Chapter 24

WKB quantization

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

$$-\frac{\hbar^2}{2m}\psi''(q) + V(q)\psi(q) = E\psi(q)\,. \tag{24.1}$$

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

$$p(q) = \sqrt{2m(E - V(q))}, \quad p(q) = \hbar k(q)\,. \tag{24.2}$$

Then

$$\psi'' + k^2(q)\psi = 0\,. \tag{24.3}$$

Substitution $\psi = Ae^{\frac{i}{\hbar}S}$, A, S real functions of q, yields

$$\begin{aligned} (S')^2 &= p^2 + \hbar^2\frac{A''}{A} && (24.4)\\ S''A + 2S'A' &= \frac{1}{A}\frac{d}{dq}(S'A^2) = 0\,. && (24.5) \end{aligned}$$

(D-dimensional version of these equations will be given below, in (26.3) and (26.4).) The Wentzel-Kramers-Brillouin *(WKB)* or *semiclassical* approximation consists in dropping the $\hbar^2$ term in (24.4). Recalling that $p = \hbar k$, dropping this term amounts to claiming that $k^2 \gg \frac{A''}{A}$ which in turn implies that the phase of the wavefunction is changing much faster than its overall

amplitude. This justifies the standard interpretation as a short wavelength approximation. This approximation is also consistent with saying $\hbar \ll 1$.

Integrating (24.4) we obtain the phase increment of a wave function initially at q, at energy E

$$S(q, q', E) = \int_{q'}^{q} dq" \cdot p(q")\,. \tag{24.6}$$

Integration of (24.5) is even easier

$$A(q) = \frac{C}{|p(q)|^{\frac{1}{2}}}, \qquad C = |p(q')|^{\frac{1}{2}}\psi(q')\,, \tag{24.7}$$

where C is the integration constant, fixed by requiring that the wave function is single-valued everywhere, including the initial point q'. The WKB ansatz, or the semi-classical wave function is given by

$$\psi_{sc}(q) = \frac{C}{|p(q)|^{\frac{1}{2}}}e^{\frac{i}{\hbar}S(qq'E)}\,. \tag{24.8}$$

This is fine, except at the turning points, where all energy is potential, and

$$p(q) \to 0 \quad \text{as} \quad q \to q_T\,, \tag{24.9}$$

so that the assumption that $k^2 \gg \frac{A''}{A}$ fails. What to do? The answer is given in every quantum mechanics textbook, usually by expanding the potential close to the turning point

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

solving the Airy equation 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 face up to, in order to incorporate diffraction phenomena into semiclassical quantization. However, 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, and the motion appears singular. Not so in the full phase space: the trajectory in a smooth confining 1-d potential is always a smooth loop, with the "special" role of the turning points q_L, q_R seen to be an artifact of the particular choice of the (q,p) coordinate frame. Maslov's idea was to proceed from (q',p') to (q_A,p_A) in the $\psi(q)$ representation, then switch by means of a Fourier transform to the momentum representation

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dq\, e^{-\frac{i}{\hbar}qp}\psi(q)\,, \tag{24.10}$$

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

$$\psi(q) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{\frac{i}{\hbar}qp}\,\widetilde{\psi}(p)\,, \tag{24.11}$$

and so on.

The only rub is that we do not know how to evaluate these transforms exactly. As the WKB wave function (24.8) is anyhow approximate, it suffices to estimate these transforms with leading order in $\hbar$ accuracy. This we do by the stationary phase method.

24.1 Method of stationary phase

Semiclassical approximations are based on saddlepoint evaluations of integrals of the type

$$I = \int d^d x\, A(x)\, e^{is\Phi(x)}\,, \qquad x, \Phi(x) \in \mathbb{R}, \tag{24.12}$$

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* $\Phi'(x_0) = 0$, where $\Phi''(x_0) \neq 0$ but can have either sign. 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 one-dimensional integral, and expand $\Phi(x_0 + \delta x)$ around x_0 to second order in δx,

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

If $A(x)$ varies slowly around x_0 compared to 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

$$I \approx A(x_0) e^{is\Phi(x_0)} \int_{-\infty}^{\infty} dx\, e^{is\Phi''(x_0)\frac{x^2}{2}}\,.$$

24.6
page 460

Using the *Fresnel integral* formula

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2}\, e^{i\frac{\pi}{4}\frac{a}{|a|}} \tag{24.13}$$

we obtain

$$I \approx A(x_0) \left| \frac{2\pi}{s\Phi''(x_0)} \right|^{1/2} e^{is\Phi(x_0) \pm i\frac{\pi}{4}}\,, \tag{24.14}$$

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

24.2 WKB quantization

We can now evaluate the Fourier transforms (24.10), (24.11) to the same order in $\hbar$ as the WKB wave function by means of the stationary phase method

$$\begin{aligned} \widetilde{\psi}_{sc}(p) &= \frac{C}{\sqrt{2\pi\hbar}} \int \frac{dq}{|p(q)|^{\frac{1}{2}}}\, e^{\frac{i}{\hbar}(S(q) - qp)} \\ &\approx \frac{C}{\sqrt{2\pi\hbar}} \frac{e^{\frac{i}{\hbar}(S(q^*) - q^* p)}}{|p(q^*)|^{\frac{1}{2}}} \int dq\, e^{\frac{i}{2\hbar}S''(q^*)(q-q^*)^2}\,, \end{aligned} \tag{24.15}$$

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 (24.13)

$$\widetilde{\psi}_{sc}(p) = \frac{C}{|p(q^*)p'(q^*)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}[S(q^*) - q^* p] + \frac{i\pi}{4} sgn(S''(q^*)}\,. \tag{24.16}$$

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

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

which re-expresses everything in terms of the p variable

$$q^* = q(p), \quad \frac{d}{dq}q = 1 = \frac{dp}{dq}\frac{dq(p)}{dp} = q'(p)p'(q^*) . \tag{24.17}$$

As it crosses q_L, the weight in (24.16)

$$\frac{d}{dq}p^2(q_L) = 2p(q_L)p'(q_L) = -2mV'(q) \tag{24.18}$$

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 (24.16) is $-\frac{\pi}{4}$. To go back from p to q representation, just turn the phase space loop a quarter turn anticlockwise. Everything is the same if you replace $(q, p) \to (-p, q)$; so, without much ado we get at the point (q_B, p_B)

$$\psi_{sc}(q) = \frac{e^{\frac{i}{\hbar}(\tilde{S}(p^*)+qp^*)-\frac{i\pi}{4}}}{|q^*(p^*)|^{\frac{1}{2}}}\,\widetilde{\psi}_{sc}(p^*) = \frac{e^{\frac{i}{\hbar}S(q)-\frac{i\pi}{2}}}{|p(q)|^{\frac{1}{2}}}C . \tag{24.19}$$

The extra $|p'(q^*)|^{1/2}$ weight in (24.16) is cancelled by the $|q'(p^*)|^{1/2}$ term, by the Legendre relation (24.17).

We note in passing that the Fresnel integral phase slip requires a potential with finite slope $V'(q)$. In case of infinite wall (billiards) a different argument applies: the wave function must vanish at the wall, and the phase slip due to a specular reflection is $-\pi$, not $-\pi/2$.

The main message is that going through a smooth potential turn-back the WKB wave function phase slips by $-\frac{\pi}{2}$. This is equally true for the right and the left turn-backs, as can be seen by turning the phase space loop by $\frac{1}{2}$ turn, and flipping coordinates $(q, p) \to (-q, -p)$. While a turn-back is not an invariant concept (for a short trajectory segment, it can be undone by a 45^o turn), for a complete period $(q(T), p(T)) = (q', p')$ the total phase slip is always by $2 \cdot \pi/2$, as a loop always has $m = 2$ turn-backs.

The *WKB quantization condition* follows by demanding that the wave function computed after a complete period be single-valued. With normalization (24.7) we obtain

$$\psi(q') = \psi(q(T)) = \left|\frac{p(q')}{p(q(T))}\right|^{\frac{1}{2}} e^{i(\frac{1}{\hbar}\oint p(q)dq - \pi)}\psi(q') .$$

The prefactor equals 1 by the periodic orbit condition $q(T) = q'$, hence the phase must be a multiple of 2π

$$\frac{1}{\hbar}\oint p(q)dq = 2\pi\left(n + \frac{m}{4}\right) . \tag{24.20}$$

By definition, the action integral in (24.20) is the area enclosed by the phase space loop, and the quantization condition says that eigenenergies correspond to loops whose action is an integer multiple of the basis quantum of action, the Planck constant $\hbar$. Plus the extra topological phase, which, even though it had been discovered many times in centuries past, had to wait for its quantum mechanical (re)birth until 1970's. This result involves only canonically invariant classical quantities (action and phase) despite its derivation in terms of noninvariant coordinates.

24.2.1 Harmonic oscillator quantization

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

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

The phase space loop is now a circle in the (mwq, p) plane, action is its area $S = 2\pi E/w$, and the WKB spectrum

$$E_n = \hbar w(n + 1/2) \tag{24.21}$$

turns out to be the *exact* harmonic oscillator spectrum. Morally, stationary phase condition (24.15) keeps $V(q)$ accurate to order q^2, which in this case is the whole answer (but we were plain lucky, really). Nevertheless, for many 1-d problems WKB spectrum turns out to be very accurate. Surprisingly so, if one interprets dropping the $\hbar^2$ term in (24.4) as a short wavelength approximation.

Commentary

Remark 24.1 Airy function. The stationary phase approximation is all that is needed for the semiclassical approximation, with the proviso that D in (26.35) 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 [27.12].

24.9
page 461