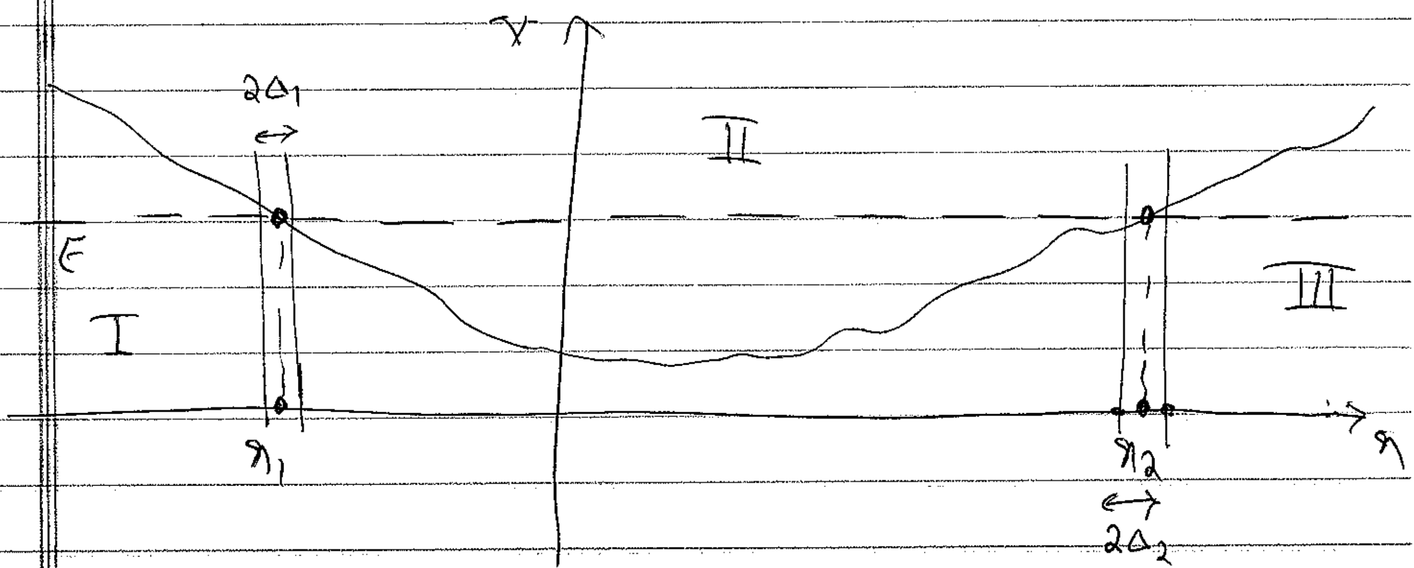
Lec 28: 11/02/2009

WKB Approximation and Bound States:

The WKB approximation can be used to estimate energy eigenvalues of bound states.

Consider the following potential that can (in general) support bound states:



In region II we have $E > V$, while $E < V$ in regions I, III. Note that x_1, x_2 are classical turning points, hence the WKB approximation is not valid.

There are small intervals around these two points that we must use another approximation for ψ, and then match these solutions to those from WKB.

Thus:

$$\psi_{I}(x) = \frac{A_1}{\sqrt{P(x)}} \exp\left[\frac{1}{\hbar}\int_{x_1-\Delta_1}^{x} \sqrt{2m(V(x)-E)}\, dx'\right]$$

$$\psi_{II}(x) = \frac{A_2}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar}\int_{x_1+\Delta_1}^{x} \sqrt{2m(-V(x)+E)}\, dx' + \theta_1\right] =$$

$$\frac{A_2}{\sqrt{P(x)}} \cos\left[\frac{1}{\hbar}\int_{x_2-\Delta_2}^{x} \sqrt{2m(-V(x)+E)}\, dx' + \theta_2\right]$$

$$\psi_{III}(x) = \frac{A_3}{\sqrt{P(x)}} \exp\left[-\frac{1}{\hbar}\int_{x_2+\Delta_2}^{x} \sqrt{2m(V(x)-E)}\, dx'\right]$$

Here the signs of exponentials in ψ_I, ψ_{III} are chosen such that $\psi \to 0$ as $x \to \pm\infty$.

Δ_1, Δ_2 are chosen such that $\left|\frac{d\lambda}{dx}\right| \simeq 1$ at $x_1 \pm \Delta_1$ and $x_2 \pm \Delta_2$ (the condition for slow variation of the potential).

$$\underbrace{\left|\frac{d\lambda}{dx}\right|}_{\lambda = \frac{h}{p}} \simeq 1 \Rightarrow \left|\frac{dp}{dx}\right| \frac{h}{p^2} \simeq 1 \Rightarrow \left|\frac{dp}{dx}\right| \simeq \frac{p^2}{h}$$

Around x_1, x_2 we have:

$$E - V \simeq \alpha_1 (x - x_1) \quad , \quad E - V \simeq \alpha_2 (x - x_2)$$

Therefore:

$$\left|\frac{dp}{dx}\right| \simeq \frac{p^2}{h} \Rightarrow \Delta_1 \simeq \left(\frac{h}{\sqrt{8m\alpha_1}}\right)^{\frac{2}{3}} , \quad \Delta_2 \simeq \left(\frac{h}{\sqrt{8m\alpha_2}}\right)^{2/3}$$

The Schrodinger equation near x_1, x_2 becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \simeq \alpha_1 (x - x_1)\psi \qquad x_1 - \Delta_1 < x < x_1 + \Delta_1$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \simeq \alpha_2 (x - x_2)\psi \qquad x_2 - \Delta_2 < x < x_2 + \Delta_2$$

This can be cast in the form of Airy equation

$\frac{d\psi}{dz^2} = z\psi$, whose solutions are Airy functions.

Without going into detail, we find:

$$\psi(x_1 \pm \Delta_1) \simeq \psi(x_1) \pm \frac{d\psi(x_1)}{dx}\Delta_1$$

$$\psi(x_2 \pm \Delta_2) \simeq \psi(x_2) \pm \frac{d\psi}{dx}(x_2)\Delta_2$$

At a classical turning point $\frac{d^2\psi}{dx^2} = 0$, and so the above

approximation is very good because the next order term is $\propto (x-x_{1,2})^3$ that can be comfortably dropped.

Now we need to ~~do~~ matching. The continuity conditions require that at point $x_1 - a_1$ we have:

$$\psi_I(x_1 - a_1) = \psi(x_1) - \frac{d\psi}{dx}(x_1)\,a_1$$

$$\frac{d\psi_I}{dx}(x_1 - a_1) = \frac{d\psi(x_1)}{dx}$$

This leads to:

$$\frac{A_1}{\sqrt{P(x_1 - a_1)}} = \psi(x_1) - \frac{d\psi}{dx}(x_1)\,a_1 \simeq \psi(x_1) \qquad (1)$$

$$\frac{A_1}{\sqrt{P(x_1 - a_1)}}\,\frac{1}{\hbar}\sqrt{2m\alpha_1 a_1} = \frac{d\psi}{dx}(x_1) \qquad (2)$$

Taking the derivative of the exponential function in ψ_I, we have dropped $\frac{d}{dx}\left(\frac{1}{\sqrt{P(x)}}\right)$ term since it is subdominant in the validity region of the WKB approximation.

Matching at point $x_1 + a_1$ leads to:

$$\frac{A_2 \cos\theta_1}{\sqrt{P(x_1 + a_1)}} \simeq \psi(x_1) \qquad (3)$$

$$\frac{-A_2}{\sqrt{P(x_1 + a_1)}}\,\frac{1}{\hbar}\sqrt{2m\alpha_1 a_1}\,\sin\theta_1 = \frac{d\psi}{dx}(x_1) \qquad (4)$$

Now, dividing the two sides of 2 by the two sides of 1 gives us;

$$\frac{1}{\hbar}\sqrt{2m\alpha_1 \Delta_1} = \frac{\frac{d\psi}{dx}(x_1)}{\psi(x_1)} \qquad *$$

Similarly, dividing the two sides of 4 by the two sides of 3, we find;

$$-\frac{1}{\hbar}\sqrt{2m\alpha_1 \Delta_1}\tan\theta_1 = \frac{\frac{d\psi}{dx}(x_1)}{\psi(x_1)} \qquad **$$

Comparing *, ** we see that;

$$\tan\theta_1 = -1 \Rightarrow \boxed{\theta_1 = -\frac{\pi}{4}}$$

Performing the matching of solutions at $x_2 - \Delta_2$ and $x_2 + \Delta_2$ we find;

$$\frac{1}{\hbar}\sqrt{2m\alpha_2 \Delta_2} = \frac{\frac{d\psi}{dx}(x_2)}{\psi(x_2)} \qquad ***$$

$$\frac{1}{\hbar}\sqrt{2m\alpha_2 \Delta_2}\tan\theta_2 = \frac{\frac{d\psi}{dx}(x_2)}{\psi(x_2)} \qquad ****$$

Note the sign difference between the left hand side of ⋆⋆ and ⋆⋆⋆⋆. This is due to opposite signs of the exponential functions in ψ_I and ψ_{III}. From ⋆⋆⋆ and ⋆⋆⋆⋆ we see that:

$$\tan\theta_2 = +1 \Rightarrow \boxed{\theta_2 = +\frac{\pi}{4}} \quad \left(\text{or } \frac{5\pi}{4}, \frac{9\pi}{4}, \dots\right)$$

From the two equivalent expressions of ψ_{II} we see that:

$$\theta_2 - \theta_1 = \frac{1}{\hbar}\int_{x_1+\Delta_1}^{x_2-\Delta_2} \sqrt{2m(E-V_{(x)})}\, dx \simeq \frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(E-V_{(x)})}\, dx$$

This results in the following quantization law for the energy eigen values of bound states:

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

The integral is taken between the turning points.

Note that the assumption has been that $V_{(x)}$ changes smoothly near the turning points.