Part-3
T.I.S.E. in 2D and 3D

Now, let's take a quick look back…

Schrödinger Equation : $\hat{E}\,\Psi(r,t) = \hat{H}\,\Psi(r,t)$

- in 3D and time: $$i\hbar\,\frac{\partial\Psi(r,t)}{\partial t} = V(r,t)\,\Psi(r,t) - \frac{\hbar^2}{2m}\,\nabla^2\Psi(r,t)$$

- in 1D and time: $$i\hbar\,\frac{\partial\Psi(x,t)}{\partial t} = V(x,t)\,\Psi(x,t) - \frac{\hbar^2}{2m}\,\frac{\partial^2\Psi(x,t)}{\partial x^2}$$

General solution : $\Psi(x,t) = \psi(x)\,\phi(t) = \psi(x)\;e^{-iwt} = \psi(x)\,e^{-iEt/\hbar}$

$\Psi(x,t)$ is called wave function, $\psi(x)$ is called eigen function.

Schrödinger Equation,
- time independent & 1D:
(when V doesnot explicitly depends on time)

$$E\,\psi(x) = V(x)\,\psi(x) - \frac{\hbar^2}{2m}\,\frac{\partial^2\psi(x)}{\partial x^2}$$

$$\Rightarrow \frac{\hbar^2}{2m}\,\frac{d^2\psi(x)}{dx^2} + [E - V(x)]\,\psi(x) = 0$$

S.T.I.E in 2D :

Schrödinger Equation in 3D and time :

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = V(r,t)\,\Psi(r,t) - \frac{\hbar^2}{2m}\,\nabla^2\Psi(r,t)$$

Schrödinger time independent equation (S.T.I.E.) in 3D :

$$E\,\Psi(r,t) = V(r,t)\,\Psi(r,t) - \frac{\hbar^2}{2m}\,\nabla^2\Psi(r,t)$$

$$\Rightarrow\ E\,\psi(r) = V(r)\,\psi(r) - \frac{\hbar^2}{2m}\,\nabla^2\psi(r)$$

Schrödinger time independent equation (S.T.I.E.) in 2D :

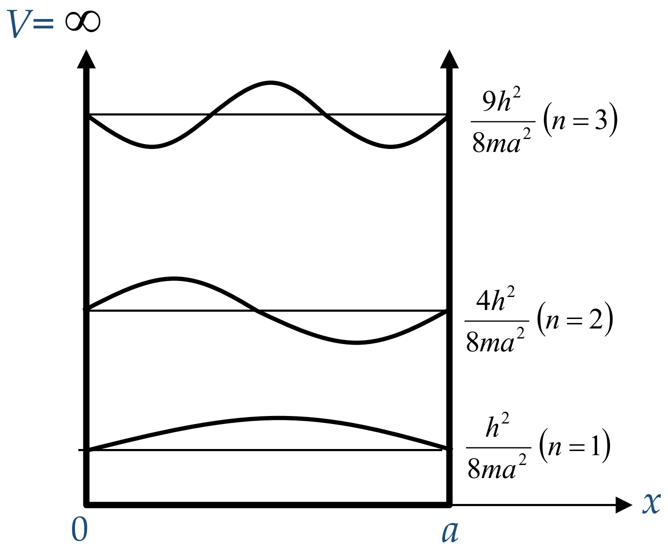
$$E\,\psi(x,y) = V(x,y)\,\psi(x,y) - \frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right]$$

$$\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right] + [E - V(x,y)]\psi(x,y) = 0$$

In 2D, by conservation of energy, $E = V(x,y) + \frac{p_x^2+p_y^2}{2m}$

Same old problem: Particle in a infinite potential well

1D



$$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + [E - V(x)]\,\psi(x) = 0$$

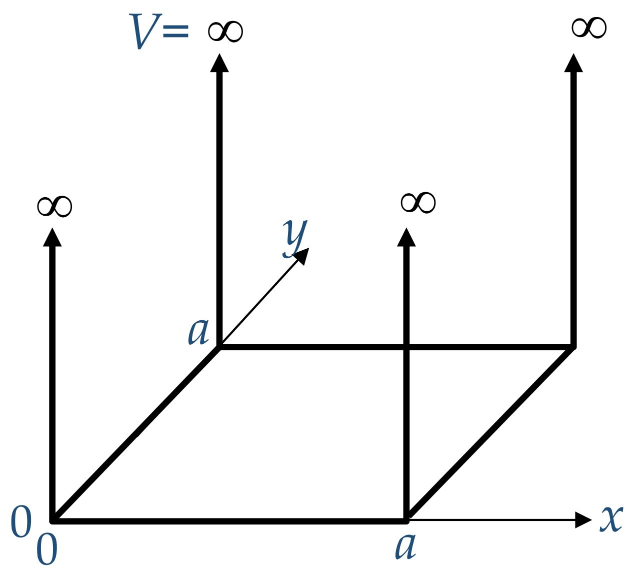
$$\psi(x) = A\sin(kx) + B\cos(kx)\,, \qquad k = \sqrt{2mE}/\hbar$$

Possible solutions are : $\sin(ka) = 0$ or $\cos(ka) = 0$

i.e. $ka = n\,\pi \quad \Rightarrow \quad k = \frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a} \quad \Rightarrow E = \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{n^2h^2}{8ma^2}$

i.e. discrete energy levels, with quantum number 'n'

2D



Aim: *to find out the eigen function and eigen values (energy states) of the particle.*

- **define potential :**

  $V(x,y) = 0$ if $0 < x,y < a$
  $= \infty$ elsewhere

- **write down T.I.S.E :**

$$\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{\partial^2\psi(x,y)}{\partial y^2}\right] + [E - V(x,y)]\,\psi(x,y) = 0$$

- **define general expression for the eigen function :**

  Assuming, x and y are independent variables in $\psi(x,y)$, we can separate out as

  $\psi(x,y) = f(x)g(y)$,

  where $f(x) = A\sin(k_x x) + B\cos(k_x x)$,

  $g(y) = C\sin(k_y y) + D\cos(k_y y)$ where $k^2 = k_x^2 + k_y^2 = 2mE/\hbar^2$

- **apply boundary conditions :**

  Since it is an infinite potential well, there is zero probability of finding the particle outside the box, as we did in the 1D case, $\psi(x,y)$ must vanish outside the well.

  ✓ $\psi(x,y)|_{x=0} = 0 \quad \Rightarrow f(x)g(y)|_{x=0} = 0 \quad \Rightarrow f(x)|_{x=0} = 0 \quad \Rightarrow B = 0$

  ✓ $\psi(x,y)|_{y=0} = 0 \quad \Rightarrow f(x)g(y)|_{y=0} = 0 \quad \Rightarrow g(y)|_{y=0} = 0 \quad \Rightarrow D = 0$

  ✓ $\psi(x,y)|_{x=a} = 0 \quad \Rightarrow f(x)g(y)|_{x=a} = 0 \quad \Rightarrow f(x)|_{x=a} = 0 \quad \Rightarrow \sin(k_x a) = 0$
  $\Rightarrow k_x a = n_x\pi$, where n_x = 1,2,3,….

  ✓ $\psi(x,y)|_{y=a} = 0 \quad \Rightarrow f(x)g(y)|_{y=a} = 0 \quad \Rightarrow g(y)|_{y=a} = 0 \quad \Rightarrow \sin(k_y a) = 0$
  $\Rightarrow k_y a = n_y\pi$, where n_y = 1,2,3,….

- **Some more algebra (normalisation) :**

$$\psi(x,y) = f(x)g(y) = A\sin(k_x x)\; C\sin(k_y y) = A'\;\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)$$

Now, normalising the eigen function over 2D space, we can find the constant A'

$$\iint_{-\infty}^{\infty} |\psi(x,y)|^2 \, dx \, dy = 1$$

$$\Rightarrow \; A'^2 \int_{-\infty}^{\infty} \sin^2\left(\frac{n_x \pi}{a} x\right) dx \int_{-\infty}^{\infty} \sin^2\left(\frac{n_y \pi}{a} y\right) dy = 1$$

$$\Rightarrow \; A'^2 \int_{0}^{a} \sin^2\left(\frac{n_x \pi}{a} x\right) dx \int_{0}^{a} \sin^2\left(\frac{n_y \pi}{a} y\right) dy = 1$$

$$\Rightarrow \; A' = 2/a$$

- **Hence, the eigen function for this particle, trapped in a 2D infinite potential well, is :**

$$\psi(x,y) = \frac{2}{a} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right)$$

- **and, can also find the eigen states…**

$$k^2 = k_x^2 + k_y^2 = \frac{2mE}{\hbar^2}$$

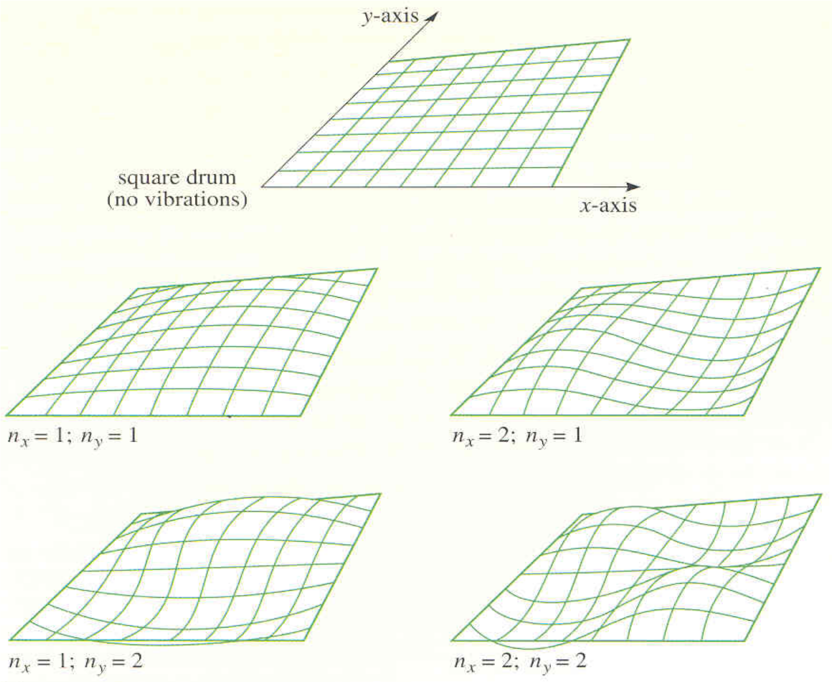
$$\Rightarrow E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right) = \frac{\hbar^2}{2m}\left(\frac{n_x^2 \pi^2}{a^2} + \frac{n_y^2 \pi^2}{a^2}\right)$$

$$\Rightarrow E = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2\right)$$

To compare with 1D case:

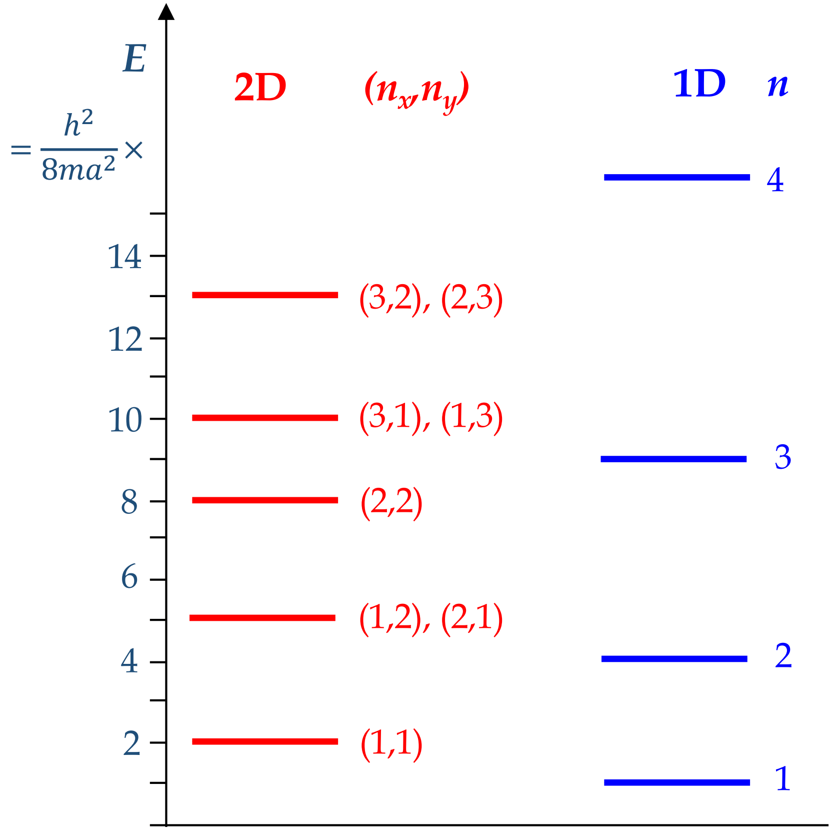
$$E_{(1D)} = \frac{h^2}{8ma^2} n^2$$

- **now, what does it mean?**
  - The energy of the particle is quantised, as in case of the 1D model, but slightly different way.
  - Note that for some of the energy levels in 2D case is associated with two eigenstates.
  - Just because there is only one energy level does not mean the eigenstates are the same (see below)



You can have different modes of vibrations associated to same energy.

i.e. can have completely different behaviour that nonetheless have same total energy.



In physics, the word that characterise this phenomena is called

Degeneracy.

And the eigen functions corresponding to the same eigen value (total energy, E) are called **degenerate states**.

Similar approach for Particle in a 3D potential well !!!

T.I.S.E :

$$\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y,z)}{\partial x^2}+\frac{\partial^2\psi(x,y,z)}{\partial y^2}+\frac{\partial^2\psi(x,y,z)}{\partial z^2}\right]+[E-V(x,y,z)]\,\psi(x,y,z)=0$$

Eigen function :

$$\psi(x,y,z)=f(x)g(y)h(z)=\left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right)$$

Eigen value :

$$E=\frac{h^2}{8ma^2}\left(n_x^2+n_y^2+n_z^2\right)$$

Note, the number of quantum numbers is related to the number of degrees of freedom of the system, **which in turn increases the degeneracy.**

If we have a non-cubical box, i.e. of sides a, b & c, for instance,

Eigen function :

$$\psi(x,y,z)=f(x)g(y)h(z)=\left(\frac{2\sqrt{2}}{\sqrt{abc}}\right)\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{b}y\right)\sin\left(\frac{n_z\pi}{c}z\right)$$

Eigen value :

$$E=\frac{h^2}{8m}\left(\frac{n_x^2}{a^2}+\frac{n_y^2}{b^2}+\frac{n_z^2}{c^2}\right)$$

This is said to lift or raise the degeneracy of the levels (i.e. the degenerate eigenstates now have unique energies). This demonstrates that **degeneracy is strongly related to symmetry.**