Lec 29: 11/04/2009

WKB Quantization Rule for Bound States:

For potentials that vary slowly and behave smoothly at the classical turning points, we found the following quantization rule for the bound state energy eigenvalues (by using the WKB approximation):

$$\int_{x_1}^{x_2} \sqrt{2m(E_n - V(x))}\, dx = \hbar\pi\left(n+\frac{1}{2}\right) \qquad n=0,1,2,\dots$$

As an example, lets apply this to find (approximate) energy eigenvalues of the simple harmonic oscillator. We denote the energy of n-th level (0-th level being the ground state) as E_n. The turning points are:

$$E_n = \frac{1}{2}m\omega^2 x^2 \Rightarrow x = \pm\sqrt{\frac{2E_n}{m\omega^2}} \qquad \left(x_0 \equiv \sqrt{\frac{2E_n}{m\omega^2}}\right)$$

The quantization rule tell us:

$$\int_{-x_0}^{+x_0} \sqrt{2m\left(E_n - \frac{1}{2}m\omega^2 x^2\right)}\, dx = \hbar\pi\left(n+\frac{1}{2}\right)$$

We need to evaluate the integral:

$$\int_{-x_0}^{+x_0} \sqrt{2m\left(E_n - \frac{1}{2}m\omega^2 x^2\right)}\, dx = \sqrt{2mE_n}\int_{-x_0}^{+x_0} \sqrt{1 - \frac{m\omega^2}{2} x^2}\, dx$$

$$= \int_{-x_0}^{+x_0} \sqrt{2mE_n}\sqrt{1 - \frac{x^2}{x_0^2}}\, dx$$

We make the following change of variable:

$$\frac{x}{x_0} = \sin\theta \Rightarrow dx = x_0 \cos\theta\, d\theta$$

Then,

$$\sqrt{2mE_n}\int_{-x_0}^{+x_0} \sqrt{1 - \frac{x^2}{x_0^2}}\, dx = \sqrt{2mE_n}\int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} x_0 \cos^2\theta\, d\theta =$$

$$\sqrt{2mE_n}\, x_0 \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \frac{1+\cos 2\theta}{2}\, d\theta = \sqrt{2mE_n}\, x_0 \left(\frac{\theta}{2} + \frac{\sin 2\theta}{4}\right)\Bigg|_{-\frac{\pi}{2}}^{+\frac{\pi}{2}}$$

$$= \sqrt{2mE_n}\, x_0 \frac{\pi}{2}$$

This must be equal to $\hbar\pi(n+\frac{1}{2})$, which implies that:

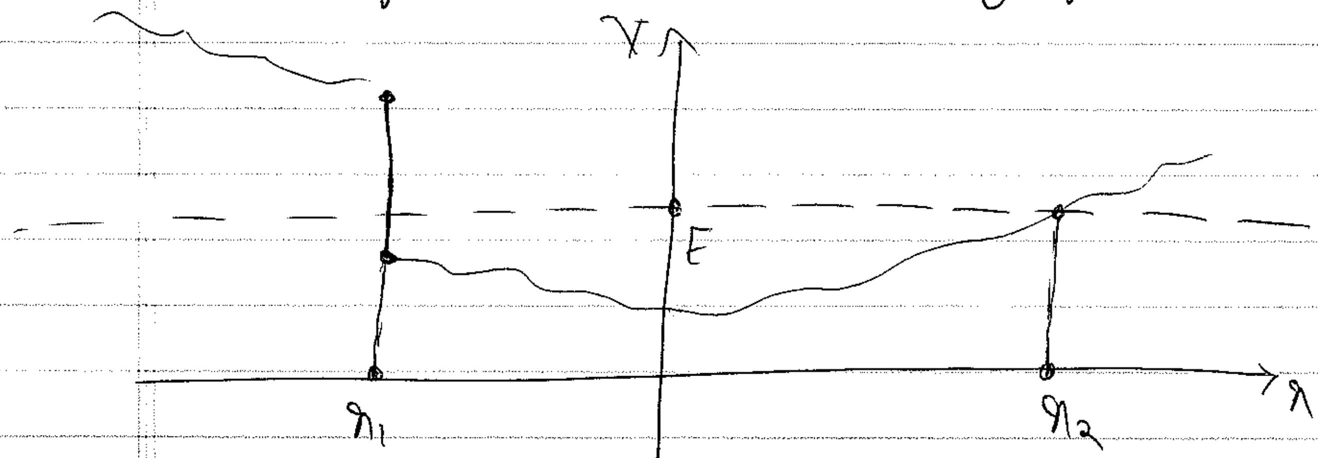
$$\sqrt{2mE_n}\, x_0 \frac{\pi}{2} = \left(n+\frac{1}{2}\right)\hbar\pi \Rightarrow \sqrt{2mE_n}\sqrt{\frac{2E_n}{m\omega^2}}\,\frac{\cancel{\pi}}{2} = \left(n+\frac{1}{2}\right)\hbar\cancel{\pi}$$

$$\Rightarrow \frac{E_n}{\omega} = \left(n+\frac{1}{2}\right)\hbar \Rightarrow \boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega}$$

The WKB approximation actually gives the exact result for the simple harmonic oscillator.

If the potential is not smooth around the turning points, then the quantization rule will not be valid. The question is how it will change.

For example consider the following potential:



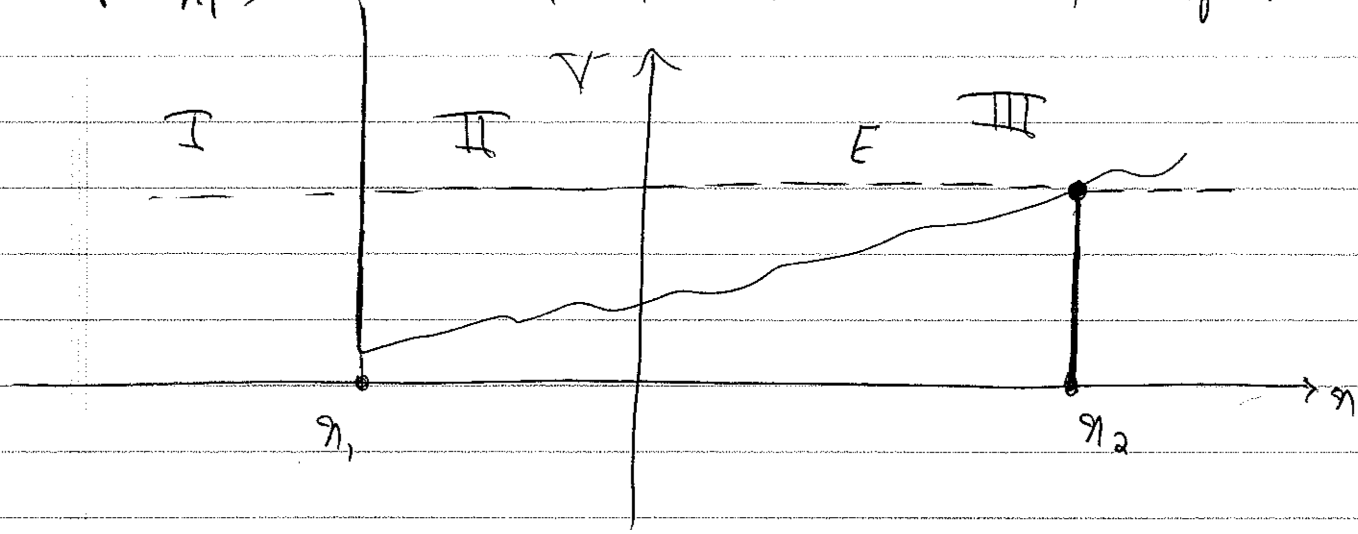
There is a discontinuity in V at one of the turning points x_1. In the region between x_1, x_2 we still have:

$$\psi_{(x)} \simeq \frac{A}{\sqrt{P_{(x)}}} \cos\left[\frac{1}{\hbar}\int_{x_1+\Delta_1}^{x}\sqrt{2m\left(E-V_{(x')}\right)}\,dx' + \theta_1\right] = \quad (\Delta_1 \to 0)$$

$$\frac{A}{\sqrt{P_{(x)}}} \cos\left[\frac{1}{\hbar}\int_{x_2-\Delta_2}^{x}\sqrt{2m\left(E-V_{(x')}\right)}\,dx' + \theta_2\right]$$

The matching of the solutions at $x<x_2$ and $x>x_2$ will yield $\theta_2 = +\frac{\pi}{4}$ (as we saw). However, the matching of the solutions at $x<x_1$ and $x>x_1$ will not result in any useful information on θ_1 because of the sudden change in the potential (do this as an exercise).

Not knowing θ_1, we cannot estimate the energy eigenvalues. However, if there exists an infinite barrier at x_1, the situation will become very simple:



Again, in the region between x_1, x_2 we have,

$$\Psi_{II}(x) \simeq \frac{A}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar} \int_{x_1+a_1\ (a_1\to 0)}^{x} \sqrt{2m(E-V(x'))}\, dx' + \theta_1 \right]$$

In region I we have $\psi = 0$. Continuity of ψ at $x = x_1$ requires that $\psi_{II}(x_1) = 0$. Note that $\int_{x_1}^{x} \sqrt{2m(E - V(x'))}\, dx'$ vanishes when $x = x_1$. Therefore:

$$\psi_{II}(x_1) \propto \cos\theta_1 , \quad \psi_{II}(x_1) = 0 \Rightarrow \boxed{\theta_1 = -\frac{\pi}{2}}$$

In the case that the potential has a smooth behavior at x_1 we have $\theta_1 = -\frac{\pi}{4}$.

Since potential behaves smoothly around the other turning point at x_2, we find (as before) $\theta_2 = \frac{\pi}{4}$.

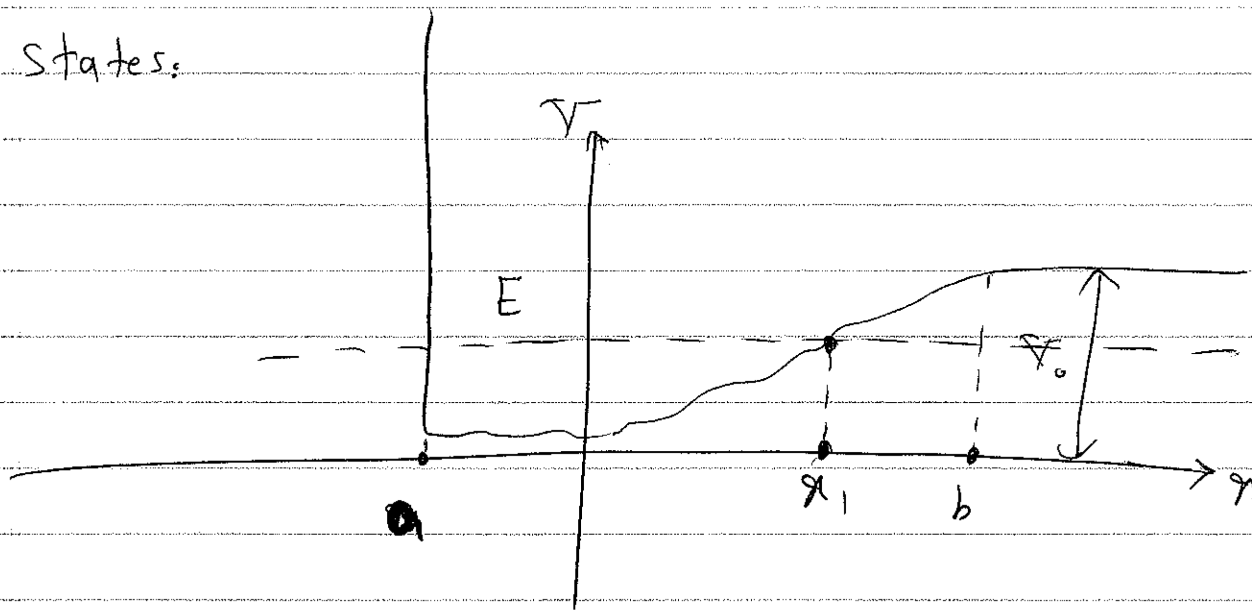
In consequence, the quantization rule when there is one infinite barrier becomes:

$$\boxed{\int_{x_1}^{x_2} \sqrt{2m(E_n - V(x))}\, dx = \left(n + \frac{3}{4}\right)\pi\hbar \qquad n = 0, 1, 2, \ldots}$$

Using the same argument, with two infinite barriers, the quantization rule is ($\theta_1 = -\frac{\pi}{2}$, $\theta_2 = +\frac{\pi}{2}$ in this case):

$$\boxed{\int_{x_1}^{x_2} \sqrt{2m(E_n - V(x))}\, dx = (n+1)\pi\hbar \qquad n = 0, 1, 2, \ldots}$$

Based on this, we can argue why a potential with one infinite barrier (as follows) may have no bound states:



According to the quantization rule:

$$\int_a^{x_1} \sqrt{2m\left(E_n - V_{(x)}\right)}\, dx = \left(n + \frac{3}{4}\right)\pi\hbar$$

The integrand is less than $\sqrt{2mE_n}$ within the limits of integral. Thus:

$$\left(n + \frac{3}{4}\right)\pi\hbar < \int_a^{x_1} \sqrt{2mE_n}\, dx < \sqrt{2mE_n}\,(b-a)$$

For a bound state $E < V_0$. This implies that:

$$\left(n + \frac{3}{4}\right)\pi\hbar < \sqrt{2mV_0}\,(b-a)$$

At least for a ground state to exist ($n=0$), we must have:

$$\frac{3}{4}\pi\hbar < \sqrt{2mV_0}\,(b-a) \Rightarrow 2mV_0(b-a)^2 > \frac{9}{16}\pi^2\hbar^2 \Rightarrow$$

$$\boxed{mV_0(b-a)^2 > \frac{9}{32}\pi^2\hbar^2}$$

If this condition is not satisfied, there will be no ground state, and hence no bound states at all.

The condition is satisfied if m, V_0 or $(b-a)$ are large enough. That is the particle is heavy enough, the well is deep enough, or the well is wide enough.

This is what we expect intuitively.