Lecture 2

WKB

I know all of you already can do WKB – but it is good to review, since the concepts of WKB will show up more. To keep things interesting I'll make some connections to semiclassics in time. The other thing which we will see which might be new to some of you is the "slick" way to derive connection formulas.

For those who are interested in history, many people refer to the WKB approximation as JWKB. The initials stand for Jeffreys, Wentzel, Kramers, and Brillouin, the scientists who came up with the approach.

A. WKB

Our starting point is the time independent Schrodinger equation

$$\frac{\hbar^2}{2m}\partial_x^2\psi = [V(x) - E]\,\psi, \tag{2.1}$$

with the condition that ψ is square integrable. We want to find the spectrum as $\hbar \to 0$. We know that as $\hbar$ is made smaller the level spacing drops, but the coarse grained density of states approaches a smooth function.

One nice way to think about WKB is that the limit $\hbar \to 0$ is the limit of a smooth potential. This is particularly transparent if you let $y = x/\hbar$. [Which we won't – but feel free to play with this.] Thus, as long as we just look locally near some point x_0, we expect the wavefunction to look like a free particle:

$$\psi(x) \approx A_x\, e^{\pm ik(x-x\ )} \tag{2.2}$$

$$k = \sqrt{2m[V(x_0) - E]}/\hbar. \tag{2.3}$$

This is essentially correct. The only tricky thing is how to piece together the wavefunctions at different positions. One clue is the continuity equation: if k is larger, then A must be smaller – that way there does not need to be any sources or sinks for probability density. Recall that the probability density is $\rho = |\psi|^2$ and the probability current is $j = (\psi^* \partial_x \psi - \psi \partial_x \psi^*)/(2i)$, and the continuity equation is

$$\partial_t \rho + \partial_x j = 0. \tag{2.4}$$

[This is nothing but the imaginary part of the time dependent Schrodinger equation.]

> **Group Activity**: Express j in terms of A and k.

Thus one must have $j = k|A|^2$ constant. This still doesn't tell us what the phase of A is though. Nor does it tell us how to get the quantization condition.

The formal trick, motivated by these thoughts, is to write

$$\psi = e^{iS/\hbar}. \tag{2.5}$$

The $\hbar$ in this expression is exactly the $\hbar$ in Eq. (2.3).

> **Group Activity**: Express $\partial_x^2 \psi$ in terms of S and its derivatives.

With this substitution, the Schrodinger equation reads

$$\frac{i}{2m} \hbar \partial_x^2 S - \frac{1}{2m} (\partial_x S)^2 = V(x) - E. \tag{2.6}$$

On one hand we have apparently made things worse: this is a nonlinear equation. On the other hand it is amenable to solution by expansion in powers of $\hbar$, writing $S = S_0 + \hbar S_1 + \hbar^2 S_2 + \cdots$. To lowest order

$$\partial_x S_0 = \sqrt{2m(E - V)}, \tag{2.7}$$

which is readily integrated to give

$$S_0(x) = \int^x dx \sqrt{2m(E - V)}. \tag{2.8}$$

The next order equation is

$$\frac{i}{2m} \partial_x^2 S_0 - \frac{1}{m} (\partial_x S_0)(\partial_x S_1) = 0 \tag{2.9}$$

> **Group Activity**: Solve for S_1.

The net result is that to second order

$$\psi_{WKB} = \frac{1}{\sqrt{p(x)}} e^{\frac{i}{\hbar}} \int^x dx\, p(x) \tag{2.10}$$

where

$$\frac{p^2}{2m} = E - V. \tag{2.11}$$

Equation (2.10) has all the features we wanted.

> **Group Activity**: What is the realm of validity of this expansion?

B. Connection Formula

You all know that the WKB expressions break down near the classical turning points. One sees this by taking the ratio

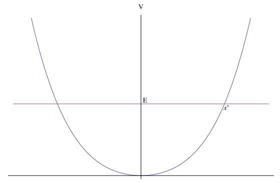
$$\left|\frac{S_1}{S_0}\right| = \frac{1}{2}\frac{\log \partial_x S_0}{S_0}, \tag{2.12}$$

which diverges when $p \to 0$.

Physically the problem is clear. The particle needs to be reflected at the turning point, but our approach always has the current going in the same direction. The classic approach to addressing this breakdown is to go back to some standard rules from asymptotic analysis.

The general rule from asymptotic analysis is that whenever you have a sum with multiple terms, then generically only two of them will be important. We have already seen that in Eq. (2.6), generically the leading behavior is given by throwing out the first term on the left. This is known as the ”outer” solution. When $p \to 0$, however, the first term is bigger than the second. The solution is to throw away the second term. One then solves the resulting “inner” equation. In order to match the two solutions one needs to add to Eq. (2.10) a term corresponding to a wave going in the other direction. The relationship between these waves (and the evanescent waves on the other side of the barrier) are the ”connection formulas”. [In practice one works directly with Eq. (2.1), and where the inner solution is an Airy function.]

There is a simpler approach which requires less thinking. This is again a general technique for solving differential equations. The idea is to recognize that Eq. (2.6) is a perfectly good approach to defining a function $S(x)$ for complex x. Let x^* be one of the points satisfying $V(x) = E$. For concreteness you can think about the following potential, and take x^* to be the right-most crossing:



For x near x^* we can approximate $p \approx \alpha\sqrt{x - x^*}$ where α is positive, and we will interpret the square root to be the principle branch. [That is we take $p > 0$ when $x < x^*$.] Let us suppose that everywhere in the complex plane

$$\psi = \frac{A}{\sqrt{p(x)}} e^{\frac{i}{\hbar}\int_x^x dx\, p(x)} \tag{2.13}$$

Since p is a multivalued function of x, so is this function. If I go from $x < x^*$ to $x > x^*$ by circling around x^* in a counterclockwise direction, then p^2 picks up a negative imaginary part, and one gets

$$\psi_{x>x^*} = \frac{Ae^{i\pi/4}}{\sqrt{|p(x)|}} e^{i\phi^*} e^{\frac{1}{\hbar}\int_{x^*}^x dx\, |p(x)|} \tag{2.14}$$

where

$$\phi^* = \frac{1}{\hbar}\int_x^{x^*} p(x)\, dx. \tag{2.15}$$

Typically Eq. (2.16) is bad. This wavefunction grows exponentially. If instead we want it to decay, we need to circle x^* in the opposite manner, instead finding

$$\psi_{x>x^*} = \frac{Ae^{-i\pi/4}}{\sqrt{|p(x)|}} e^{i\phi^*} e^{-\frac{1}{\hbar}\int_{x^*}^x dx\, |p(x)|} \tag{2.16}$$

If we keep circling back in this direction, we find that we don't come back to our original wavefunction, instead we get

$$\psi = \frac{Ae^{-i\pi/2}}{\sqrt{p(x)}} e^{i\phi^*} e^{-\frac{i}{\hbar}\int_{x^*}^x dx\, p(x)}. \tag{2.17}$$

This is the reflected wave. Putting things together we have

$$\psi_{x<x^*} = Ae^{i\phi^*}\frac{1}{\sqrt{p(x)}}\left[e^{\frac{i}{\hbar}\int_{x^*}^x dx\, p(x)} + e^{-i\pi/2}e^{-\frac{i}{\hbar}\int_{x^*}^x dx\, p(x)}\right] \tag{2.18}$$

$$\psi_{x>x^*} = \frac{Ae^{-i\pi/4}}{\sqrt{|p(x)|}} e^{i\phi^*} e^{-\frac{1}{\hbar}\int_{x^*}^x dx\, |p(x)|}. \tag{2.19}$$

In other words the wavefunction picks up a phase factor of $\pi/2$ upon reflection from a linear turning point. This is very different from reflection from a hard wall, where the wavefunction picks up a phase of π.

If we make the same argument at the other barrier, and require the wavefunction to be single-valued, we get the standard semiclassical quantization condition:

$$\oint p(x)\, dx = 2\pi\hbar(n + 1/2). \tag{2.20}$$

The standard way of interpreting this is to note that $p(x)$ defines an isoenergy contour in phase space. Looking at two sequential trajectories sattisfying Eq. (2.20),

$$\left[\oint_{E_n} - \oint_{E_{n-}}\right] p\,dx = 2\pi\hbar. \tag{2.21}$$

This can be rewritten as

$$\delta E \oint_{E_{n-}} \frac{\partial p}{\partial E} dx = 2\pi\hbar. \tag{2.22}$$

But $\partial E/\partial p = v$ is the velocity so

$$\oint \frac{\partial p}{\partial E} dx = \oint \frac{dx}{v} = T = \frac{2\pi\hbar}{\delta E} \tag{2.23}$$

C. Tunneling

How does this argument change when we have a double well potential? Clearly one needs to include not only the exponentially decaying solutio, but also the exponentially growing solution. Let x_1 and x_2 be the two turning points defining the leftmost and rightmost edge of the barrier. Inside the barrier the wavefunction should be:

$$\psi = \frac{1}{\sqrt{|p(x)|}}\left[e^{-\frac{1}{\hbar}\int_x^x dx\,|p(x)|} \pm e^{\frac{1}{\hbar}\int_x^x dx\,|p(x)|}\right] \tag{2.24}$$

Analytically continuing the first term to the left (and adding the two contributions from the two ways to go) gives

$$\psi_1 = \frac{1}{\sqrt{p(x)}}\left[e^{-i\pi/4} e^{\frac{i}{\hbar}\int_x^x dx\,p(x)} + e^{i\pi/4} e^{-\frac{i}{\hbar}\int_x^x dx\,p(x)}\right]. \tag{2.25}$$

Analytically continuing the second term gives

$$\psi_2 = \pm e^{-\Lambda}\left[e^{-i\pi/4} e^{\frac{i}{\hbar}\int_x^x dx\,p(x)} + e^{i\pi/4} e^{-\frac{i}{\hbar}\int_x^x dx\,p(x)}\right]. \tag{2.26}$$

where

$$\Lambda = \frac{1}{\hbar}\int_x^x |p(x)| dx. \tag{2.27}$$

Adding these together gives

$$\psi = \frac{A}{\sqrt{p(x)}}\left[e^{-i\chi/2} e^{\frac{i}{\hbar}\int_x^x dx\,p(x)} + e^{i\chi/2} e^{-\frac{i}{\hbar}\int_x^x dx\,p(x)}\right], \tag{2.28}$$

where

$$Ae^{i\chi/2} = e^{i\pi/4} \pm e^{-\Lambda} e^{-i\pi/4} \tag{2.29}$$

$$= e^{i\pi/4}[1 \mp ie^{-\Lambda}] \tag{2.30}$$

$$\approx \exp[i\pi/4 \mp ie^{-\Lambda}], \tag{2.31}$$

which gives quantization condition

$$\frac{1}{\hbar}\oint p\,dx = 2\pi(n+1/2) \pm 2e^{-\Lambda} \tag{2.32}$$

Taking the difference between the + and − one has

$$\frac{T\Delta}{\hbar} = 4e^{-\Lambda}. \tag{2.33}$$

Thus the splitting is $\Delta = (2\hbar\omega/\pi)e^{-\Lambda}$. This seems to be a factor of 2 larger than what most books say. I think I am right, but bonus points to anyone who finds my error.

Actually, I tried numerically calculating Δ, and I seem to get a bigger prefactor than this. More bonus points for identifying the missing physics.

Problem 2.1. Consider the eigenvalue problem:

$$\partial_x^2\psi - x\psi = 0.$$

According to our arguments here, there are two independent solutions with asymptotic behavior:

$$\begin{aligned}\psi_1(x<0) &= |x|^{-1/4}e^{i(2/3)|x|^{3/2}+i\pi/4} + x^{-1/4}e^{-i(2/3)|x|^{3/2}-i\pi/4}\\ \psi_1(x>0) &= |x|^{-1/4}e^{-(2/3)x^{3/2}}\end{aligned}$$

and

$$\begin{aligned}\psi_2(x<0) &= |x|^{-1/4}e^{i(2/3)|x|^{3/2}-i\pi/4} + x^{-1/4}e^{-i(2/3)|x|^{3/2}+i\pi/4}\\ \psi_2(x>0) &= |x|^{-1/4}e^{(2/3)x^{3/2}}.\end{aligned}$$

Look up the solution to this differential equation and verify that these are correct.

D. Top of the barrier

Near the top of the barrier, Eq. (2.34) still holds, but the approximation below it fails. Instead $\Lambda \to 0$ and

$$\begin{aligned}Ae^{i\chi/2} &= e^{i\pi/4} \pm e^{-\Lambda}e^{-i\pi/4} && (2.34)\\ &= e^{i\pi/4}[1 \mp i] && (2.35)\\ &\propto \exp[i\pi/4 \mp i\pi/4], && (2.36)\end{aligned}$$

Thus the quantization condition for the two modes are:

$$\frac{1}{\hbar}\oint p\,dx = 2\pi(n+1/4) \tag{2.37}$$

$$\frac{1}{\hbar}\oint p\,dx = 2\pi(n+3/4). \tag{2.38}$$

This integral is taken around the path that circles one well. This is the same result that you would get if you took paths that circled both wells.

E. Mathematics

The arguments made here were purely heuristic. I know no way to make them rigorous – but it turns out they are correct.