Chapter 30

WKB quantization

The wave function for a particle of energy E moving in a constant potential V is

$$\psi = A e^{\frac{i}{\hbar} pq} \tag{30.1}$$

with a constant amplitude A, and constant wavelength $\lambda = 2\pi/k$, $k = p/\hbar$, and $p = \pm\sqrt{2m(E-V)}$ is the momentum. Here we generalize this solution to the case where the potential varies slowly over many wavelengths. This semiclassical (or WKB) approximate solution of the Schrödinger equation fails at classical turning points, configuration space points where the particle momentum vanishes. In such neighborhoods, where the semiclassical approximation fails, one needs to solve locally the exact quantum problem, in order to compute connection coefficients which patch up semiclassical segments into an approximate global wave function.

Two lessons follow. First, semiclassical methods can be very powerful - classical mechanics computations yield suprisingly accurate estimates of quantal spectra, without solving the Schrödinger equation. Second, semiclassical quantization does depend on a purely wave-mechanical phenomena, the coherent addition of phases accrued by all fixed energy phase space trajectories that connect pairs of coordinate points, and the topological phase loss at every turning point, a topological property of the classical flow that plays no role in classical mechanics.

30.1 WKB ansatz

Consider a time-independent Schrödinger equation in 1 spatial dimension:

$$-\frac{\hbar^2}{2m}\psi''(q) + V(q)\psi(q) = E\psi(q)\,, \tag{30.2}$$

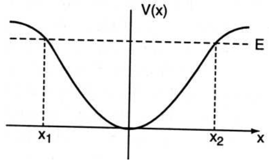

Figure 30.1: A 1-dimensional potential, location of the two turning points at fixed energy E.

with potential $V(q)$ growing sufficiently fast as $q \to \pm\infty$ so that the classical particle motion is confined for any E. Define the local momentum $p(q)$ and the local wavenumber $k(q)$ by

$$p(q) = \pm\sqrt{2m(E - V(q))}, \quad p(q) = \hbar k(q)\,. \tag{30.3}$$

The variable wavenumber form of the Schrödinger equation

$$\psi'' + k^2(q)\psi = 0 \tag{30.4}$$

sugests that the wave function be written as $\psi = A e^{\frac{i}{\hbar} S}$, A and S real functions of q. Substitution yields two equations, one for the real and other for the imaginary part:

$$(S')^2 = p^2 + \hbar^2 \frac{A''}{A} \tag{30.5}$$

$$S''A + 2S'A' = \frac{1}{A}\frac{d}{dq}(S'A^2) = 0\,. \tag{30.6}$$

The Wentzel-Kramers-Brillouin *(WKB)* or *semiclassical* approximation consists of dropping the $\hbar^2$ term in (30.5). Recalling that $p = \hbar k$, this amounts to assuming that $k^2 \gg \frac{A''}{A}$, which in turn implies that the phase of the wave function is changing much faster than its overall amplitude. So the WKB approximation can interpreted either as a short wavelength/high frequency approximation to a wave-mechanical problem, or as the semiclassical, $\hbar \ll 1$ approximation to quantum mechanics.

Setting $\hbar = 0$ and integrating (30.5) we obtain the phase increment of a wave function initially at q, at energy E

$$S(q, q', E) = \int_{q'}^{q} dq'' p(q'')\,. \tag{30.7}$$

This integral over a particle trajectory of constant energy, called the *action*, will play a key role in all that follows. The integration of (30.6) is even easier

$$A(q) = \frac{C}{|p(q)|^{\frac{1}{2}}}, \qquad C = |p(q')|^{\frac{1}{2}}\psi(q')\,, \tag{30.8}$$

where the integration constant C is fixed by the value of the wave function at the initial point q'. The *WKB* (or *semiclassical*) *ansatz* wave function is given by

$$\psi_{sc}(q, q', E) = \frac{C}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar} S(q,q',E)} . \tag{30.9}$$

In what follows we shall supress dependence on the initial point and energy in such formulas, $(q, q', E) \to (q)$.

The WKB ansatz generalizes the free motion wave function (30.1), with the probability density $|A(q)|^2$ for finding a particle at q now inversely proportional to the velocity at that point, and the phase $\frac{1}{\hbar} q\, p$ replaced by $\frac{1}{\hbar}\int dq\, p(q)$, the integrated action along the trajectory. This is fine, except at any turning point q_0, figure 30.1, where all energy is potential, and

$$p(q) \to 0 \quad \text{as} \qquad q \to q_0 , \tag{30.10}$$

so that the assumption that $k^2 \gg \frac{A''}{A}$ fails. What can one do in this case?

For the task at hand, a simple physical picture, due to Maslov, does the job. In the q coordinate, the turning points are defined by the zero kinetic energy condition (see figure 30.1), and the motion appears singular. This is not so in the full phase space: the trajectory in a smooth confining 1-dimensional potential is always a smooth loop, with the "special" role of the turning points q_L, q_R seen to be an artifact of a particular choice of the (q, p) coordinate frame. Maslov's idea was to proceed from the initial point (q', p') to a point (q_A, p_A) preceeding the turning point in the $\psi(q)$ representation, then switch to the momentum representation

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dq\, e^{-\frac{i}{\hbar} qp} \psi(q) , \tag{30.11}$$

continue from (q_A, p_A) to (q_B, p_B), switch back to the coordinate representation,

$$\psi(q) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{\frac{i}{\hbar} qp}\, \widetilde{\psi}(p) , \tag{30.12}$$

and so on.

The only rub is that one usually cannot evaluate these transforms exactly. But, as the WKB wave function (30.9) is approximate anyway, it suffices to estimate these transforms to leading order in $\hbar$ accuracy. This is accomplished by the method of stationary phase.

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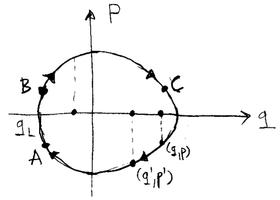

Figure 30.2: A 1-dof phase space trajectory of a particle moving in a bound potential.

30.2 Method of stationary phase

All "semiclassical" approximations are based on saddlepoint evaluations of integrals of the type

$$I = \int dx\, A(x)\, e^{is\Phi(x)} , \qquad x, \Phi(x) \in \mathbb{R} , \tag{30.13}$$

where s is assumed to be a large, real parameter, and $\Phi(x)$ is a real-valued function. In our applications $s = 1/\hbar$ will always be assumed large.

For large s, the phase oscillates rapidly and "averages to zero" everywhere except at the *extremal points* $\Phi'(x_0) = 0$. The method of approximating an integral by its values at extremal points is called the *method of stationary phase*. Consider first the case of a 1-dimensional integral, and expand $\Phi(x_0 + \delta x)$ around x_0 to second order in δx,

$$I = \int dx\, A(x)\, e^{is(\Phi(x_0) + \frac{1}{2}\Phi''(x_0)\delta x^2 + \ldots)} . \tag{30.14}$$

Assume (for time being) that $\Phi''(x_0) \neq 0$, with either sign, $\mathrm{sgn}[\Phi''] = \Phi''/|\Phi''| = \pm 1$. If in the neighborhood of x_0 the amplitude $A(x)$ varies slowly over many oscillations of the exponential function, we may retain the leading term in the Taylor expansion of the amplitude, and approximate the integral up to quadratic terms in the phase by

$$I \approx A(x_0) e^{is\Phi(x_0)} \int dx\, e^{\frac{1}{2} is\Phi''(x_0)(x - x_0)^2} . \tag{30.15}$$

Using the *Fresnel integral formula*

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2} e^{i\frac{\pi}{4}\frac{a}{|a|}} \tag{30.16}$$

we obtain

$$I \approx A(x_0) \left| \frac{2\pi}{s\Phi''(x_0)} \right|^{1/2} e^{is\Phi(x_0) \pm i\frac{\pi}{4}} , \tag{30.17}$$

where $\pm$ corresponds to the positive/negative sign of $s\Phi''(x_0)$.

30.3 WKB quantization

We can now evaluate the Fourier transforms (30.11), (30.12) to the same order in $\hbar$ as the WKB wave function using the stationary phase method,

$$\begin{aligned} \widetilde{\psi}_{sc}(p) &= \frac{C}{\sqrt{2\pi\hbar}} \int \frac{dq}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}(S(q)-qp)} \\ &\approx \frac{C}{\sqrt{2\pi\hbar}} \frac{e^{\frac{i}{\hbar}(S(q^*)-q^*p)}}{|p(q^*)|^{\frac{1}{2}}} \int dq\, e^{\frac{i}{2\hbar}S''(q^*)(q-q^*)^2} , \end{aligned} \tag{30.18}$$

where q^* is given implicitly by the stationary phase condition

$$0 = S'(q^*) - p = p(q^*) - p$$

and the sign of $S''(q^*) = p'(q^*)$ determines the phase of the Fresnel integral (30.16)

$$\widetilde{\psi}_{sc}(p) = \frac{C}{|p(q^*)p'(q^*)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}[S(q^*)-q^*p] + \frac{i\pi}{4}\mathrm{sgn}[S''(q^*)]} . \tag{30.19}$$

As we continue from (q_A, p_A) to (q_B, p_B), nothing problematic occurrs - $p(q^*)$ is finite, and so is the acceleration $p'(q^*)$. Otherwise, the trajectory would take infinitely long to get across. We recognize the exponent as the Legendre transform

$$\tilde{S}(p) = S(q(p)) - q(p)p$$

which can be used to expresses everything in terms of the p variable,

$$q^* = q(p), \quad \frac{d}{dq}q = 1 = \frac{dp}{dq}\frac{dq(p)}{dp} = q'(p)p'(q^*) . \tag{30.20}$$

As the classical trajectory crosses q_L, the weight in (30.19),

$$\frac{d}{dq}p^2(q_L) = 2p(q_L)p'(q_L) = -2mV'(q) , \tag{30.21}$$

is finite, and $S''(q^*) = p'(q^*) < 0$ for any point in the lower left quadrant, including (q_A, p_A). Hence, the phase loss in (30.19) is $-\frac{\pi}{4}$. To go back from the p to the q representation, just turn figure 30.2 90^o anticlockwise. Everything is the same if you replace $(q,p) \to (-p,q)$; so, without much ado we get the semiclassical wave function at the point (q_B, p_B),

$$\psi_{sc}(q) = \frac{e^{\frac{i}{\hbar}(\tilde{S}(p^*)+qp^*) - \frac{i\pi}{4}}}{|q^*(p^*)|^{\frac{1}{2}}} \widetilde{\psi}_{sc}(p^*) = \frac{C}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S(q) - \frac{i\pi}{2}} . \tag{30.22}$$

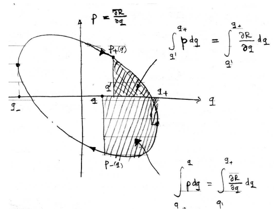

Figure 30.3: $S_p(E)$, the action of a periodic orbit p at energy E, equals the area in the phase space traced out by the 1-dof trajectory.

The extra $|p'(q^*)|^{1/2}$ weight in (30.19) is cancelled by the $|q'(p^*)|^{1/2}$ term, by the Legendre relation (30.20).

The message is that going through a smooth potential turning point the WKB wave function phase slips by $-\frac{\pi}{2}$. This is equally true for the right and the left turning points, as can be seen by rotating figure 30.2 by 180^o, and flipping coordinates $(q,p) \to (-q,-p)$. While a turning point is not an invariant concept (for a sufficiently short trajectory segment, it can be undone by a 45^o turn), for a complete period $(q,p) = (q',p')$ the total phase slip is always $-2 \cdot \pi/2$, as a loop always has $m = 2$ turning points.

The *WKB quantization condition* follows by demanding that the wave function computed after a complete period be single-valued. With the normalization (30.8), we obtain

$$\psi(q') = \psi(q) = \left|\frac{p(q')}{p(q)}\right|^{\frac{1}{2}} e^{i(\frac{1}{\hbar}\oint p(q)dq - \pi)} \psi(q') .$$

The prefactor is 1 by the periodic orbit condition $q = q'$, so the phase must be a multiple of 2π,

$$\frac{1}{\hbar}\oint p(q)dq = 2\pi\left(n + \frac{m}{4}\right) , \tag{30.23}$$

where m is the number of turning points along the trajectory - for this 1-dof problem, $m = 2$.

The action integral in (30.23) is the area (see figure 30.3) enclosed by the classical phase space loop of figure 30.2, and the quantization condition says that eigenenergies correspond to loops whose action is an integer multiple of the unit quantum of action, Planck's constant $\hbar$. The extra topological phase, which, although it had been discovered many times in centuries past, had to wait for its most recent quantum chaotic (re)birth until the 1970's. Despite its derivation in a noninvariant coordinate frame, the final result involves only canonically invariant classical quantities, the periodic orbit action S, and the topological index m.

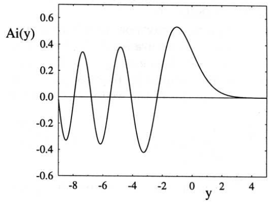

Figure 30.4: Airy function $Ai(q)$.

30.3.1 Harmonic oscillator quantization

Let us check the WKB quantization for one case (the only case?) whose quantum mechanics we fully understand: the harmonic oscillator

$$E = \frac{1}{2m}\left(p^2 + (m\omega q)^2\right) .$$

The loop in figure 30.2 is now a circle in the $(m\omega q, p)$ plane, the action is its area $S = 2\pi E/\omega$, and the spectrum in the WKB approximation

$$E_n = \hbar\omega(n + 1/2) \tag{30.24}$$

turns out to be the *exact* harmonic oscillator spectrum. The stationary phase condition (30.18) keeps $V(q)$ accurate to order q^2, which in this case is the whole answer (but we were simply lucky, really). For many 1-dof problems the WKB spectrum turns out to be very accurate all the way down to the ground state. Surprisingly accurate, if one interprets dropping the $\hbar^2$ term in (30.5) as a short wavelength approximation.

30.4 Beyond the quadratic saddle point

We showed, with a bit of Fresnel/Maslov voodoo, that in a smoothly varying potential the phase of the WKB wave function slips by a $\pi/2$ for each turning point. This $\pi/2$ came from a $\sqrt{i}$ in the Fresnel integral (30.16), one such factor for every time we switched representation from the configuration space to the momentum space, or back. Good, but what does this mean?

The stationary phase approximation (30.14) fails whenever $\Phi''(x) = 0$, or, in our the WKB ansatz (30.18), whenever the momentum $p'(q) = S''(q)$ vanishes. In that case we have to go beyond the quadratic approximation (30.15) to the first nonvanishing term in the Taylor expansion of the exponent. If $\Phi'''(x_0) \neq 0$, then

$$I \approx A(x_0)e^{is\Phi(x_0)} \int_{-\infty}^{\infty} dx\, e^{is\Phi'''(x_0)\frac{(x-x_0)^3}{6}} . \tag{30.25}$$

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Airy functions can be represented by integrals of the form

$$Ai(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dy\, e^{i(xy - \frac{y^3}{3})} . \tag{30.26}$$

Derivations of the WKB quantization condition given in standard quantum mechanics textbooks rely on expanding the potential close to the turning point

$$V(q) = V(q_0) + (q - q_0)V'(q_0) + \cdots ,$$

solving the Airy equation

$$\psi'' = q\psi , \tag{30.27}$$

and matching the oscillatory and the exponentially decaying "forbidden" region wave function pieces by means of the *WKB connection formulas*. That requires staring at Airy functions and learning about their asymptotics - a challenge that we will have to eventually overcome, in order to incorporate diffraction phenomena into semiclassical quantization.

2) what does the wave function look like?

3) generically useful when Gaussian approximations fail

The physical origin of the topological phase is illustrated by the shape of the Airy function, figure 30.4. For a potential with a finite slope $V'(q)$ the wave function pentrates into the forbidden region, and accomodates a bit more of a stationary wavelength then what one would expect from the classical trajectory alone. For infinite walls (i.e., billiards) a different argument applies: the wave function must vanish at the wall, and the phase slip due to a specular reflection is $-\pi$, rather than $-\pi/2$.

Commentary

Remark 30.1 Airy function. The stationary phase approximation is all that is needed for the semiclassical approximation, with the proviso that D in (31.36) has no zero eigenvalues. The zero eigenvalue case would require going beyond the Gaussian saddle-point approximation, which typically leads to approximations of the integrals in terms of Airy functions [30.10].

Remark 30.2 Bohr-Sommerfeld quantization. Bohr-Sommerfeld quantization condition was the key result of the old quantum theory, in which the electron trajectories were purely classical. They were lucky - the symmetries of the Kepler problem work out in such a way that the total topological index $m = 4$ amount effectively to numbering the energy levels starting with $n = 1$. They were unlucky - because the hydrogen $m = 4$ masked the topological index, they could never get the helium spectrum right - the semiclassical calculation had to wait for until 1980, when Leopold and Percival [?] added the topological indices.

Résumé

The WKB ansatz wave function for 1-degree of freedom problems fails at the turning points of the classical trajectory. While in the q-representation the WKB ansatz a turning point is singular, along the p direction the classical trajectory in the same neighborhood is smooth, as for any smooth bound potential the classical motion is topologically a circle around the origin in the (q, p) space. The simplest way to deal with such singularities is as follows; follow the classical trajectory in q-space until the WKB approximation fails close to the turning point; then insert $\int dp|p\rangle\langle p|$ and follow the classical trajectory in the p-space until you encounter the next p-space turning point; go back to the q-space representation, an so on. Each matching involves a Fresnel integral, yielding an extra $e^{-i\pi/4}$ phase shift, for a total of $e^{-i\pi}$ phase shift for a full period of a semiclassical particle moving in a soft potential. The condition that the wave-function be single-valued then leads to the 1-dimensional WKB quantization, and its lucky cousin, the Bohr-Sommerfeld quantization.

Alternatively, one can linearize the potential around the turning point a, $V(q) = V(a) + (q - a)V'(a) + \cdots$, and solve the quantum mechanical constant linear potential $V(q) = qF$ problem exactly, in terms of an Airy function. An approximate wave function is then patched together from an Airy function at each turning point, and the WKB ansatz wave-function segments inbetween via the WKB connection formulas. The single-valuedness condition again yields the 1-dimensional WKB quantization. This a bit more work than tracking the classical trajectory in the full phase space, but it gives us a better feeling for shapes of quantum eigenfunctions, and exemplifies the general strategy for dealing with other singularities, such as wedges, bifurcation points, creeping and tunneling: patch together the WKB segments by means of exact QM solutions to local approximations to singular points.

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