Lec 11: 09/18/2009

Particle in a Box:

Next we consider particle in a box:

$$\begin{cases} V(x) = 0 & |x| < \frac{L}{2} \\ V(x) = \infty & |x| \geq \frac{L}{2} \end{cases}$$

The only nontrivial region is inside the box, Due to infinite potential outside we have $\psi(x) = 0$ for $|x| \geq \frac{L}{2}$.

The eigenvalue problem for the Hamiltonian is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx} = E\psi(x) \qquad -\frac{L}{2} < x < +\frac{L}{2}$$

And the boundary condition is $\psi(-\frac{L}{2}) = \psi(+\frac{L}{2}) = 0$.

General solutions are:

$$\psi(x) = A\sin kx + B\cos kx$$

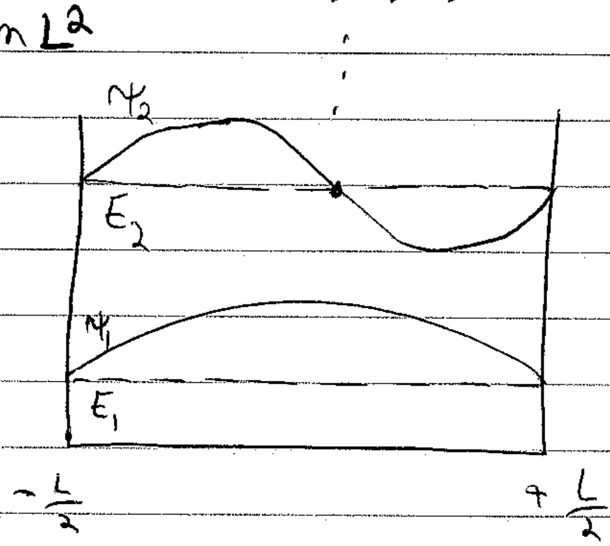
The boundary condition implies that $A=0$ or $B=0$. The solutions are therefore divided into two classes, namely even and odd solutions:

$\psi_n(x) = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) \qquad n = 1, 3, 5, \ldots$ (even solutions)

$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad n = 2, 4, 6, \ldots$ (odd solutions)

The $\sqrt{\frac{2}{L}}$ factor is the normalization factor. The corresponding energy eigenvalues are:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \qquad n = 1, 2, 3, \ldots$$



The evenness or oddness of the eigenstates can be understood from the symmetry under $x \to -x$. For both of these $|\psi(x)|^2$ is an even function as expected.

Some features (that can be generalized) to note:

1- The particle can be found anywhere inside the box, i.e. $|\Psi(x)|^2 \neq 0$ for an infinte number of points. This is in sharp contrast to the calssical mechanics.

2- The minimum energy, i.e. smallest energy eigenvalue, is nonzero. Again, this is against our "classical intuition": the zero-point quantum energy is nonzero.

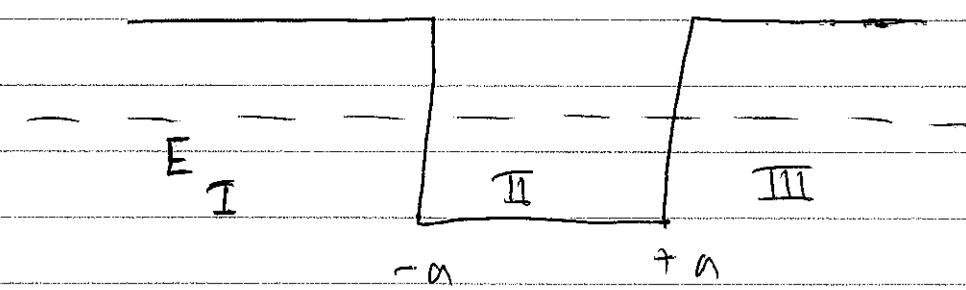
3- The "ground state", state with the lowest energy eigenvalue, has no nodes. That is $\Psi(x)$ does not change sign. This is true in general (can be proved).

4- There is no degeneracy, i.e. only one state for a given energy eigenvalue. This is associated with the fact that there is no continuous symmetry under which H is invariant.

Square Well Potential:

This is similar to the particle in a box, but potential outside is now finite:

$$\begin{cases} V(x) = 0 & |x| < a \\ V(x) = V_0 & |x| \geq a \end{cases}$$



We are interested in eigenstates whose energy $E < V_0$.

This is the first example of having various nontrivial regions. The eigenvalue problem is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = (E - V_0)\,\psi_I$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = E\,\psi_{II}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{III}}{dx^2} = (E - V_0)\,\psi_{III}$$

Again notice the symmetry under $x \to -x$. This implies that the solutions are either even or odd functions. Even solutions are (up to a normalization constant):

$$\begin{cases} \psi_I(x) = e^{+\kappa x} & (e^{-\kappa x} \text{ not acceptable}) \\ \psi_{II}(x) = A\cos kx & \\ \psi_{III}(x) = e^{-\kappa x} & (e^{+\kappa x} \text{ not acceptable}) \end{cases}$$

Similarly, the odd solutions are (up to a normalization constant):

$$\begin{cases} \psi_I(x) = e^{+\kappa x} & (e^{-\kappa x} \text{ not acceptable}) \\ \psi_{II}(x) = A\sin kx & \\ \psi_{III}(x) = -e^{-\kappa x} & (e^{+\kappa x} \text{ not acceptable}) \end{cases}$$

In both cases:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Note that $k^2 + \kappa^2 = \dfrac{2mV_0}{\hbar^2}$.

Since the potential is finite everywhere, then

$\psi_{(x)}$ and $\frac{d\psi_{(x)}}{dx}$ must be continuous. Thus:

$$\psi_{I}(-a) = \psi_{II}(-a) \qquad \frac{d\psi_{I}}{dx}(-a) = \frac{d\psi_{II}(-a)}{dx}$$

$$\psi_{II}(+a) = \psi_{III}(+a) \qquad \frac{d\psi_{II}(+a)}{dx} = \frac{d\psi_{III}(+a)}{dx}$$

For even slou tions these result in:

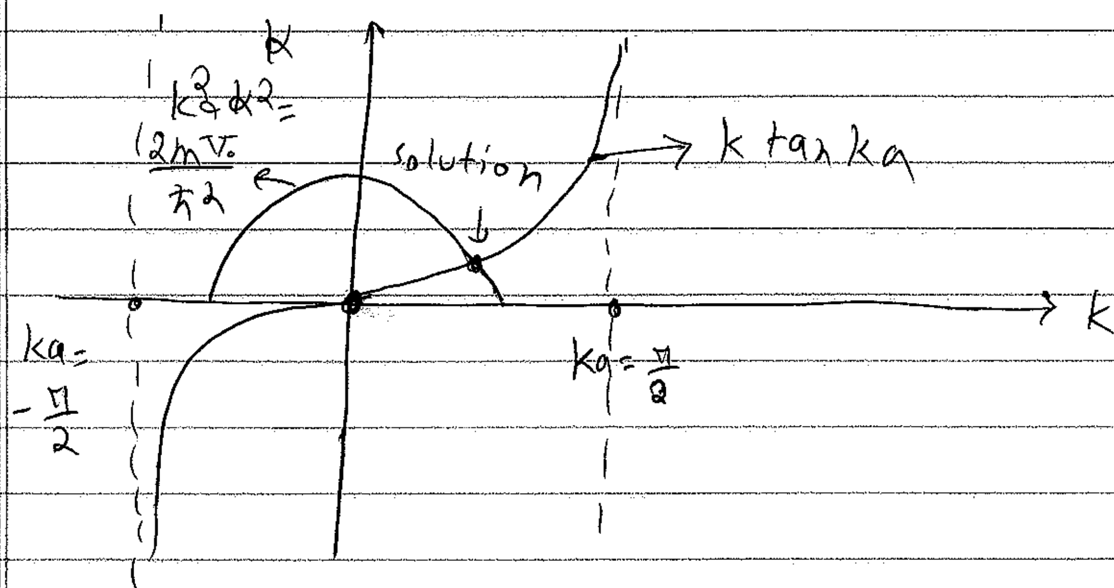
$k \tan ka = +\kappa$

And for odd solutions:

$k \cot ka = -\kappa$

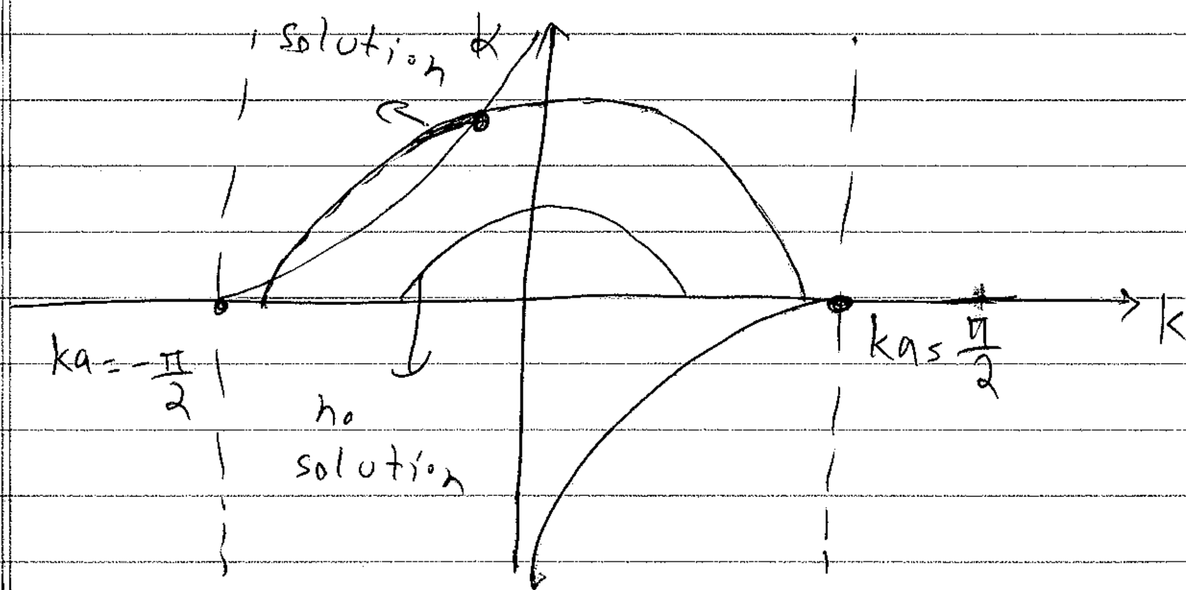
Lets consider the even solutions first. In the

k-κ plane we have:



The intersection of the circle and $ka \tan ka$ curve will be a solution to the eigenvalue problem. Note that there is alway at least one even solution, no matter how small V_0 is.

For the odd solutions we have:



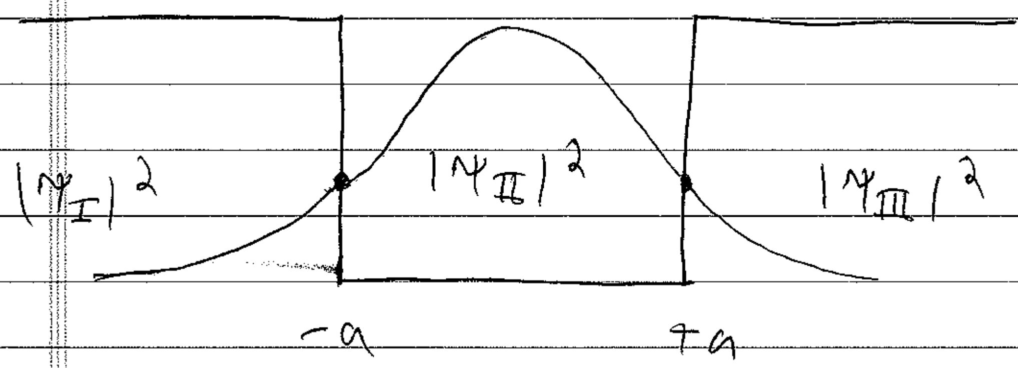
There may be no odd solutions. If V_0 is too small, we will not find an intersection between the circle and $-k \cot ka$ curve.

The important points are:

1- The square well always have a

ground state.

2- The probability to find the particle in regions I, III is not zero:



This is completely different from classical mechanics. For $E < V_0$ the particle can penetrate into regions I, III in quantum mechanics.