221A Lecture Notes
WKB Method

1 Hamilton–Jacobi Equation

We start from the Schrödinger equation for a single particle in a potential

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t)=\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2+V(\vec{x})\right]\psi(\vec{x},t). \tag{1}$$

We can rewrite this equation by using $\psi(\vec{x},t)=e^{iS(\vec{x},t)/\hbar}$:

$$-\frac{\partial S}{\partial t}\psi=\left[\frac{1}{2m}(\vec{\nabla}S)^2-\frac{i\hbar}{2m}(\vec{\nabla}^2S)+V\right]\psi. \tag{2}$$

Assuming $\psi\neq 0$, this leads to an equation

$$-\frac{\partial S}{\partial t}=\frac{1}{2m}(\vec{\nabla}S)^2-\frac{i\hbar}{2m}(\vec{\nabla}^2S)+V. \tag{3}$$

Now taking the formal limit $\hbar\to 0$, it becomes the same as the classical Hamilgon–Jacobi equation

$$-\frac{\partial S}{\partial t}=\frac{1}{2m}(\vec{\nabla}S)^2+V. \tag{4}$$

It is often said that the $\hbar\to 0$ limit is indeed the classical mechanics because it reduces to the Hamilton–Jacobi equation.

2 Classical Limit

The fact that the exponent S satisfies the Hamilton–Jacobi equation may not mean the classical behavior to you right away. The way to see it is by forming a wave packet, and ask the question how does the wave packet moves as a whole. To simplify the discussion, let us consentrate on the case where the Hamiltonian does not depend explicitly on time, and we can separate the variable as

$$S(\vec{x},t)=\tilde{S}(\vec{x},E)-Et. \tag{5}$$

The inverse Legendre transformation says

$$t = \frac{\partial \tilde{S}(\vec{x}, E)}{\partial E}. \tag{6}$$

This condition can be viewed as an implicit equation to determine the position of the particle $\vec{x}$ as a function of time t.

To form a wave packet, we need to put together waves of slighly different energies. We can write

$$\psi(\vec{x}, t) = \int dE g(E) e^{i(\tilde{S}(\vec{x},E) - Et)/\hbar}, \tag{7}$$

The question here is where the wave packet is. At most places, the averaging over E makes the phase oscillate very fast because of the small $\hbar$, and there is a strong cancellation. Only at special points where the phase factor is stationary with respect to E, the wave function is sizable. Therefore, the position of the wave packet is determined by the stationary condition

$$\frac{\partial}{\partial E}\left(\tilde{S}(\vec{x}, E) - Et\right) = \frac{\partial \tilde{S}(\vec{x}, E)}{\partial E} - t = 0. \tag{8}$$

This is nothing but Eq. (6). In other words, the wave packet is sizable only where the position satisfies the classical equation of motion. Therefore, the wave packet follows the classical equation of motion.

3 $\hbar$ Expansion

Now that we have rederived classical mechanics from quantum mechanics, our interest now turns to quantum mechanics itself. We will use the fact that $\hbar$ is indeed small to find a useful approximation method in quantum mechanics.

The Eq. (3) is exact as long as $\psi \neq 0$. One can use this equation, and consider an expansion

$$S(\vec{x}, t) = S_0 + \hbar S_1 + \hbar^2 S_2 + \cdots. \tag{9}$$

This is an expansion in $\hbar$, and hence called $\hbar$-expansion or semi-classical expansion. Plugging in the expansion into Eq. (3), we find

$$-\frac{\partial S_0}{\partial t} = \frac{1}{2m}(\vec{\nabla} S_0)^2 + V, \tag{10}$$

$$-\frac{\partial S_1}{\partial t} = \frac{1}{2m}\left[-i\vec{\nabla}^2 S_0 + 2(\vec{\nabla} S_0)(\vec{\nabla} S_1)\right], \tag{11}$$

and similarly for higher terms in $\hbar$. The leading equation has only S_0, and it is exactly the same as Hamilton–Jacobi equation. Once you solve these equations starting from S_0, S_1, etc, you have solved the wave function ψ in a systematic expansion in $\hbar$.

There is one importance difference between the "classical limit" which reduces to the Hamilton–Jacobi equation and the idea of expansion in $\hbar$. In the classical limit, S is of course *real* because it does not make sense otherwise. However, in the sense of an expansion in $\hbar$, we don't know if S_0 has to be real. In fact, in many interesting cases, S_0 turns out to be *complex*. We will see these examples below.

4 WKB Approximation

WKB Approximation, due to Wentzel, Kramers, and Brillouin, keeps terms up to $O(\hbar)$ in the $\hbar$ expansion. It is used mostly for the time-independent case, or in other words, for an eigenstate of energy E. Then the wave function has the ordinary time dependence $e^{-iEt/\hbar}$. We also restrict ourselves to the one-dimensional problem. In terms of S, it corresponds to

$$S(\vec{x}, t) = S(\vec{x}) - Et. \tag{12}$$

Therefore only S_0 has the time dependence $S_0(x,t) = S_0(x) - Et$, while higher order terms $S_i = S_i(x)$ for $i \neq 0$ do not depend on time.

The lowest order term S_0 satisfies the Hamilton–Jacobi equation (see Eq. (10)

$$E = \frac{1}{2m}(S_0')^2 + V(x). \tag{13}$$

The differential equation can be solve immediately as

$$S_0(x) = \pm \int^x \sqrt{2m(E - V(x'))}dx' = \int^x p(x')dx' \tag{14}$$

up to an integration constant which can be determined only after imposing a boundary condition on the wave function. We used the notation $p(x) = \pm\sqrt{2m(E - V(x))}$ because it is nothing but the momentum of the particle in the classical sense. Once we know S_0, we can also solve for S_1. Starting from Eq. (11), and using $\partial S_1/\partial t = 0$, we find

$$2S_0'S_1' = iS_0'', \tag{15}$$

which has a solution

$$S_1(x) = i\int^x \frac{S_0''(x')}{2S_0'(x')}dx' = \frac{i}{2}\log p(x) + \text{constant}. \tag{16}$$

Therefore the general solution to the Schrödinger equation up to this order is

$$\begin{aligned}\psi(x,t) &= e^{i(S_0(x)+\hbar S_1(x))/\hbar}e^{-iEt/\hbar} \\ &= c\frac{1}{p(x)^{1/2}}\exp\left(\pm\frac{i}{\hbar}\int^x\sqrt{2m(E-V(x'))}dx'\right)e^{-iEt/\hbar},\end{aligned} \tag{17}$$

and the overall constant c is of course undetermined from this analysis.

This solution makes it immediately clear that this approximation breaks down when $p(x)$ goes to zero. Or in other words, the approximation is bad where the classical particle *stops* and *turns* because of the potential. Such points are called "classical turning points."

4.1 Validity of the WKB Approximation

The approximation to stop with S_1 in the $\hbar$ expansion is valid only when S_1 is much smaller than S_0. Or in other words, if the term with $\hbar$ in Eq. (2) is much smaller than the other terms. In particular, we require

$$|(\vec{\nabla}S)^2| \gg \hbar|\vec{\nabla}^2 S|. \tag{18}$$

In the one-diimensional time-independent case discussed above, this is

$$p(x)^2 \gg \hbar|p'(x)|. \tag{19}$$

Using the definition of $p(x) = \pm\sqrt{2m(E-V(x))}$, we find

$$\left|\frac{\hbar dV(x)/dx}{2(E-V(x))p(x)}\right| \ll 1. \tag{20}$$

Again we find the same conclusion: the WKB approximation breaks down close to the classical turning point $V(x) = E$ (*e.g.*, $p(x) = 0$).

For example, take a harmonic oscillator $V(x) = \frac{1}{2}m\omega^2x^2$. The validity condition Eq. (20) can be rewritten as

$$8\left|E - \frac{1}{2}m\omega^2x^2\right|^3 \gg (\hbar\omega)^2 m\omega^2 x^2. \tag{21}$$

This inequality is always satisfied exactly at the origin $x = 0$, but once away from the origin, it is impossible to satisfy unless $E \gg \hbar\omega$. In this sense, we are indeed in the classical regime. However, even for a large $E \gg \hbar\omega$, the approximation is not valid close to the classical turning points $E = \frac{1}{2}m\omega^2 x^2$.

Here is the surprise. The validity condition Eq. (20) may be satisfied even in the region where the particle cannot enter classicaly $E < V(x)$. For example with the harmonic oscillator again, the validity condition is always satisfied for large $x \gg \sqrt{2E/m\omega^2}$ for any value of E. In other words, the WKB approximation is good away from the classical turning points both where a classical particle exists and where a classical particle cannot exist. This is why the WKB approximation is not really a classical limit. It applies also where physics is truly quantum mechanical.

In the classically forbidden region, the solution Eq. (17) needs to be modified to

$$\begin{aligned}\psi(x,t) &= e^{i(S_0(x)+\hbar S_1(x))/\hbar} e^{-iEt/\hbar} \\ &= c\frac{1}{(2m(V(x)-E))^{1/4}} \exp\left(\pm\frac{1}{\hbar}\int^x \sqrt{2m(V(x')-E)}dx'\right) e^{-iEt/\hbar}\end{aligned} \quad (22)$$

by following the same steps as in the classically allowed region.

4.2 Matching

WKB approximation can be good both in the region $E > V(x)$ and the region $E < V(x)$ but cannot be good in between the regions close to the classical turning point $E = V(x_c)$. In order to utilize the WKB approximation to work out wave functions, we need to somehow overcome this limitation. The standard method is to expand around x_c and solve for the wave function "exactly." Then you can match on to the WKB solutions away from x_c to determine the entire wave function.

The common method is to approximate the potential around the classical turning point x_c by a linear one:

$$V(x) = V(x_c) + V'(x_c)(x - x_c) + O(x - x_c)^2, \quad (23)$$

and ignore the second order term. By definition $V(x_c) = E$. Schrödinger equation around this point is therefore

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) - E\right)\psi = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V'(x_c)(x - x_c)\right)\psi = 0. \quad (24)$$

Using the new variable

$$u = \left(\frac{2m}{\hbar^2}\frac{dV}{dx}(x_c)\right)^{1/3}(x - x_c), \tag{25}$$

the differential equation simplifes drastically to

$$\left(\frac{d^2}{du^2} - u\right)\psi = 0. \tag{26}$$

The solution to this equation is known as the Airy function

$$\mathrm{Ai}(u) = \frac{1}{\pi}\int_0^\infty dt \cos\left(\frac{1}{3}t^3 + ut\right). \tag{27}$$

This can be checked as follows. By acting the differential operator in Eq. (26) on the definition of the Airy function, we find

$$\left(\frac{d^2}{du^2} - u\right)\mathrm{Ai}(u) = -\frac{1}{\pi}\int_0^\infty dt \frac{d}{dt}\sin\left(\frac{1}{3}t^3 + ut\right). \tag{28}$$

The boundary term at $t = 0$ obviously vanishes. The behavior at $t = \infty$ is trickier. The point is that the argument of the sin grows as t^3 and oscillates more and more rapidly as $t \to \infty$. Therefore for any infinitesimal interval of large t, the oscillation basically cancels the integrand except for a "left-over" that goes down as $\sim 1/t^2$. Therefore the boundary term for $t \to \infty$ can also be dropped.

It can be shown using the steepest descent method that the asymptotic behavior of the Airy function smoothly matches to the WKB solutions. The asymptotic behavior is

$$\mathrm{Ai}(u) \sim \begin{cases} \frac{1}{2}\left(\frac{1}{\pi\sqrt{u}}\right)^{1/2}\exp\left(-\frac{2}{3}u^{3/2}\right) & u \gg 0 \\ \left(\frac{1}{\pi\sqrt{-u}}\right)^{1/2}\cos\left(\frac{2}{3}u\sqrt{-u} + \frac{\pi}{4}\right) & u \ll 0 \end{cases}. \tag{29}$$

Note first that, for $u \ll 0$, the asymptotic behavior is

$$\mathrm{Ai}(u) = \left(\frac{\hbar(2mV'/\hbar^2)^{1/3}}{\pi\sqrt{2m(E-V)}}\right)^{1/2}\cos\left(\frac{1}{\hbar}\int_{x_c}^x \sqrt{2m(E-V)}dx' + \frac{\pi}{4}\right). \tag{30}$$

Here we used the linear expansion $V(x) = E + V'(x_c)(x - x_c)$ to relate powers of u to $\sqrt{2m(E-V)}$. This expression is consistent with the WKB solution for a particular choice of the overall constant. Similarly, for $u \gg 0$,

$$\mathrm{Ai}(u) = \frac{1}{2}\left(\frac{\hbar(2mV'/\hbar^2)^{1/3}}{\pi\sqrt{2m(V-E)}}\right)^{1/2} \exp\left(-\frac{1}{\hbar}\int_{x_c}^{x}\sqrt{2m(V(x')-E)}dx'\right). \quad (31)$$

4.3 Bound States

Consider the following situation. In the region I ($x < a$), $E < V$ and it is classically forbidden. In the region II ($a < x < b$), $E > V$ and the the particle is classically allowed. But again in the region III ($x > b$) it is classically forbidden. In this case, we expect bound states with discrete energy levels.

From the matching using the Airy function at $x = b$, we want the wave function in the classicaly allowed region II to be as in Eq. (30),

$$\psi(x) = c_b\left(\frac{\hbar(2mV'(b)/\hbar^2)^{1/3}}{\pi\sqrt{2m(E-V)}}\right)^{1/2} \cos\left(\frac{1}{\hbar}\int_{b}^{x}\sqrt{2m(E-V(x'))}dx' + \frac{\pi}{4}\right). \quad (32)$$

On the other hand from the matching at $x = a$, the wave function in the region II must be

$$\psi(x) = c_a\left(\frac{\hbar(2mV'(a)/\hbar^2)^{1/3}}{\pi\sqrt{2m(E-V)}}\right)^{1/2} \cos\left(\frac{1}{\hbar}\int_{a}^{x}\sqrt{2m(E-V(x'))}dx' - \frac{\pi}{4}\right). \quad (33)$$

c_b and c_a are normalization constants. The minus sign in fron of $\pi/4$ is because the classically allowed region is to the right of the turning point and hence we need to use Ai(-u) instead of Ai(u) for matching. The two behaviors obtained from matching at both sides must be the same in order to have a consistent wave function for the entire region II. Because we do not know the coefficients $c_{a,b}$, which can in particular differ in signs, we have to require

$$\frac{1}{\hbar}\int_{b}^{x}\sqrt{2m(E-V(x'))}dx' + \frac{\pi}{4} = \frac{1}{\hbar}\int_{a}^{x}\sqrt{2m(E-V(x'))}dx' - \frac{\pi}{4} - n\pi. \quad (34)$$

Further simplifying the equation we obtain

$$\int_{a}^{b}\sqrt{2m(E-V(x))}dx = \left(n + \frac{1}{2}\right)\pi\hbar. \quad (35)$$

This is reminiscent of Bohr–Sommerfeld quantization condition that appeared at the early stage of quantum mechanics,

$$\oint p dq = nh \tag{36}$$

with $h = 2\pi\hbar$ except that there is an extra contribution $1/2$ here. Remember that the Bohr–Sommerfeld quantization condition was an *ad hoc* requirement which happened to give correct energy spectra for the hydrogen-like atoms. Nonetheless, this is an important equation because it puts constraints on the allowed values of E, and hence we find discrete energy levels. Because the WKB approximation is better for larger E, the constraint Eq. (35) is expected to give correct energy levels at least for highly excited states.

Let us apply this constraint Eq. (35) for a harmonic oscillator. The condition then is

$$\int_{x_{min}}^{x_{max}} \sqrt{2mE - m^2\omega^2 x^2} dx = \left(n + \frac{1}{2}\right)\pi\hbar. \tag{37}$$

The l.h.s. is an elementary integral $\frac{2mE}{m\omega}\frac{\pi}{2}$ and we find

$$E = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{38}$$

This is precisely the energy levels of a harmonic oscillator. Of course, obtaining the exact energy levels is an accident for a harmonic oscillator. In general, we expect to get approximately correct energy levels for high n. Indeed, if we apply the same constraint for the hydrogen-like atoms (for $l = 0$ and applying the WKB method to the radial wave function), we would obtain the correct results if we drop $1/2$ (this is what Bohr–Sommerfeld) did, but don't if we keep $1/2$ as obtained by the WKB method.

What we obtain from the WKB method is not just the energy levels, but more details such as the approximate wave function. To simplify the notation, let us choose a unit system such that $m = \omega = \hbar = 1$. Then the wave function in the region II for the harmonic oscillator is

$$\psi \propto \frac{1}{(2E - x^2)^{1/4}} \cos\left(\int_{-\sqrt{2E}}^{x} \sqrt{2E - x'^2} dx' - \frac{\pi}{4}\right). \tag{39}$$

Doing the standard integral, we find

$$\psi \propto \frac{1}{(2E - x^2)^{1/4}} \cos\left[E\left(\sin^{-1}\frac{x}{\sqrt{2E}} + \frac{\pi}{2} + \frac{x}{\sqrt{2E}}\sqrt{1 - \frac{x^2}{2E}}\right) - \frac{\pi}{4}\right]. \tag{40}$$

Because $E = n + 1/2$ in this unit, it further simplifies to

$$\psi \propto \frac{1}{(2E - x^2)^{1/4}} \begin{cases} \cos\left[E\left(\sin^{-1}\frac{x}{\sqrt{2E}} + \frac{x}{\sqrt{2E}}\sqrt{1-\frac{x^2}{2E}}\right)\right] & n \text{ even} \\ \sin\left[E\left(\sin^{-1}\frac{x}{\sqrt{2E}} + \frac{x}{\sqrt{2E}}\sqrt{1-\frac{x^2}{2E}}\right)\right] & n \text{ odd} \end{cases} \tag{41}$$

4.4 Tunneling

To study a tunneling process, we again have three regions, a classically allowed region I $x < a$, where the particle initially exist, a classically forbidden region II $a < x < b$, and a classically allowed region III $x > b$ where the particle tunnels to. We follow the same matching procedure as in the bound state example. A difference is that the matching at $x = b$ uses a different version of the Airy function which rises exponentially away from $x = b$. This version of the Airy function Bi is explained in the note on steepest descent method. The bottom line is that the matching at $x = a$ is done as

$$\psi \simeq \left(\frac{\hbar(2mV'(a)/\hbar^2)^{1/3}}{\pi\sqrt{2m(E-V)}}\right)^{1/2} \cos\left(\frac{-1}{\hbar}\int_x^a \sqrt{2m(E-V)}dx' + \frac{\pi}{4}\right), \qquad (x < a)$$

$$\psi \simeq \frac{1}{2}\left(\frac{\hbar(2mV'(a)/\hbar^2)^{1/3}}{\pi\sqrt{2m(V-E)}}\right)^{1/2} \exp\left(\frac{-1}{\hbar}\int_a^x \sqrt{2m(V-E)}dx'\right). \qquad (x > a)$$

The matching at $x = b$ is, on the other hand,

$$\psi \simeq C\frac{i}{2}\left(\frac{\hbar(2mV'(b)/\hbar^2)^{1/3}}{\pi\sqrt{2m(V-E)}}\right)^{1/2} \exp\left(\frac{+1}{\hbar}\int_x^b \sqrt{2m(V-E)}dx'\right), \qquad (x < b)$$

$$\psi \simeq C\frac{i}{2}\left(\frac{\hbar(2mV'(b)/\hbar^2)^{1/3}}{\pi\sqrt{2m(E-V)}}\right)^{1/2} \sin\left(\frac{1}{\hbar}\int_b^x \sqrt{2m(E-V)}dx' + \frac{\pi}{4}\right). \qquad (x > b)$$

The overall normalization factor C is determined by the requirement that the behavior of the wave function is consistent for $a < x < b$ between two matching procedures. We therefore find

$$C = -i\left(\frac{V'(a)}{V'(b)}\right)^{1/6} \exp\left(-\frac{1}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}dx\right). \tag{42}$$

Comparing two classically allowed regions, and taking advantage of a further normalization change, the matching reduces to

$$\begin{aligned}
\psi &\simeq \frac{1}{(2m(E-V))^{1/4}} \cos\left(\frac{-1}{\hbar}\int_x^a \sqrt{2m(E-V)}dx' + \frac{\pi}{4}\right), \qquad (x<a) \\
\psi &\simeq \frac{1}{2}\exp\left(-\frac{1}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}dx\right) \frac{1}{(2m(E-V))^{1/4}} \sin\left(\frac{1}{\hbar}\int_b^x \sqrt{2m(E-V)}dx' + \frac{\pi}{4}\right).
\end{aligned}$$

In other words, the amplitude in the region $x > b$ due to tunneling from the region $x < a$ is suppressed by

$$\frac{1}{2}\exp\left(-\frac{1}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}dx\right). \tag{43}$$

Usually people refer to Gamov's transmission coefficient

$$\exp\left(-2\frac{1}{\hbar}\int_a^b \sqrt{2m(V(x)-E)}dx\right) \tag{44}$$

as a suppression factor for the tunneling rate (square of the amplitude).