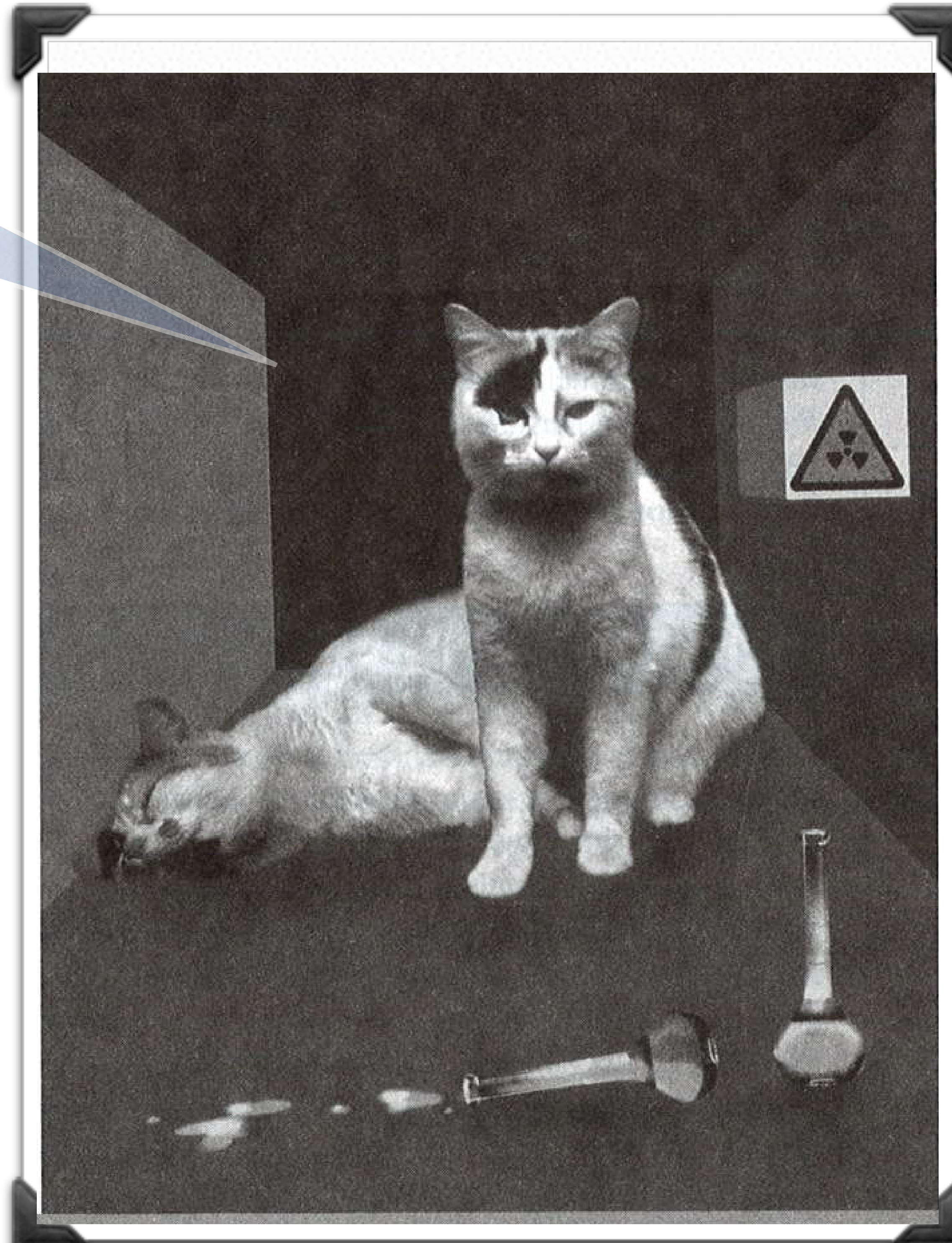
Welcome back to PHY 3305

Today's Lecture:

More Schrodinger Equation: Particle in a Finite Well



Schrödinger's Cat
Alive or Dead?

Last Lecture:

Time-Independent SWE

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

Bound State: Particle in an Infinite Well

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L}) & (0 < x < L) \\ 0 & x < 0; \;\; x > L \end{cases}$$

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Bound States II: Particle in a Finite Well

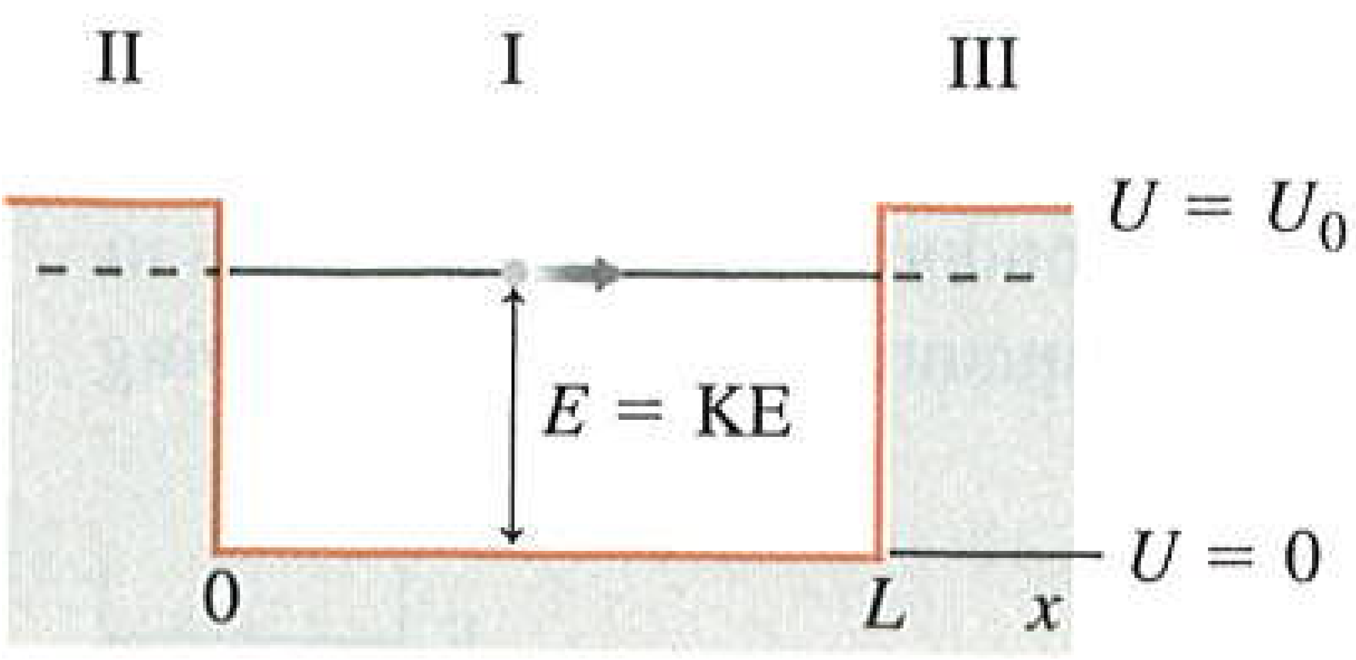
Now we need to write the SWE in 3 different regions.

Regions II and III:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U_0\psi(x)=E\psi(x)$$

Regions I:

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



Regions II and III:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U_0\psi(x) = E\psi(x)$$

Step 1: Rewrite

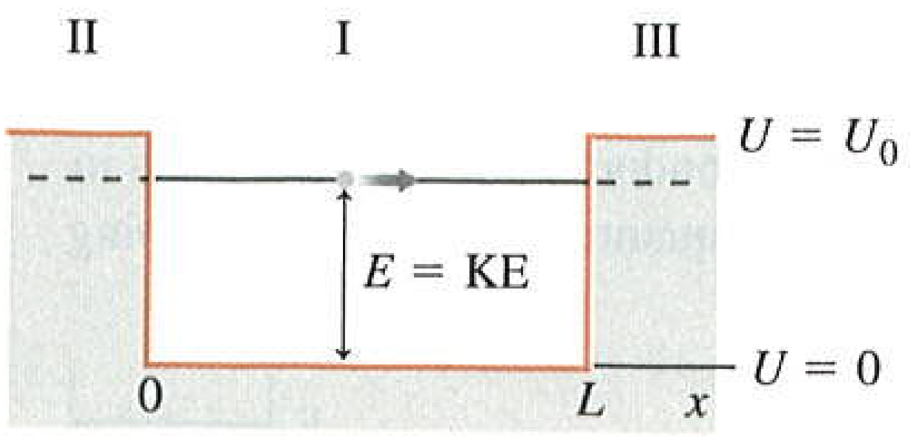
$$\frac{d^2\psi(x)}{dx^2} = \frac{2m(U_0 - E)}{\hbar^2}\psi(x)$$

Step 2: Guess a solution

$$\psi(x) = Ce^{\alpha x} + De^{-\alpha x}$$

where

$$\alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$



Step 3: Apply continuity conditions to Region II & III.

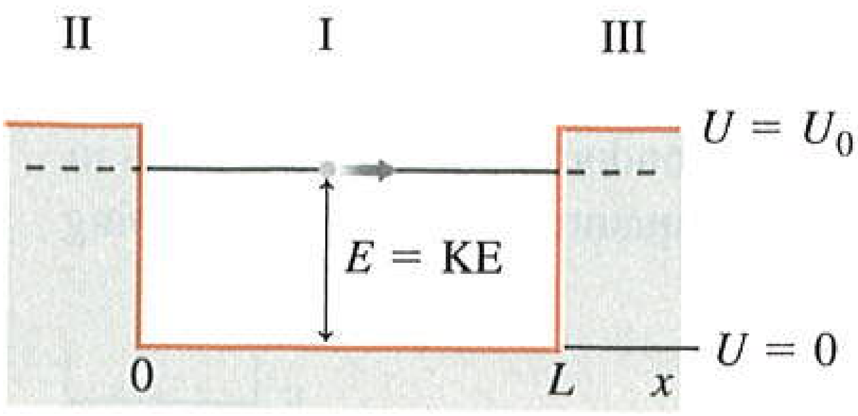
$$\psi(x)_{II} = Ce^{\alpha x} + De^{-\alpha x}$$

$$\psi(x)_{III} = Fe^{\alpha x} + Ge^{-\alpha x}$$

Problem: $e^{-\alpha x}$ diverges as x -> negative infinity. Similarly, $e^{\alpha x}$ diverges as x -> positive infinity.

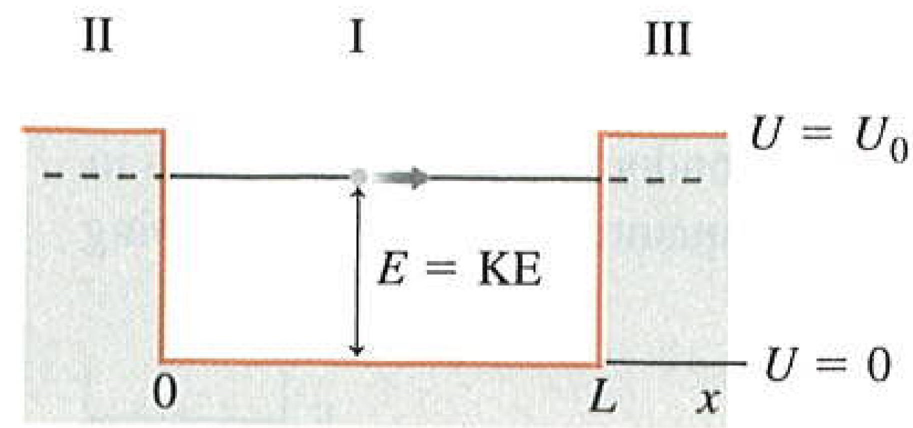
$$\psi(x)_{II} = Ce^{\alpha x}$$

$$\psi(x)_{III} = Ge^{-\alpha x}$$



Region I:

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



We found the general solution to be

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

This time we can not toss the cosine term as the solution does not need to be 0 at x = 0.

How do we solve for A, B, C and G?

Apply smoothness (continuity) condition.

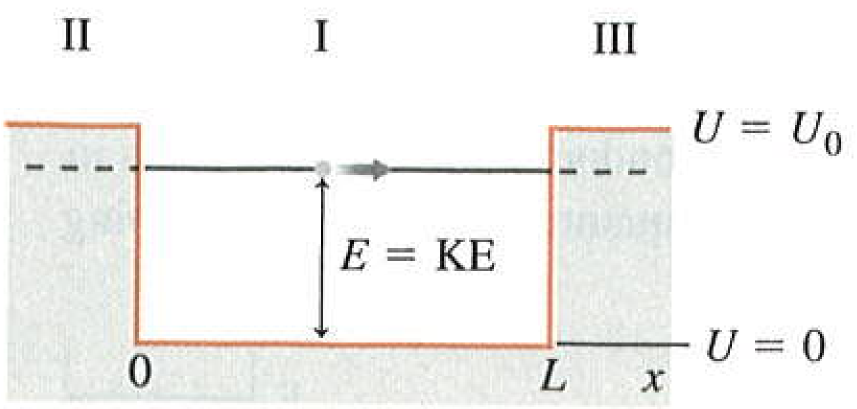
Apply Continuity

$$\psi(x=0)_{II} = \psi(x=0)_{I}$$

$$\psi(x=L_I) = \psi(x=L)_{III}$$

$$\frac{d\psi(x)_{II}}{dx}|(x=0) = \frac{d\psi(x)_{I}}{dx}|(x=0)$$

$$\frac{d\psi(x)_{I}}{dx}|(x=L) = \frac{d\psi(x)_{III}}{dx}|(x=L)$$



$$\psi(x=0)_{II} = \psi(x=0)_I$$

evaluate at x = 0
$$\begin{cases} \psi(x)_{II} = Ce^{\alpha x} \;\; = C \\ \psi(x)_I = A\sin(kx) + B\cos(kx) \;\; = B \end{cases}$$

$$\boxed{C = B}$$

$$\frac{d\psi(x)_{II}}{dx}|(x=0) = \frac{d\psi(x)_I}{dx}|(x=0)$$

evaluate at x = 0
$$\begin{cases} \psi(x)_{II} = \alpha Ce^{\alpha x} \;\; = \alpha C \\ \psi(x)_I = kA\cos(kx) - kB\sin(kx) \;\; = kA \end{cases}$$

$$\boxed{\alpha C = kA}$$

$$\psi(x = L_I) = \psi(x = L)_{III}$$

evaluate at x = L

$$\left\{\begin{aligned} \psi(x)_I &= A\sin(kx) + B\cos(kx) \\ &= A\sin(kL) + B\cos(kL) \\ \psi(x)_{III} &= Ge^{-\alpha x} \quad = Ge^{-\alpha L} \end{aligned}\right.$$

$$\boxed{A\sin(kL) + B\cos(kL) = Ge^{-\alpha L}}$$

$$\frac{d\psi(x)_I}{dx}|(x = L) = \frac{d\psi(x)_{III}}{dx}|(x = L)$$

evaluate at x = L

$$\left\{\begin{aligned} \psi(x)_I &= kA\cos(kx) - kB\sin(kx) \\ &= kA\cos(kL) - kB\sin(kL) \\ \psi(x)_{III} &= -\alpha Ge^{-\alpha x} \quad = -\alpha Ge^{-\alpha L} \end{aligned}\right.$$

$$\boxed{kA\cos(kL) - kB\sin(kL) = -\alpha Ge^{-\alpha L}}$$

$$\left.\begin{aligned} C &= B \\ \alpha C &= kA \\ A\sin(kL) + B\cos(kL) &= Ge^{-\alpha L} \\ kA\cos(kL) - kB\sin(kL) &= -\alpha G e^{-\alpha L} \end{aligned}\right\}$$

These equations impose a quantization condition on the solution.

The solution to these equations is:

$$2\cot(kL) = \frac{k}{\alpha} - \frac{\alpha}{k}$$

Details of the solution to these 4 equations are on page 162 of your textbook. You should work through them!

Let's examine this solution:

$$\boxed{2\cot(kL) = \frac{k}{\alpha} - \frac{\alpha}{k}}$$

This is a transcendental equation - it can not be solved using paper and pencil.

What does k equal?

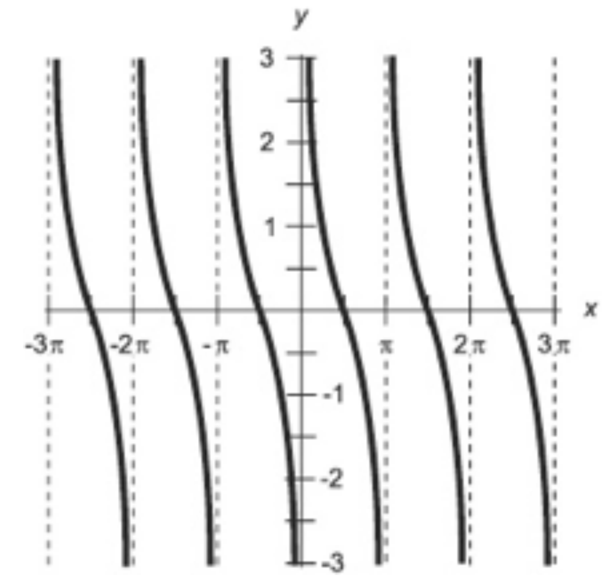
$$k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

What does α equal?

$$\alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

So, k and α depend on E and U_0. Thus for a given well depth, U_0, our equation hold for discrete values of E.

$$2\cot(kL) = \frac{k}{\alpha} - \frac{\alpha}{k} \qquad k \equiv \sqrt{\frac{2mE}{\hbar^2}} \qquad \alpha = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$



Limiting Case: U_0 -> infinity:

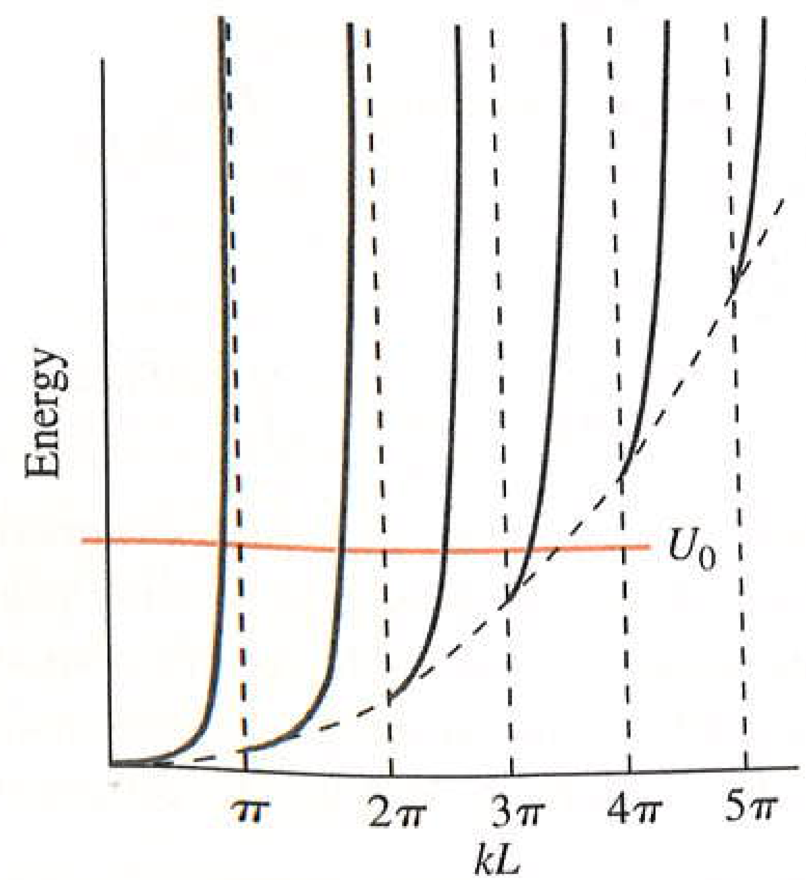
α -> infinity.

$$\cot(kL) = -\infty$$

$$kL = n\pi$$

This is the same as the infinite square well!

Graph this quantization -
A little math
(substitute k and α)
puts the transcendental
eqn ito energy (U_0).



WEIRD SCIENCE?

There exists some probability of finding the particle in the classically forbidden region in a finite square well.

In this region, E_{tot} is less than U_0. This implies that there is negative KE. Classically this is not allowed.

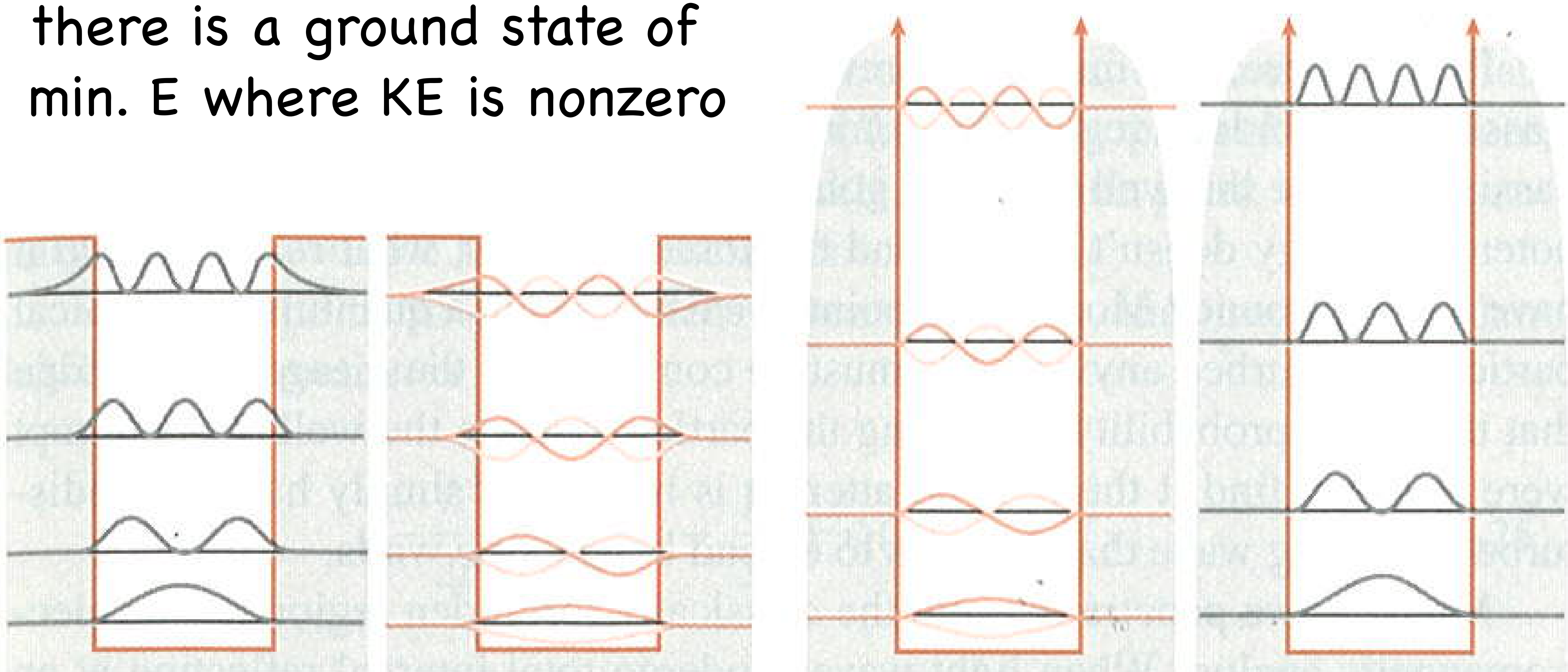
The measure of how far $\psi(x)$ extends into the forbidden region is given by α.

$$\boxed{\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U_0 - E)}}}$$

STOP AND THINK

same

energy is quantized
there is a ground state of
min. E where KE is nonzero



$|\psi(x)|^2$ Finite well $\psi(x)$ $\psi(x)$ Infinite well $|\psi(x)|^2$

different

Finite well - waves penetrate into forbidden region
energy levels are closer together

Can you see particles in the forbidden region?

- You need to conduct an experiment whose spacial precision is better than or comparable to δ (δ = Δx).
- The uncertainty principle gives the momentum uncertainty as

$$\Delta p \geq \frac{\hbar}{2\delta} \sim \frac{\hbar}{\delta}$$

- The kinetic energy would then be

$$KE = \frac{p^2}{2m} \geq \frac{\hbar^2}{2m\delta^2} = U_0 - E$$

Remember - this is negative kinetic energy.

- No experiment can be certain that the particle has negative KE, which is what is required to be certain the particle has entered the forbidden region.

What We Can Say

- The particle is a standing wave whose physical extend penetrates into the classically forbidden region until we make the observation of the particle.

- Once we make the observation, there is a finite probability of finding it outside the box.

THE END
(FOR TODAY)