Lecture 18 Highlights
Phys 402

WKB Approximation

We now go back to one-dimensional quantum mechanics and investigate some very useful approximation schemes. Note that the Schrödinger equation for the hydrogen atom reduces, in part, to a one-dimensional Schrödinger problem for the radial coordinate, so these approximation schemes can also work for aspects of 3D problems.

First consider the approximation due to Wentzel, Kramers and Brillouin, known as the WKB approximation. This approximation works in the "semi-classical limit" of quantum mechanics. The lowest lying states of a quantum problem are said to be in the extreme quantum limit. Look at the eigenfunctions for the 1D harmonic oscillator on the top of page 53 of Griffiths, for example (or similar wavefunctions here). The wave nature of the solution is crucial for understanding the properties of such states. On the other hand we know that classical mechanics should be recovered if we consider solutions to the Schrödinger equation at very high quantum number ("$n \to \infty$"). In this limit the deBroglie wavelength of the particle is so small that it plays essentially no role in the dynamics of the particle or wave packet. In between these two extremes we have the semi-classical limit, where both the wave nature and the high quantum number are of roughly equal significance. The harmonic oscillator wavefunction shown on the bottom of page 53 of Griffiths is a good example of a semi-classical wavefunction. It has both quantum and classical character, as we shall see. In other fields of physics very similar approximations are made, but given different names: Eikonal approximation (quantum scattering theory in the semi-classical limit) and paraxial approximation (wave optics in the short wavelength limit).

The WKB approximation is basically good for two things: 1) estimating eigen-energies in the semi-classical limit for complicated 1D potentials $V(x)$, and 2) estimating tunneling rates in the semi-classical limit through complicated barriers. Here we look at eigen-energies in the 1D semi-classical limit, and we examine the tunneling case in the next lecture.

The lecture followed the book (Griffiths, pages 354-357) quite closely. The basic idea is that in the semi-classical limit we can construct solutions to the 1D Schrödinger equation which are basically modulated traveling waves, in which the amplitude and phase vary on the scale of the variation of the potential:

$$\psi(x) = A(x)\exp\left[\pm i\phi(x)\right],$$

where it is assumed that the wavelength of the particle $2\pi/k(x)$ (treating $\phi(x) = k(x)x$) is much smaller than the length scale on which the potential $V(x)$ is changing. With this ansatz (which is exact at this point), the Schrödinger equation reduces to two real equations for the two unknown functions;

$$A'' = A(\phi')^2 - \frac{p_{class}^2}{\hbar^2}A$$

$$\frac{d}{dx}\left(A^2\phi'\right) = 0,$$

where $A'' = d^2A/dx^2$, etc., $p_{class} = \sqrt{2m(E - V(x))}$ is the classical momentum of the particle, and it is assumed that the amplitude $A \neq 0$. The WKB approximation basically

consists of ignoring the second derivative term in the first equation because the amplitude is expected to vary slowly if the above constraint on the length scale of variation of $V(x)$ is satisfied. With this, the solutions to the Schrödinger equation become;

$$\psi(x) = \frac{D}{\sqrt{p_{class}(x)}} \exp\left[\pm \frac{i}{\hbar} \int^{x} p_{class}(x')dx' \right],$$

where D is a complex constant and x' is a dummy coordinate variable. Note that the probability density varies inversely with the classical momentum:

$$|\psi(x)|^2 \propto \frac{1}{p_{class}(x)} \propto \frac{1}{\sqrt{2m(E - V(x))}}.$$

Hence the probability density should peak at the classical turning points (i.e. the points x_{class} where $V(x_{class}) = E$). This is indeed the case with the semi-classical wavefunction shown on the bottom of page 53 in Griffiths, and <u>not</u> the case for the extreme quantum wavefunctions on the top of page 53.

As an example of computing eigen-energies, consider a 1D infinite square well with an arbitrary potential $V(x) \neq 0$ on the bottom, going from $x = 0$ to $x = a$. We can solve for the eigen-energies in the semi-classical limit (assuming $E > V(x)$ everywhere in the well) where the wavelength of the particle is small compared to the spatial variation length scale of $V(x)$. The solutions are of the form;

$$\psi(x) = \frac{1}{\sqrt{p_{class}(x)}} \{D_1 \sin(\phi(x)) + D_2 \cos(\phi(x))\},$$

where $\phi(x) = \frac{1}{\hbar} \int_0^{x} p_{class}(x')dx'$. Enforcing the boundary conditions $\psi(0) = \psi(a) = 0$ gives $D_2 = 0$ (from $\psi(0) = 0$, and the fact that $\phi(0) = 0$), and because $\psi(a) = 0$ we require $\sin\left(\frac{1}{\hbar} \int_0^{a} p_{class}(x')dx' \right) = 0$, which in turn requires $\frac{1}{\hbar} \int_0^{a} p_{class}(x')dx' = \pi n$, where n is a positive integer. The value of n should start at the eigen-number that first enters the semi-classical limit, coming up the ladder of states from the quantum limit (in other words, $n \gg 1$). This value will depend on the problem, of course. For a given potential $V(x)$ on the bottom of the well, we now have a numerical problem to solve for the eigenenergies (E_n) in the semiclassical limit: $\frac{1}{\hbar} \int_0^{a} \sqrt{2m(E_n - V(x))}\, dx = \pi n$, with $n = 50, 51, 52,$ ...., where the numbers should not be taken literally but are meant to represent that the eigenenergy estimate must be done in the semi-classical limit ($n \gg 1$).

As a specific example, consider the flat infinite square well in which $V(x) = 0$, and $p_{class} = \sqrt{2mE}$. The integral is easy to do, and one gets the exact result for the eigenenergies of the infinite square well:

$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$, with n being a positive integer. This is a little too good to be true, but the potential varies on an infinite length scale, so perhaps the WKB approximation can

be justified down to small quantum numbers. This situation is a bit artificial because of the infinite square well boundary conditions.

The case of the harmonic oscillator potential is more challenging. In this case one has a potential $V(x)$ that varies with position. In addition there are classical turning points where the WKB approximation formally breaks down because p_{class} goes to zero there, rendering the WKB $\psi(x)$ undefined. We must deal with this next.

Fixing WKB at the Classical Turning Points

The WKB approximation method is essentially for a "free" particle that is travelling over a slowly-varying "bumpy" potential $V(x)$. The approximate wavefunction is of the form

$$\psi(x) = \frac{D}{\sqrt{p_{class}(x)}} \exp\left[\pm \frac{i}{\hbar} \int^{x} p_{class}(x')dx' \right], \text{ where } p_{class}(x) = \sqrt{2m\left(E - V(x)\right)} \text{ is the}$$

spatially-varying classical momentum of the particle. In an infinite square well potential between $x = 0$ and $x = a$ this gives rise to a quantization condition that allows one to find the eigen-energies in the semi-classical limit:

$$\frac{1}{\hbar} \int_0^a \sqrt{2m\left(E_n - V(x)\right)}\, dx = \pi n \text{ , with } n = 50, 51, 52, ...,$$

where the numbers should not be taken literally, but represent the idea that the approximation works only in the semi-classical limit ($n \gg 1$).

This is fine for infinite square wells, but there is a problem when the potential varies slowly near the classical turning point, such as the harmonic oscillator. At the classical turning points the WKB approximation formally breaks down because p_{class} goes to zero there, rendering the WKB $\psi(x)$ undefined. We sketched a solution to this problem by solving the Schrodinger equation near the classical turning point by linearizing the potential there, and then matching it to the WKB solutions further away from the classical turning point. This led to a slightly revised quantization condition that applies to potentials with "ordinary" classical turning points (like the harmonic oscillator):

$$\int_{x_1}^{x_2} \sqrt{2m\left(E_n - V(x)\right)}\, dx = \pi\hbar\left(n - \frac{1}{2} \right), \text{ with } n = 50, 51, 52, ...,$$

where the integral is taken between the two classical turning points x_1 and x_2.

Applying this to the harmonic oscillator potential with $V(x) = \frac{m\omega^2 x^2}{2}$ with total energy $E = \frac{m\omega^2 A^2}{2}$ (classical amplitude of oscillation A), yields the following quantization condition: $E = \hbar\omega\left(n - \frac{1}{2}\right)$, with $n = 51, 52, 53, ...$ Re-defining n, this can be written in a more familiar form: $E = \hbar\omega\left(n + \frac{1}{2}\right)$, with $n = 50, 51, 52, 53, ...$ Surprisingly, this works all the way down to $n = 0$.

The bottom line is that the eigen-energies of complex 1D potentials can be estimated without solving the Schrodinger equation directly, or solving for the eigenfunctions, at least in the semi-classical limit.