Potential wells, potential walls ...

Free-moving particle of constant energy E
=> constant momentum p : $E = p^2/2m$
=> eigenstates of $\hat{p}_x$

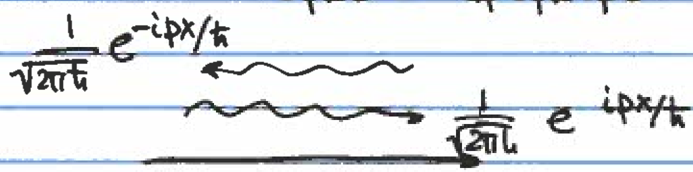
wavefunction $\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ip\cdot x/\hbar}$

$$\hat{p}_x|p\rangle = -i\hbar \frac{\partial}{\partial x}\left[\frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}\right] =$$

$$= (-i\hbar)\left(\frac{ip}{\hbar}\right)\left[\frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}\right] = p\cdot|p\rangle$$

The ~~max~~ $\langle \hat{p}_x\rangle = \langle p|\hat{p}_x|p\rangle = p > 0$ momentum is in $+x$-direction, the particle is moving along the x-axis

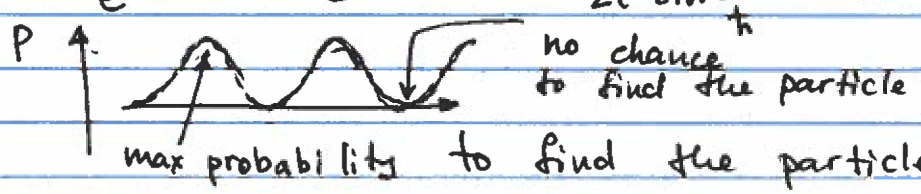
Correspondingly $\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\, e^{-ipx/\hbar}$ describes the particle moving against the x-axis
$\langle p_x\rangle = \langle p|\hat{p}_x|p\rangle = -p < 0$



Standing wave : the sum of the two waves moving in the opposite directions

$$e^{ipx/\hbar} + e^{-ipx/\hbar} = 2\cos\frac{px}{\hbar}$$
or
$$e^{ipx/\hbar} - e^{-ipx/\hbar} = 2i\sin\frac{px}{\hbar}$$

depends on how the two waves ar combined



Of course, we can find the same solution in x-representation using the Schrodinger equation

$$\hat{H}\psi(x) = E\psi(x) \qquad \hat{H} = \frac{\hat{p}^2}{2m} = \frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2$$

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

$$\frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \qquad k^2 = \frac{2mE}{\hbar^2}$$

General form of the solution

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

$\psi(0) = 0 \Rightarrow A = 0$

$\psi(L) = 0 \Rightarrow B\sin kL = 0 \qquad kL = \pi \cdot n$

$$E_n = \frac{\pi^2 n^2 \hbar^2}{2mL^2} \qquad \sqrt{\frac{2mE_n}{\hbar^2}} = \frac{\pi n}{L}$$

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

Any other state of a particle inside the well can be decomposed in the basis of $\{\psi_n(x,t)\}$

$$\langle x|\psi\rangle = \psi(x) = c_1\psi_1(x) + c_2\psi_2(x) + \ldots$$
$$= c_1\sin\frac{\pi x}{L} + c_2\sin\frac{2\pi x}{L} + \ldots$$

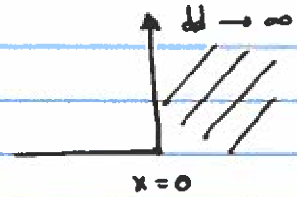
Mathematically, this is Fourier series

Time evolution

$$\psi(x,t) = c_1\sin\frac{\pi x}{L}e^{-iE_1t/\hbar} + c_2\sin\frac{2\pi x}{L}e^{-iE_2t/\hbar} + \ldots$$

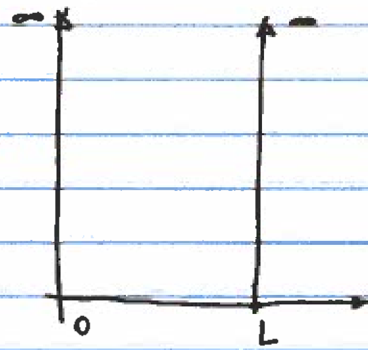
$$c_i = \langle\psi_i|\psi\rangle = \int_{-\infty}^{+\infty}\langle\psi_i|x\rangle\langle x|\psi\rangle\,dx = \int_{-\infty}^{+\infty}\psi_i^*(x)\,\psi(x)\,dx$$

Infinite square well



a particle of finite energy cannot exist for $x>0$

→ equivalent to a perfect mirror !

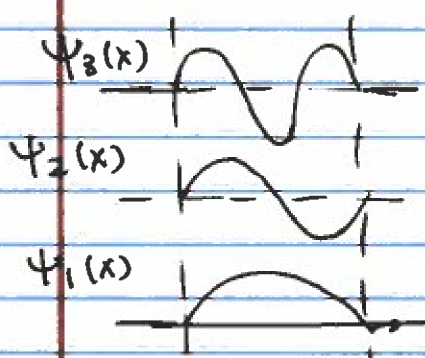


Infinite square well

→ light bouncing b/w two perfect mirrors

→ standing waves !

Since the probability to find a particle at the wall's locations must be zero, only certain wavelength values are possible



$$3\lambda/2 = L$$

$$2\lambda/2 = L \qquad \frac{2\pi\hbar}{p_2} = L,\ p_2 = \frac{2\pi\hbar}{L},\ E_2 = \frac{4\pi^2\hbar^2}{2mL^2}$$

$$\lambda/2 = L \qquad \frac{1}{2}\,\frac{2\pi\hbar}{p_1} = L \Rightarrow p_1 = \frac{\cancel{2}\pi\hbar}{L}\quad E_1 = \frac{\pi^2\hbar^2}{2mL^2}$$

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

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

These are stationary states

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

Constant potential $\cancel{E = \frac{p^2}{2m} + U}$

$\vec{p}_0$

$$\psi(x) = e^{ipx/\hbar} \qquad p_0 = \sqrt{2mE}$$

$\xrightarrow[x]{}$ $U=0$

$$\lambda_0 = \frac{2\pi\hbar}{p_0} = \frac{2\pi\hbar}{\sqrt{2mE}}$$

Now we change the potential energy, same E

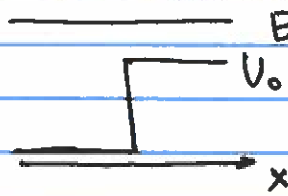
$$E = \frac{p^2}{2m} + U_0 \implies p = \sqrt{2m(E-U_0)}$$

$$\lambda = \frac{2\pi\hbar}{p} = \frac{2\pi\hbar}{\sqrt{2m(E-U_0)}}$$

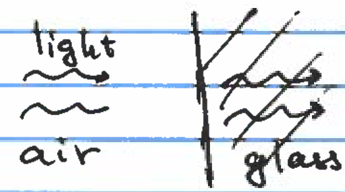
$U_0 > 0$ $\quad p < p_0$ (particle moves slower)
wavelengh increases

$U_0 < 0$ $\quad p > p_0$ (particle moves faster)
wavelengh decreases

This is similar to light propagating in materials with different refractive index!



$\Longleftrightarrow$

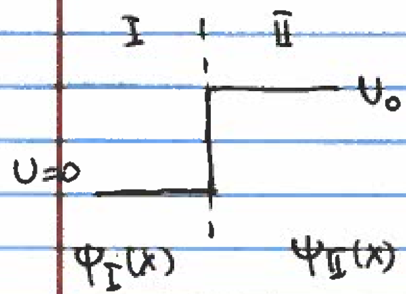


when light hits the boundary (a potential step), the light can

- reflect (wave moving in opposite direction)

- transmit (wave moving in the next region with different momentum)

Boundary conditions: if there is a finite discontinuity in the potential energy, the wave function stays continuous and smooth



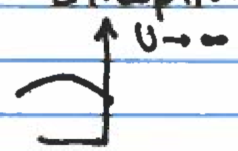
Solution of the Shrodinger equation
in region I : $\psi_I(x)$
in region II : $\psi_2(x)$

On the boundary $\psi_I(a) = \psi_{II}(a)$ (continuous)
$\psi_I'(a) = \psi_{II}'(a)$ (smooth)

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

If $U(x)$ has a finite step, then $\frac{d^2\psi}{dx^2}$ has a step, and $\frac{d\psi(x)}{dx}$ is continuous (no steps)

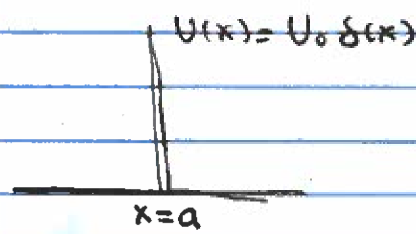
Exception – ~~δ-function~~ infinite step



$$\psi(x) \sim \begin{cases} \sin kx & x < L \\ 0 & x > L \end{cases}$$

continuous but not smooth

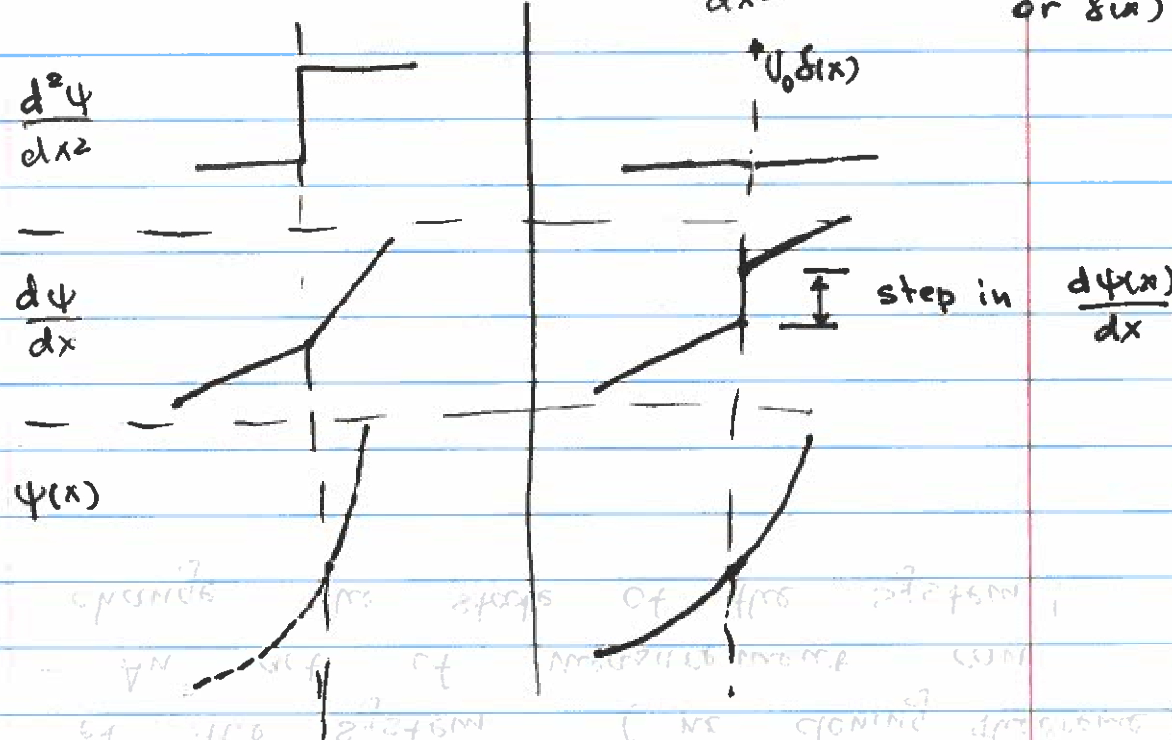
Another example – $\delta(x)$



Anywhere except $x=a$
same $\psi(x)$ solution function
~~But Integrate~~ but $d\psi/dx$
has a break at $x=a$

To illustrate

if $U(x)$ and thus $\frac{d^2\psi(x)}{dx^2}$ has a step or $\delta(x)$



How to calculate this step? Integrate Shrodinger Eqn around discontinuity

$$\lim_{\Delta x \to 0} \int_{-\Delta x}^{+\Delta x} \left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}\right) dx + \int_{-\Delta x}^{+\Delta x} U_0\,\delta(x)\psi\,dx = \int_{-\Delta x}^{\Delta x} E\psi(x)\,dx$$

$$-\frac{\hbar^2}{2m}\left(\left.\frac{d\psi(x)}{dx}\right|_{x=+\Delta x} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\Delta x}\right) + U_0 = 0$$

$$\left.\frac{d\psi(x)}{dx}\right|_{x=0+} - \left.\frac{d\psi(x)}{dx}\right|_{x=0-} = \frac{2mU_0}{\hbar^2}$$