Lecture 38 Highlights

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 certain 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 58 of Griffiths, for example. 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. 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 58 of Griffiths is a good example of a semi-classical wavefunction. It has both quantum and classical character, as we shall see.

The WKB approximation is basically good for two things: 1) estimating eigen-energies in the semi-classical limit for complicated 1D potentials, 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.

The lecture followed the book (Griffiths, pages 315-320) 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 $2\pi/k(x)$ is much smaller than the length scale on which the potential $V(x)$ is changing. With this ansatz (which is exact), 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., $p_{class} = \sqrt{2m\left(E - V(x)\right)}$ 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 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 58 in Griffiths, and not the case for the extreme quantum wavefunctions on the top of page 58.

As an example of computing eigen-energies, consider a 1D infinite square well with an arbitrary potential $V(x)$ on the bottom, going from $x = 0$ to $x = a$. We can solve for the eigen-energies in the semi-classical limit 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 $D_2 = 0$, and since $\sin\left(\frac{1}{\hbar}\int_0^a p_{class}(x')dx'\right) = 0$, we must have $\frac{1}{\hbar}\int_0^a p_{class}(x')dx' = \pi n$, 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. 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: $\frac{1}{\hbar}\int_0^a \sqrt{2m(E_n - V(x))}\,dx = \pi n$.

As a specific example, consider the flat infinite square well in which $p_{class} = \sqrt{2mE}$. 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.