in the region $0 < x^2 < E$. Now in a neighborhood of $\Sigma = \left\{ t \mid t = 0 \left(\text{mod } \frac{\pi}{4} \right) \right\}$ we have $H_h \Phi_h(x) = O(h^2)$ because either $e_X = 0$ or $e_P = 0$ there.

We have thus shown that

$$\left(\int_{x^2 \leq E} |(H_h \Phi_h)(x)|^2 dx \right)^{\frac{1}{2}} = O(h^2).$$

Also for $x^2 \geq E$,

$$\begin{aligned} (H_h \Phi_h)(x) &= (\tilde{H}_h(\psi_{P,h} e_P)^\wedge) \sim (x) \\ &= (e^{\frac{i}{h}\tilde{\sigma}} h^2 g_{P,h} e_P^\wedge) \sim (x) + (e^{\frac{i}{h}\tilde{\sigma}} [\tilde{H}'_h, e_P^\wedge] f_P) \sim (x) = A(x) + B(x). \end{aligned}$$

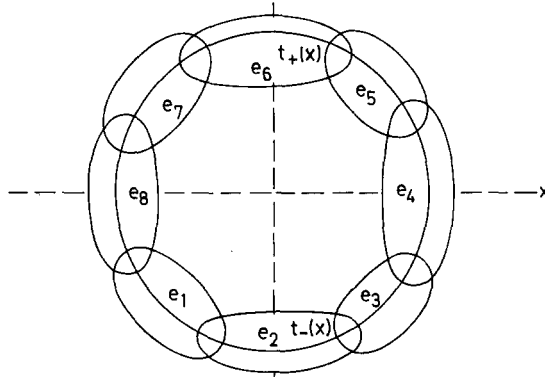


Figure 2

Now

$$\left(\int_{x^2 \geq E} |A(x)|^2 dx \right)^{\frac{1}{2}} \leq \left(\int |A(x)|^2 dx \right)^{\frac{1}{2}} = h^2 \left(\int |(g_{p,h} \hat{e}_p)(p)|^2 dp \right)^{\frac{1}{2}} = O(h^2),$$

and

$$\left(\int_{x^2 \geq E} |B(x)|^2 dx \right)^{\frac{1}{2}} = O(h^N), \quad N=1, 2, \dots,$$

because B is the Fourier transform of a C^∞ function which has support away from $p=0$ (see Corollary A1). The theorem is thus proved.

Before we determine the connection between Φ_h and the exact solution φ_h we prove

Lemma 6. As $h \rightarrow 0$ we have

$$\|\Phi_h\|_{L_2} = 1 + O(h).$$

Remark. A difficulty here is the fact that

$$(\psi_{p,h} e_p)^{\sim}(\pm E^{\frac{1}{2}}) = O(h^{-\frac{1}{2}})$$

(see Lemma A3). That is, while $\Phi_h(\pm E^{\frac{1}{2}})$ is finite (in contrast with the situation for the usual WKB approach) it is not uniformly bounded in h .

Proof. We write e_x as a sum of six real functions. This yields a partition of unity on Γ into the sum of eight terms e_j (with supports as indicated in Fig. 2), namely

$$\sum_{j=1, 2, 3, 5, 6, 7} e_j = e_x, \quad e_4 + e_8 = e_p.$$

If we write $e_j(t(x))$ below, it is always understood that $t(x) = t_+(x)$ for $j=5, 6, 7$, $t(x) = t_-(x)$ for $j=1, 2, 3$, with similar agreements for e_4 and e_8 . By definition

$$\begin{aligned} \pi \|\Phi_h\|_{L_2}^2 &= \int \left| \sum_{j=1, 2, 3, 5, 6, 7} e^{iI_x + \frac{i}{h} \int_0^{t(x)} p dx} e_j(t(x)) \right| \left| \frac{dx}{dt}(x) \right|^{-\frac{1}{2}} \\ &\quad + \int dp' \sum_{j=4, 8} e^{iI_p + \frac{i}{h} (p'x - \int_0^{t(p')} x dp)} e_j(t(p')) \left| \frac{dp}{dt}(p') \right|^{-\frac{1}{2}} \Big|^2 dx \\ &= \int \sum_{j, j'=1}^8 A_{jj'}(x) dx, \end{aligned}$$

where $A_{jj'}$ comes from the cross term containing the factor $e_j e_{j'}$. We bound $\|\Phi_h\|_{L^2}^2$ by distinguishing eight cases for $A_{jj'}$.

(1) A_{jj} with $j \in \{1, 2, 3, 5, 6, 7\}$. Here

$$\int A_{jj}(x) dx = \int e_j(t(x))^2 \left| \frac{dx}{dt}(x) \right|^{-1} dx = \int e_j(t)^2 dt.$$

(2) A_{jj} with $j \in \{4, 8\}$. Here

$$\int A_{jj}(x) dx = \int e_j(t(p))^2 \left| \frac{dp}{dt}(p) \right|^{-1} dp = \int e_j(t)^2 dt,$$

where the first equality is Parseval's formula.

(3) $A_{j, j+1}$ with $j \in \{1, 2, 5, 6\}$. Here

$$\int A_{j, j+1}(x) dx = \int e_j(t(x)) e_{j+1}(t(x)) \left| \frac{dx}{dt}(x) \right|^{-1} dx = \int e_j(t) e_{j+1}(t) dt,$$

since the $t(x)$ are either both $t_+(x)$ or both $t_-(x)$.

(4) $A_{j, j+1}$ with $j \in \{3, 4, 7, 8\}$. These terms are typically of the form

$$\begin{aligned} & \int e_j(t(x)) \left| \frac{dx}{dt}(x) \right|^{-\frac{1}{2}} e^{iI_X + \frac{i}{h} \int^t p dx} \cdot \int e_{j+1}(t(p')) \left| \frac{dp}{dt} \right|^{-\frac{1}{2}} e^{-iI_{P'} - \frac{i}{h} (p'x - \int^x p' dp')} dp' \\ &= \int_{\text{supp } e_j} e_j(t(x)) \left| \frac{dx}{dt}(x) \right|^{-\frac{1}{2}} e^{iI_X + \frac{i}{h} \int^t p dx} \left(e_{j+1}(t(x)) \left| \frac{dx}{dt} \right|^{-\frac{1}{2}} e^{-iI_X - \frac{i}{h} \int^t p dx} + O(h) \right) dx \\ & \text{(by Lemma 1)} \\ &= \int e_j(t(x)) \left| \frac{dx}{dt} \right|^{-1} e_{j+1}(t(x)) dx + O(h) = \int e_j(t) e_{j+1}(t) dt + O(h). \end{aligned}$$

(5) $A_{jj'}$ and $A_{j'j}$ with $\{j, j'\} = \{1, 3\}, \{1, 5\}, \{3, 7\}, \{5, 7\}$. These terms are zero since

$$e_j(t(x)) e_{j'}(t(x)) = 0.$$

(6) Terms $A_{jj'}$ with $j, j' \in \{1, 2, 3, 5, 6, 7\}$, but not treated above. Consider for example the pair $j=5, j'=3$. Then

$$\int A_{53}(x) dx = \int e_5(t_+(x)) e_3(t_-(x)) \left| \frac{dx}{dt} \right|^{-1} \exp i \left(\frac{1}{h} \int_0^{t_+(x)} p dx - \frac{1}{h} \int_0^{t_-(x)} p dx + c \right) dx.$$

This phase is not stationary on $\text{supp } e_5 e_3$ since it is given by

$$-\frac{1}{h} \int_{t_+(x)}^{\frac{\pi}{2} - t_+(x)} p dx + \text{const.}$$

which has the derivative $2 \frac{1}{h} p(x) \neq 0$. Therefore, by Lemma A1,

$$\int A_{jj'}(x) dx = O(h^N), \quad N=1, 2, 3, \dots$$

(7) $A_{4,8}, A_{8,4}$. We use the same argument as in (6) together with Parseval's identity. Thus

$$\int A_{4,8}(x) dx = O(h^N), \quad N = 1, 2, 3, \dots$$

(8) Terms $A_{jj'}$ and $A_{j'j}$ with $j \in \{1, 2, 3, 5, 6, 7\}, j' \in \{4, 8\}$ but not treated above. Here

$$\int A_{jj'}(x) dx = \int e^{\frac{i}{h} \int^x p dx - \frac{i}{h} (p'x - \int^x p' dx) + \text{const.}} \cdot e_j(t(x)) e_{j'}(t(p')) \left| \frac{dx}{dt} \right|^{-\frac{1}{2}}(x) \left| \frac{dp}{dt} \right|^{-\frac{1}{2}}(p') dx dp'.$$

The gradient of the phase $\frac{i}{h} \varphi$ is not stationary on $\text{supp } e_j e_{j'}$. Indeed

$$\frac{d}{dx} \varphi = p(x) - p', \quad \frac{d}{dp'} \varphi = -x + x(p')$$

and these expressions cannot vanish on $\text{supp } e_j e_{j'}$, because e_j and $e_{j'}$ have non-overlapping support on Γ . The two dimensional version of Lemma A1 shows that

$$\int A_{jj'}(x) dx = O(h^N), \quad N = 1, 2, 3, \dots$$

We have thus shown that

$$\int \sum_{j,j'=1}^8 A_{jj'}(x) dx = \int_0^\pi \sum_{j,j'=1}^8 e_j(t) e_{j'}(t) dt + O(h) = \pi + O(h);$$

the lemma is therefore proved.

Before turning to the main result, we note that $H(x, -ih\partial_x)$ has isolated eigenvalues of multiplicity one at $2h(n + \frac{1}{2}), n = 0, 1, 2, \dots$ (It is not clear whether this holds in more general cases*.) (14)

Let $E > 0$ be fixed. For $h = E/2(n + \frac{1}{2})$ let φ_h be a normalized eigenfunction of $H(x, -ih\partial_x)$ with eigenvalue E , and if $h \neq E/2(n + \frac{1}{2})$, set $\varphi_h = 0$. Our main result is

Theorem 7.

$$|(\Phi_h, \varphi_h)| - \|\varphi_h\|_{L_2}^2 = O(h) \quad \text{as } h \rightarrow 0.$$

That is, Φ_h asymptotically lies in the subspace spanned by φ_h .

Proof. Suppose $h = \frac{E}{2(n + \frac{1}{2})}$, the other case being trivial. Let

$$P\Phi_h = \Phi_h - (\Phi_h, \varphi_h) \varphi_h.$$

With $H_h = H(x, -ih\partial_x) - E$, we find by Theorem 5 that

$$\|H_h P\Phi_h\|_{L_2} = \|H_h \Phi_h\|_{L_2} = O(h^2).$$

Now $P\Phi_h \in (\varphi_h)^\perp$, and H_h is invertible on $(\varphi_h)^\perp$; in fact by (14)

$$\|(H_h|_{(\varphi_h)^\perp})^{-1}\|_{L_2} = \frac{1}{2h} = O(h^{-1}).$$

* As an illustration we give a possible generalization in Lemma A4.

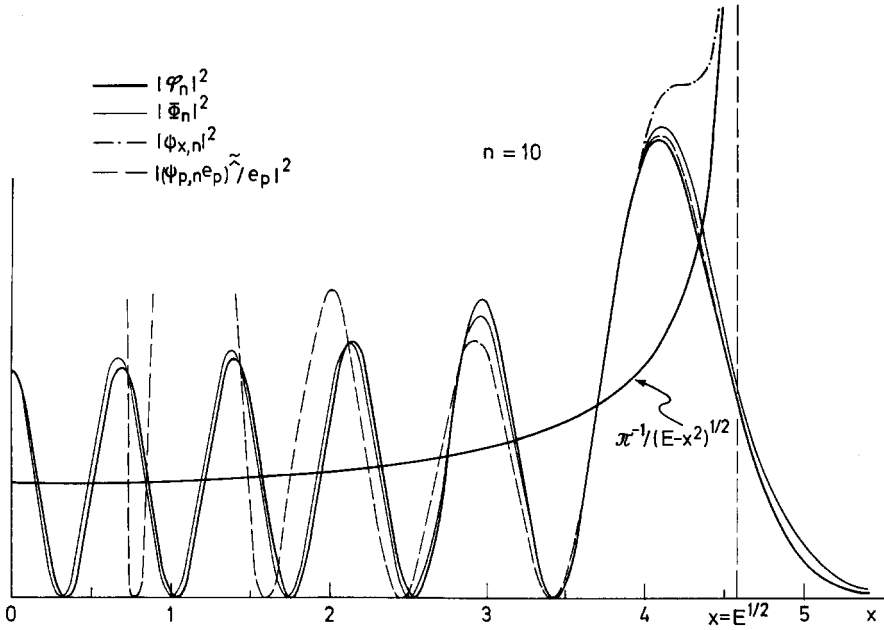


Figure 3

Thus

$$\|P\Phi_h\|_{L_2} = O(h),$$

or

$$\begin{aligned} O(h^2) &= \|P\Phi_h\|_{L_2}^2 \\ &= \|\Phi_h\|_{L_2}^2 - 2|(\Phi_{h, \varphi_h})|^2 + |(\Phi_{h, \varphi_h})|^2 \\ &= 1 + O(h) - |(\Phi_{h, \varphi_h})|^2 \end{aligned}$$

by Lemma 6, from which the assertion follows.

Example. In Figure 3 we show the graphs of the different functions discussed in this paper for the case $E=21$, $h=1$, $n=10$ (h need not be small in the case of the harmonic oscillator, provided that n is large, as can be seen by a scaling argument). For computational reasons we have chosen e_p so that $\hat{e}_p(p) = \cos\left(\frac{\pi p}{2 E^{\frac{1}{2}}}\right)$. This function is neither C^∞ nor has it the correct support properties, but since we are only doing numerical integration these things do not matter. Note in particular the good agreement between $|\varphi_n|^2$ and $|\Phi_n|^2$. One can also see clearly how $\psi_{x,h}$ (the usual WKB approximation) diverges at $x = E^{\frac{1}{2}}$, and how $(\psi_{p,h} e_p)^{\sim}$ is a good approximation in the region $x \sim E^{\frac{1}{2}}$, $x \geq E^{\frac{1}{2}}$. The function $\pi^{-1/2}(E-x^2)^{-\frac{1}{2}}$ is the probability distribution for the position of the classical particle. (It is well-known that in this case φ_h is the 10th Hermite function.)

Discussion. In summary, given a Hamiltonian H and an energy $E(>0)$ MASLOV's method provides us with a function Φ_h which for $h \rightarrow 0$ has the following properties:

- (i) It is normalized.
- (ii) It is in the domain of $H - E$.
- (iii) It is an approximate solution in the subspace of the Hilbert space corresponding to the spectral interval $(-O(h), O(h))$ of $H - E$.
- (iv) If in addition E is an isolated eigenvalue of H of multiplicity one, separated from the rest of the spectrum by $O(h)$, then Φ_h is an L_2 approximation to the corresponding eigenspace.
- (v) The conclusion of (iv) is valid even if the eigenvalue is separated from the remainder of the *discrete* spectrum by $O(h)$.
- (vi) All results except Lemma 3 remain valid if the quantization condition is replaced by

$$\frac{1}{h} \oint p dx - \pi = O(h) \pmod{2\pi}$$

and if Φ_h is defined with $M = 1$.

The results obtained in this paper generalize to systems in several variables under the following conditions:

- (1) The system is almost integrable.
- (2) There is a compact Lagrangian manifold associated with the system.
- (3) One trajectory is dense on this manifold.

For this situation the appropriate formulas are obtained by replacing the factor

$$\left| \frac{dx}{dt} \right|^{-\frac{1}{2}} \text{ by } \left| \frac{dx_1 \dots dx_k dp_{k+1} \dots dp_n}{dt d\alpha_1 \dots d\alpha_{n-1}} \right|^{-\frac{1}{2}}$$

in the representation whose local coordinates are $x_1, \dots, x_k, p_{k+1}, \dots, p_n$ where $\alpha_1, \dots, \alpha_{n-1}$ are integrals of the motion.

It is not clear if the results remain true in more general situations but it seems to the authors that (1) is the essential condition, whereas (2) and (3) can probably be somewhat relaxed.

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Appendix

Lemma A 1. Let $f(p) \in C_0^\infty$ and $\varphi(p) \in C^\infty$. If the integral on the right hand side below exists for some $N = 1, 2, 3, \dots$, then

$$\int dp e^{\frac{i}{h}\varphi(p)} f(p) = \left(-\frac{h}{i} \right)^N \int dp e^{\frac{i}{h}\varphi(p)} \underbrace{\frac{d}{dp} \left(\frac{1}{\varphi'} \frac{d}{dp} \left(\frac{1}{\varphi'} \dots \frac{d}{dp} \left(\frac{f}{\varphi'} \right) \dots \right) \right)}_{N \text{ derivatives}} (p),$$

where ' denotes the derivative.

In particular, if $\varphi'(p) \neq 0$ on $\text{supp } f$, then

$$\int dp e^{\frac{i}{h}\varphi(p)} f(p) = O(h^N) \quad \text{for } N = 1, 2, 3, \dots$$

Proof. The first formula is obvious. The second formula follows if

$$\frac{d}{dp} \left(\frac{1}{\varphi'} \frac{d}{dp} \left(\frac{1}{\varphi'} \cdots \frac{d}{dp} \frac{f}{\varphi'} \right) \cdots \right) \in C_0^\infty.$$

But this is easily checked by observing that the expression is of the form

$$\sum_{k=N}^{2N} \left(\frac{1}{\varphi'} \right)^k f_k$$

where f_k is a sum of derivatives of f and φ , and is hence C_0^∞ .

Corollary A1. *Let*

$$\varphi(p, x) = px - \int^t x dp.$$

If $f \in C_0^\infty$ has support away from $p = p(x)$ and $p = -p(x)$, then

$$\int e^{\frac{i}{\hbar} \varphi(p, x)} f(p) dp = O(\hbar^N) \quad \text{for } N = 1, 2, 3, \dots$$

If $f \in C_0^\infty$ has support away from $p = 0$ then

$$\int_{x^2 \geq E} \left| \int e^{\frac{i}{\hbar} \varphi(p, x)} f(p) dp \right|^2 dx = O(\hbar^{2N}), \quad N = 1, 2, 3, \dots$$

Proof. The first assertion is obtained from Lemma A1 by observing that

$$|\partial_p \varphi(p, x)|_{p \in \text{supp } f} \geq \text{dist}(x, x(\text{supp } f)) > 0.$$

The second assertion follows by observing that

$$\left| \int e^{\frac{i}{\hbar} \varphi(p, x)} f(p) dp \right| \leq \hbar^N (|x| - E^{\frac{1}{2}} - \varepsilon)^{-N} f_N(x) \quad \text{for } N = 1, 2, 3, \dots,$$

where f_N is bounded; indeed

$$|\partial_p \varphi(p, x)|_{p \in \text{supp } f} \geq \text{dist}(x, x(\text{supp } f)) = |x| - E^{\frac{1}{2}} - \varepsilon \quad \text{for some } \varepsilon > 0.$$

Furthermore, $\partial_p^k \varphi(p, x)$ is uniformly bounded in x on $\text{supp } f$ for $k = 2, 3, 4, \dots$. This proves the assertion.

Lemma A2. (The Stationary Phase Theorem.) *Let $f \in C_0^\infty$, $\varphi \in C^\infty$, let $\varphi'(p) \neq 0$ on $\text{supp } f \setminus \{0\}$, and let $\varphi'(0) = 0$, $\varphi''(0) \neq 0$. Then*

$$\int e^{\frac{i}{\hbar} \varphi(p)} f(p) dp = (2\pi \hbar)^{\frac{1}{2}} \frac{f(0)}{|\varphi''(0)|^{\frac{1}{2}}} e^{\frac{i}{\hbar} \varphi(0)} e^{\frac{i\pi}{4} \text{sign} \varphi''(0)} + O(\hbar^{\frac{3}{2}}).$$

Proof. We sketch the argument for the special case $\varphi(p) = \frac{a}{2} p^2$, $a \in \mathbb{R} \setminus \{0\}$. The general case follows by the implicit function theorem.

We note that for $\mu \in \mathbb{C}$, $\mu \neq 0$, $\text{Re } \mu \geq 0$,

$$\int_{-\infty}^{+\infty} \left(-\frac{x^2}{2} \right)^m e^{-\mu \frac{x^2}{2}} dx = \frac{d^m}{d\mu^m} \int_{-\infty}^{+\infty} e^{-\mu \frac{x^2}{2}} dx = \frac{d^m}{d\mu^m} \left(\frac{2\pi}{\mu} \right)^{\frac{1}{2}} = O(\mu^{-m-\frac{1}{2}}).$$

Setting $\mu = -i\frac{a}{h}$, we find that

$$\begin{aligned} & \int_{-\infty}^{+\infty} e^{\frac{i}{h}\frac{a}{2}p^2} f(p) dp \\ &= f(0) \int_{-\infty}^{+\infty} e^{\frac{i}{h}\frac{a}{2}p^2} dp + f'(0) \int_{-\infty}^{+\infty} p e^{\frac{i}{h}\frac{a}{2}p^2} dp + \int_{-\infty}^{+\infty} p^2 \Theta(p) e^{\frac{i}{h}\frac{a}{2}p^2} dp \\ &= f(0) \left(\frac{2\pi h}{-ia}\right)^{\frac{1}{2}} + 0 + O(h^{\frac{3}{2}}) \end{aligned}$$

because locally $\Theta(p)$ is a constant. Finally

$$\left(\frac{1}{-ia}\right)^{\frac{1}{2}} = e^{i\frac{\pi}{4}\text{sign} a} \frac{1}{|a|^{\frac{1}{2}}},$$

so that the assertion follows in the special case.

Lemma A3. *With the notations of the main section,*

$$|\Phi_h(\pm E^{\pm})| = O(h^{-\frac{1}{2}}).$$

Proof. We use the general stationary phase argument [1, (4.7) p.135]: If

$$\begin{aligned} f \in C_0^\infty, \quad \varphi \in C^\infty, \quad f(0) = 1, \quad \varphi(p) = a + bp^3(1 + \Theta(p)), \\ b \neq 0, \quad \Theta(p) \in C^\infty, \quad \Theta(0) = 0, \quad \varphi'(p) \neq 0 \text{ on } \text{supp } f \setminus \{0\}, \end{aligned}$$

then

$$|\int e^{\frac{i}{h}\varphi(p)} f(p) dp| = O(h^{\frac{1}{2}}).$$

We treat only the case $\Phi_h(+E^{\pm})$, the other case being similar. We apply the above argument with

$$\begin{aligned} \varphi(p) &= p\sqrt{E} - \int_0^p d\rho(E - \rho^2)^{\frac{1}{2}}, \\ f(p) &= \hat{e}_p(p)(E - p^2)^{-\frac{1}{2}}. \end{aligned}$$

The stated conditions are fulfilled, and in particular

$$\begin{aligned} \varphi'(p) &= E^{\frac{1}{2}} - (E - p^2)^{\frac{1}{2}} && (> 0 \text{ if } p \neq 0), \\ \varphi''(p) &= p(E - p^2)^{-\frac{1}{2}} && (= 0 \text{ if } p = 0), \\ \varphi'''(p) &= (E - p^2)^{-\frac{3}{2}} + p^2(E - p^2)^{-\frac{5}{2}} && (= E^{-\frac{3}{2}} \neq 0 \text{ if } p = 0), \end{aligned}$$

so that $b = E^{-\frac{1}{2}}/6 \neq 0$. Therefore the result follows from the relation

$$|\Phi_h(E^{\pm})| = \text{const.} (2\pi h)^{-\frac{1}{2}} |\int e^{\frac{i}{h}\varphi(p)} (E - p^2)^{-\frac{1}{2}} \hat{e}_p(p) dp|.$$

Lemma A4. *(An a priori estimate.) Let $V(x)$ be a positive convex potential and let $H = -h^2 \partial_x^2 + V(x)$. Consider the eigenvectors ψ of H with boundary condition $\psi(0) + k\psi'(0) = 0$ for a fixed $k \in (-\infty, \infty)$. Then all suitably large eigenvalues are of multiplicity one and separated by $O(h)$.*

Proof. Let $x(\lambda) > 0$ be defined by $V(x(\lambda)) = \lambda$. Then the number of eigenvalues in $[0, \lambda]$ of $-\partial_x^2 + V(x)$ with boundary condition $\psi(0) + k\psi'(0) = 0$ is

$$N(\lambda) \sim \frac{1}{\pi} \int_0^{x(\lambda)} (\lambda - V(x))^{\frac{1}{2}} dx$$

[2; XIII. 7.58]. Consider now

$$H = -h^2 \partial_x^2 + V(x).$$

By a change of variables this is unitarily equivalent to $\bar{H} = -\partial_x^2 + V(x \cdot h)$, so that we have

$$N(\lambda) \sim \frac{1}{\pi} \int_0^{x(\lambda)/h} (\lambda - V(x \cdot h))^{\frac{1}{2}} dx = \frac{1}{\pi h} \int_0^{x(\lambda)} (\lambda - V(x))^{\frac{1}{2}} dx.$$

Fix λ so large that

$$N(\lambda) = \frac{1}{\pi h} \int_0^{x(\lambda)} (\lambda - V(x))^{\frac{1}{2}} dx + \varepsilon(\lambda, h) \tag{A2}$$

with $|\varepsilon(\lambda', h)| \leq \frac{1}{3}$, for all $\lambda' > \lambda$, $h \leq 1$. Such a λ can be found because of the uniformity of the estimates in [2]. Now for $N(\lambda)$ to increase by 1, the integral in (A2) must increase by more than $\frac{\pi}{3} h$. For small h this means that

$$\int_0^{x(\lambda')} (\lambda' - V(x))^{\frac{1}{2}} dx - \int_0^{x(\lambda)} (\lambda - V(x))^{\frac{1}{2}} dx \geq \frac{\pi h}{3}$$

or, by approximating the difference,

$$(\lambda - \lambda') \int_0^{x(\lambda)} \frac{dx}{2(\lambda - V(x))^{\frac{1}{2}}} \geq \frac{\pi h}{3}$$

so that $\lambda - \lambda' = O(h)$.

A5. We shall derive the equations for the WKB approximation in the anharmonic case by manipulating formal power series. The result is valid without further hypotheses if $H(q, p)$ is a polynomial.

The x-space: We want

$$(H(x, -ih\partial_x) - E) e^{+\frac{i}{h}s(x)} f(x) = O(h^2),$$

locally. Now

$$H(x, -ih\partial_x) e^{\frac{i}{h}s(x)} = e^{\frac{i}{h}s(x)} H(x, -ih\partial_x + s'(x))$$

because of

$$-ih\partial_x e^{\frac{i}{h}s(x)} = e^{\frac{i}{h}s(x)} (-ih\partial_x + s'(x))$$

and by virtue of the quantization used (footnote page 157). The equation of order zero in h is therefore

$$H(x, s'(x)) = E.$$

To remove terms of order h , we have to solve for $f(x)$ in

$$(H(x, -ih\partial_x + s'(x)) - E) f(x) = -ih(Kf)(x) + O(h^2),$$

where K is the following operator (obtained by calculating with the power series):

$$(Kf)(x) = \frac{1}{2} H_{pp}(x, s'(x)) s''(x) f(x) + H_p(x, s'(x)) f'(x),$$

where lower indices denote derivatives of $H(q, p)$ with respect to q or p . Alternately,

$$(Kf)(x) = \frac{1}{2} \frac{d}{dx} (H_p(x, s'(x))) f(x) - \frac{1}{2} H_{pq}(x, s'(x)) f(x) + H_p(x, s'(x)) f'(x),$$

so that

$$\frac{f'}{f} = -\frac{1}{2} \frac{H_p(x, s'(x))'}{H_p(x, s'(x))} + \frac{1}{2} \frac{H_{pq}(x, s'(x))}{H_p(x, s'(x))}.$$

The trick is now to work locally with the time coordinate. Putting

$$H_p(x, s'(x)) = \frac{dx}{dt}$$

we get

$$(\ln f)' = -\frac{1}{2} (\ln H_p)' + \frac{1}{2} H_{pq}(x, s'(x)) \frac{dt}{dx}$$

or

$$f(x) = \text{const.} \frac{1}{\sqrt{\left| \frac{dx}{dt} \right|}} \exp\left(\frac{1}{2} \int^{t(x)} H_{pq}(x(\tau), p(\tau)) d\tau\right)$$

because $s'(x(\tau)) = p(\tau)$ by the first equation.

One checks in the same way that the result in p -space is

$$(H(ih\partial_p, p) - E) e^{-\frac{i}{h}\sigma(p)} g(p) = O(h^2),$$

$$H(\sigma'(p), p) = E,$$

$$g(p) = \text{const.} \frac{1}{\sqrt{\left| \frac{dp}{dt} \right|}} \exp\left(\frac{1}{2} \int^{t(p)} H_{pq}(x(\tau), p(\tau)) d\tau\right),$$

the derivative $ih\partial_p$ acting on p in $H(ih\partial_p + \sigma'(p), p)$ compensating for the changes in signs.

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