Moving to 2D and 3D world

So far we considered 1D motion

1 spatial coordinate $\hat{x} \leftrightarrow \hat{p}_x$

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

Two-dimentional motion: 2 spatial coordinates

$\hat{x} \rightarrow \hat{p}_x \qquad \hat{p}_x = i\hbar\frac{\partial}{\partial x}$

$\hat{y} \rightarrow \hat{p}_y \qquad \hat{p}_y = i\hbar\frac{\partial}{\partial y}$

} cartesian coordinates

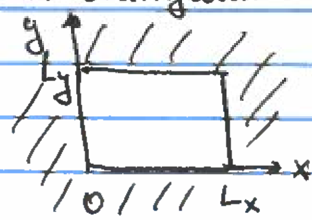
$$\hat{H} = \frac{\hat{p}^2}{2m} + U(\hat{r}) = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2m} + U(\hat{x},\hat{y})$$

Shrodinger equation $\hat{H}\psi(x,y) = E\psi(x,y)$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right] + U(x,y)\psi(x,y) = E\psi$$

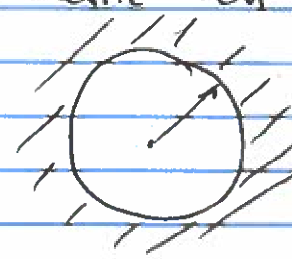
Two common geometries for a 2D potential wells

Ractangular well



Natural to use Cartesian coordinates

Radially / spherically symmetric well



Will use polar (2D) or spherical (3D) coordinates.

Ractangular or square potential well

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

A particle will bounce freely b/w four walls. Note, that the motion along x and y are <u>independent</u> degrees of freedom.
That is why each of these motion is described by an independent wave function

$$\psi(x,y) = \underbrace{X(x)}_{\text{a wave function for x-motion}} \cdot \underbrace{Y(y)}_{\text{a wave function for y-motion}}$$

Each of these wave functions describes the particle behavior in two corresponding potential wells

along x: $U(x) = \begin{cases} 0 & 0<x<L \\ \infty & \text{otherwise} \end{cases}$ $\qquad U(y) = \begin{cases} 0 & 0<y<L \\ \infty & \text{otherwise} \end{cases}$

$$\cancel{-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} + U(x)X(x) = EX(x)}$$

We know solutions for these problems!

$$X_n(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi n x}{L} \qquad Y_s(y) = \sqrt{\frac{2}{L}}\sin\frac{\pi s y}{L}$$

$n = 1, 2 \ldots \qquad s = 1, 2 \ldots$

$\cancel{A/s=1}$

Two dimentional wave function

$$\psi_{ns}(x,y) = \frac{2}{L}\sin\frac{\pi n x}{L}\sin\frac{\pi s y}{L}$$

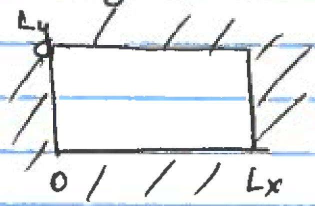
This is the eigenstate of the 2D Shrodinger eq

Corresponding eigenvalue: $\qquad \hat{H}\psi_{ns}(x,y) = E_{ns}\psi_{ns}(x,y)$

$$E_{ns} = \frac{\pi^2\hbar^2}{2mL^2}(n^2+s^2)$$

Aside:

Easy to show that for (ractangular) non-square well



$$\psi_{ns}(x,y) = \frac{2}{\sqrt{L_x L_y}} \sin\frac{\pi n x}{L_x} \sin\frac{\pi n y}{L_y}$$

$$E_{ns} = \frac{\pi^2 \hbar^2}{2m}\left[\frac{n^2}{L_x^2} + \frac{s^2}{L_y^2}\right]$$

Let's get back to a symmetric well

2D $\quad E_{ns} = \frac{\pi^2\hbar^2}{2mL^2}(n^2+s^2)$ $\qquad$ 3D $\quad E_{nsj} = \frac{\pi^2\hbar^2}{2mL^2}(n^2+s^2+j^2)$

Energy spectrum (possible particle energies)

	1D		2D		3D	
Ground state	$n=1$	$E_1 = \frac{\hbar^2\pi^2}{2mL^2}$	$n=1, s=1$	$2E_1$	$n=1, s=1, j=1$	$3E_1$
First excited state	$n=2$	$4E_1$	$n=1\ s=2$ $n=2\ s=1$ twice degenerate	$5E_1$	$n=1, s=1, j=2$ and ↻ 3x degenerate	$6E_1$
Second excited state	$n=3$	$9E_1$				

After the first excited state we have to carefully analize which combination gives lower energy

$s^2 \backslash n^2$	1	4	9	16
1	2	5	10	17
4	5	8	13	20
9	10	13	18	23
16	17	20	23	32

2D square well

(1,1) $E_1 = 2\varepsilon$ (ground) single)

(1,2) $E_2 = 5\varepsilon$ 2x degenerate

(2,2) $E_3 = 8\varepsilon$ singlet

(1,3) $E_4 = 10\varepsilon$ 2-x (doublet)

(2,3) $E_5 = 13\varepsilon$ — " —

(1,4) $E_6 = 17\varepsilon$ — " —

(3,3) $E_7 = 18\varepsilon$ singlet

(2,4) $E_8 = 20\varepsilon$ doublet

Proper mathematical solution of the 2D Schrodinger eqn $\longrightarrow$ separation of variables

Inside the well $\qquad U(x,y)=0$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2}+\frac{\partial^2\psi(x,y)}{\partial y^2}\right)=E\psi(x,y)$$

As we discussed $\quad \psi(x,y)=X(x)\,Y(y)$

$$-\frac{\hbar^2}{2m}\left(Y(y)\frac{d^2X}{dx^2}+X(x)\frac{d^2Y}{dy^2}\right)=E\cdot X\cdot Y$$

$$Y\cdot X''+X\cdot Y''+\frac{2mE}{\hbar^2}XY=0 \qquad \times\frac{1}{XY}$$

$$\underbrace{\frac{X''}{X}}_{\text{depends only on } x}+\underbrace{\frac{Y''}{Y}}_{\text{depends only on } y}+\frac{2mE}{\hbar^2}=0$$

must be true for any x,y inside the well

$\downarrow$ must be constant $\downarrow$

$$C_1=-\cancel{\frac{\hbar^2}{2m}}k_x^2 \qquad C_2=-\cancel{\frac{\hbar^2}{2m}}k_y^2$$

$$\frac{X''}{X}=C_1=\cancel{-\frac{\hbar^2}{2m}}=-k_x^2 \qquad \frac{Y''}{Y}=C_2=\cancel{-\frac{\hbar^2}{2m}}=-k_y^2$$

$$X''+\cancel{\frac{\hbar^2}{2m}}k_x^2X=0 \qquad Y''+k_y^2Y=0$$

general solution:

$$X(x)=A\cos k_xx+B\sin k_xx \qquad Y(y)=\tilde{A}\cos k_yy+\tilde{B}\sin k_yy$$

Accounding for the boundary conditions (wavefunction vanishes at $x,y=0$ & $x,y=L$)

$$X_n(x)=\sqrt{\frac{2}{L}}\sin\frac{\pi nx}{L} \qquad Y_s(y)=\sqrt{\frac{2}{L}}\sin\frac{\pi sy}{L}$$

$$k_{x_n}=\frac{\pi n}{L} \qquad k_{y_s}=\frac{\pi s}{L}$$

Substituting found values of k,s into the Schrodinger equ

$$-k_x^2 - k_y^2 + \frac{2mE}{\hbar^2} = 0 \qquad E = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m}$$

$$E_{n,s} = \frac{\pi^2 \hbar^2}{2mL^2} (n^2 + s^2)$$