Brief summary of what we have learned about wavefunctions so far.

- They don't physically exist - and thus they can take positive, negative or imaginary values. What matters physically is the probability density $P(x,t) = |\Psi(x,t)|^2 \geq 0$
- If $P(x) = 0$ there is no chance to detect a particle in that location
- The probability to find a particle b/w points $a<x<b$ is $P_{ab} = \int_a^b |\Psi(x)|^2 dx$
- If particle can only be found b/w $a<x<b$, then $\int_a^b |\Psi(x)|^2 dx = 1$ Normalization conditions
- For any potential energy $U(x)$ the time-dependent wave-function is described by the Shrodinger equation

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t)$$

To find state with distinct values of ~~each~~ total energy E_n (which happen to be stationary states in which $P_n(x) = |\Psi_n(x,t)|^2$ does not depend on time), we solve time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n(x)}{\partial x^2} + U(x)\psi_n(x) = E_n \psi_n(x)$$

$$\Psi_n(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$$

If the motion of particle is restricted in a potential well, the spectrum of the stationary states is descreate (we can label states $n = 1, 2, 3 \ldots$)

For any other state we can find its time evolution by decomposing it into the combitation of eigenstate $\psi_n(x)$ at $t=0$, and then using known ~~deco~~ time evolution of these states.

I.e., if $\psi(x,t=0) = c_1\psi_1(x) + c_2\psi_2(x)$

then $\psi(x,t) = c_1\psi_1(x,t) + c_2\psi_2(x,t) = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-\frac{iE_2t}{\hbar}}$

However, if the energy of the particle in this state is measured, one can obtain ~~to~~ different outcomes: E_1 with the probability $|c_1|^2$

E_2 —— " —— $|c_2|^2$

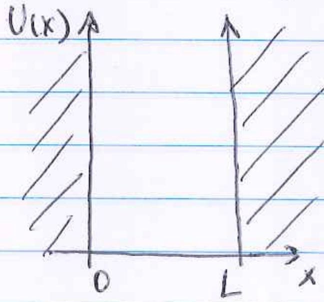
so only average value can be found ~~$\langle E\rangle$~~

$\langle E\rangle = |c_1|^2 E_1 + |c_2|^2 E_2$

Also, the probability density is not ~~set~~ time-independent any more

$$P(x,t) = |c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar}|^2$$

One example we considered: infinite potential well



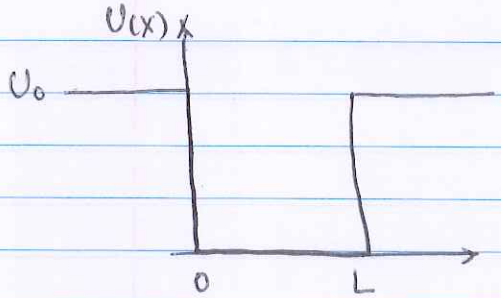
$$U(x) = \begin{cases} 0 & 0<x<L \\ \infty & x<0,\ x>L \end{cases}$$

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

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi n x}{L}$$

$$\psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\frac{\pi n x}{L}\, e^{-i\frac{\hbar\pi^2 n^2}{2mL^2}t}$$

Finite potential well



$$U(x) = \begin{cases} 0 & 0<x<L \\ U_0 & x<0 \quad x>L \end{cases}$$

~~Classical parti~~

For now we consider only cases with $E<U_0$. (bound states)

Classical particle: since $E = U_0 + K$ and K must be >0, then particle can only be b/w $0<x<L$, but does not have enough energy to penetrate the walls.

$0<x<L$ – classically allowed region $(E>U(x))$

$x<0$ and $x>L$ – classically forbidden region $(E<U(x))$

A quantum particle can be found in both regions (although ~~As~~ the probability density to find it in the classically forbidden region is usually small).

Schrodinger eqn for the classically allowed region (same as for the infinite well)

$U=0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} + \overbrace{\frac{2mE}{\hbar^2}}^{k^2}\psi = 0$$

General form of the solution:

$$\psi_{CAR} = A\cos kx + B\sin kx$$

Schrodinger eqn for the classically forbidden region

$U = U_0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U_0\psi = E\psi \qquad \frac{d^2\psi}{dx^2} - \overbrace{\frac{2m(U_0-E)}{\hbar^2}}^{\alpha^2}\psi = 0$$

General solution

$$\psi_{CFR} = Ce^{-\alpha x} + De^{\alpha x}$$

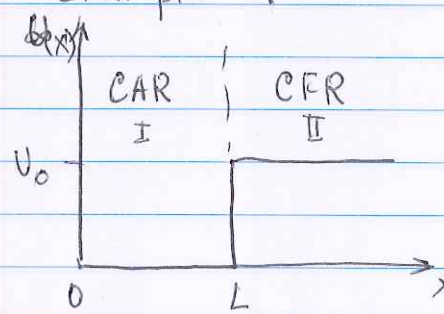
The Parameters we don't know:
coefficient A, B, C, D
energy E

How we find them:
- normalization $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$

- boundary conditions
  1. A wavefunction is always continuous
  2. A wave function is smooth (i.e. its derivative is continuous) unless $U(x) = \infty$

To use the boundary conditions, we need to know a specific potential

Example 1:



$$U(x) = \begin{cases} \infty & x<0 \\ 0 & 0<x<L \\ U_0 & x>L \end{cases}$$

$\psi(x) = 0$ for $x<0$ (impossible region)

CAR: $0<x<L$ $\quad \psi_I = A\cos kx + B\sin kx \qquad k = \sqrt{2mE/\hbar^2}$

CFR: $x>L$ $\quad \psi_{II} = \cancel{Ce^{+\alpha x}} + De^{-\alpha x} \qquad \alpha = \sqrt{2m(U_0-E)/\hbar^2}$

blows out!

Boundaries:

$x=0$

1. cont: $\psi_I(x=0) = 0$
   $A = 0$

$x = L$

1. cont $\psi_I(L) = \psi_2(L)$: $B\sin kL = De^{-\alpha L}$
2. smooth $\psi_I'(L) = \psi_2'(L)$: $kB\cos kL = -\alpha De^{-\alpha L}$

Once you've applied all boundary conditions, you can hire a math major to solve them for you!

$$De^{-\alpha L} = B\sin kL$$
$$-\alpha(\cancel{B}\sin kL) = \cancel{B}k\cos kL$$

(B can be found from normalization conditions)

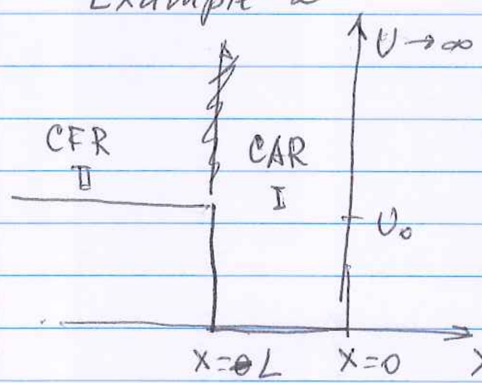
$$\tan kL = -k/\alpha \quad \leftarrow \text{depends only on } E$$

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

$$\tan\left(\sqrt{\frac{2mE}{\hbar^2}}\,L\right) = -\sqrt{\frac{E}{U_0-E}}$$

Transidental equation, can only be solved numerically

Example 2



Same potential, but $x \to -\infty$

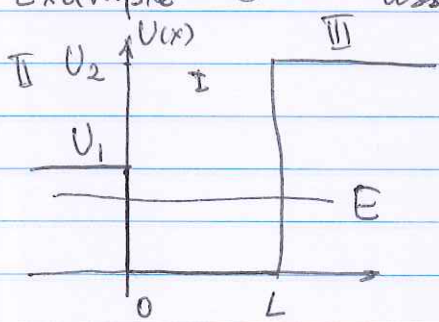
$$U(x) = \begin{cases} \infty & x>0 \\ 0 & -L<x<0 \\ U_0 & x<-L \end{cases}$$

$$\psi_I(x) = B\sin kx \qquad k=\sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_{II}(x) = Ce^{\alpha x} \qquad \alpha=\sqrt{\frac{2m(U_0-E)}{\hbar^2}}$$

since $x<0$ $e^{-\alpha x}$ blows out!

Example 3 assymmetric well



$$U(x) = \begin{cases} U_1 & x<0 \\ 0 & 0<x<L \\ U_2 & x>L \end{cases}$$

$E<U_1$ (bound motion)

Three regions: $x<0$, $x>L$ classically forbidden
$0<x<L$ classically allowed

$$\psi_{I}(x) = A\cos kx + B\sin kx \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\psi_{II}(x) = Ce^{+\alpha_1 x} + \cancel{De^{-\alpha_1 x}} \qquad \alpha_1 = \sqrt{\frac{2m(U_1-E)}{\hbar^2}}$$

blows out

$$\psi_{III}(x) = \cancel{Ee^{\alpha_2 x}} + Fe^{-\alpha_2 x} \qquad \alpha_2 = \sqrt{\frac{2m(U_2-E)}{\hbar^2}}$$

blows out

Boundary conditions

$x=0$

① cont $\quad C = A \quad \psi_{II}(0) = \psi_{I}(0)$

② smooth $\quad \psi_{II}'(0) = \psi_{I}'(0) \quad \alpha_1 C = kB$

$x = L$

① cont $\quad \psi_1(L) = \psi_{III}(L) \Rightarrow A\cos kL + B\sin kL = Fe^{-\alpha_2 L}$

② smooth $\quad \psi_{I}'(L) = \psi_{III}'(L) \Rightarrow -kA\sin kL + kB\cos kL = -\alpha_2 Fe^{-\alpha_2 L}$

then ... lets the math begin