Few important properties of Wave function

Orthogonality

For the particle in a rigid box,

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

$$\psi_m = \sqrt{\frac{2}{L}} \sin \frac{m\pi x}{L}$$

It can be seen that $\int_0^L \psi_m(x)^* \psi_n(x)\,dx = 0$

This property is called orthogonality.

If m = n, the integral is 1 (normalization)

Orthonormality

$$\int_0^L \psi_m(x)^* \psi_n(x)\,dx = \delta_{mn}$$

$$i.e., = 1\, if\ m = n$$

$$= 0\, if\ m \neq n$$

This is true for any two eigen functions of any operator, in any qm system.

Completeness

Any acceptable function f(x)

that is zero outside x = 0 and L

can be written as $\sum_{\mathrm{n}} \mathrm{c}_{\mathrm{n}} \psi_n(\mathrm{x})$, *where*

$$c_n = \int_0^L \psi_n(x)^* f(x) dx$$

(Using orthonormality condition)

Superposition and related effects

SUPERPOSITION OF WAVE FUNCTION

The wave functions must be able to superpose. One can see that following is a solution of time Dependent Schrödinger Equation,

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-i\frac{E_n t}{\hbar}}$$

$$Here\,|c_n|^2\ is\ the\ probability\ of\ getting\ E_n$$
$$as\ a\ result\ in\ the\ energy\ measurement.$$

$$Normalization\ demands$$

$$\sum |c_n|^2 = 1$$

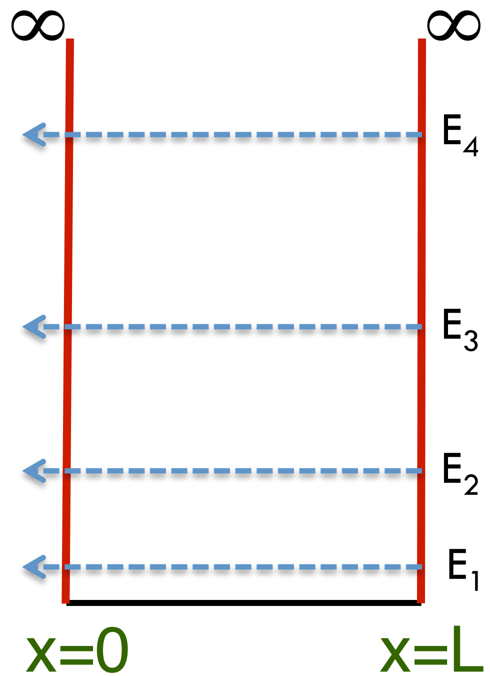
Note that the possible energy values are not continuous, but discrete.

Infinite potential well again

Following are the two normalized wave functions corresponding to n=1 and n=4 states.

$$\psi_1(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}$$

$$\psi_4(x) = \sqrt{\frac{2}{L}}\sin\frac{4\pi x}{L}$$



Following superposed wave function is **not** a normalized wave function.

$$\Psi(x,0) = \sqrt{\frac{2}{L}}\, sin\frac{\pi x}{L} + \sqrt{\frac{2}{L}}\, sin\frac{4\pi x}{L}$$

$$\text{since} \int_0^L \left(\sqrt{\frac{2}{L}}\, sin\frac{\pi x}{L} + \sqrt{\frac{2}{L}}\, sin\frac{4\pi x}{L} \right)^2 dx \neq 1$$

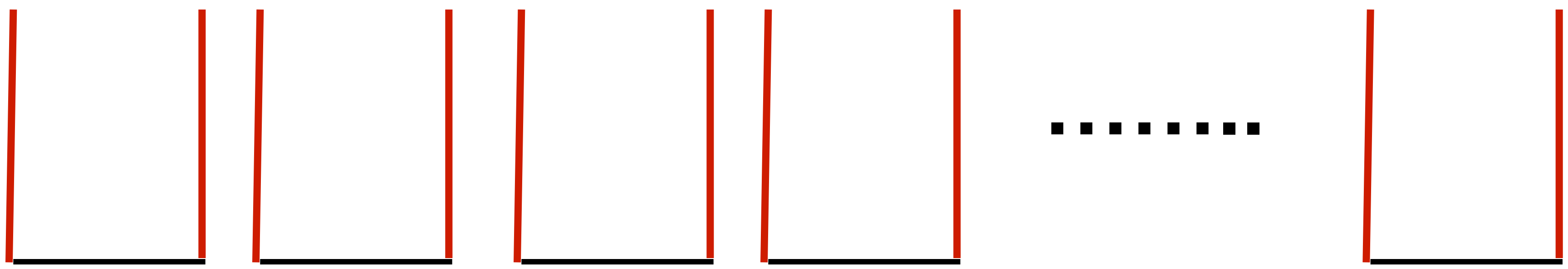
$$or \sum c_n{}^2 = 1 + 1 = 2$$

$\therefore$ *The normalized wave function is*

$$\Psi(x,0) = \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L} + \frac{1}{\sqrt{2}}\sqrt{\frac{2}{L}}\sin\frac{4\pi x}{L}$$

$$= \sqrt{\frac{1}{L}}\sin\frac{\pi x}{L} + \sqrt{\frac{1}{L}}\sin\frac{4\pi x}{L}$$

The physical interpretation implies imagining a large number of boxes where the wave function of the particle is given by above. If a measurement of energy is done, in half of them we shall find the particle to be in n=1 and in another half in n=4 state.



Question 1: Is the following wave function a normalized one ?

$$\Psi(x,0) = \sqrt{\frac{2}{5L}}\sin\frac{\pi x}{L} + \sqrt{\frac{8}{5L}}\sin\frac{4\pi x}{L}$$

We can write the above as follows.

$$\Psi(x,0)=\sqrt{\frac{1}{5}}\psi_1(x)+\sqrt{\frac{4}{5}}\psi_4(x)$$

Yes, it is normalized since $\frac{\mathbf{1}}{\mathbf{5}}+\frac{4}{5}=1$

In this case 20% of the boxes will give an energy corresponding to n=1 and 80% corresponding to n=4.

Question 2: What would be the expectation value of energy in such a case?

$$\langle E \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n = 0.2E_1 + 0.8E_4$$

Question 3: If no measurement was done what would be the wave function at a time t.

$$\Psi(x,t) = \sqrt{\frac{2}{5L}} \sin\frac{\pi x}{L} e^{-\frac{iE_1 t}{\hbar}} + \sqrt{\frac{8}{5L}} \sin\frac{4\pi x}{L} e^{-\frac{iE_4 t}{\hbar}} \quad (1)$$

We can check that this is a **non-stationary** state and the probability of finding the particle at a location would be a function of time. This is a state of indefinite energy.

For this state, $\langle E \rangle = 0.2E_1 + 0.8E_4$

$$\langle E^2 \rangle = 0.2E_1{}^2 + 0.8E_4{}^2$$

$$\therefore \Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2} = 0.8E_4 - 0.2E_1$$

That is, there is an uncertainty with respect to the energy of this state.

Question 4: If a measurement is done in one of the boxes at t=0 and the energy is found to be E_4, what would be the wave function at a later time t.

The wave function now **collapses** and the time dependence would be given by.

$$\Psi(x,t) = \sqrt{\frac{2}{L}} \sin\frac{4\pi x}{L} e^{-\frac{iE_4 t}{\hbar}} \longrightarrow (2)$$

(Note the change in the normalization constant)

Question 5: What would the measurement of energy yield on this box at a later time?

The particle is now in a stationary state. Hence the measurement would lead to E_4.

In the absence of any external effects, the result will be E_4 at any time later and for any observer.

What are the probability densities in states before and after collapse?

$$In\ state\ (1), the\ probability\ density\ oscillates$$

$$with\ frequency\ \omega = \frac{(E_4 - E_1)}{\hbar}$$

[Particle oscillates and radiation comes out]

$$In\ state\ (2), the\ probability\ density\ remains$$

$$the\ same\ with\ time.$$

[Particle is stationary and no radiation]

Effect of a measurement

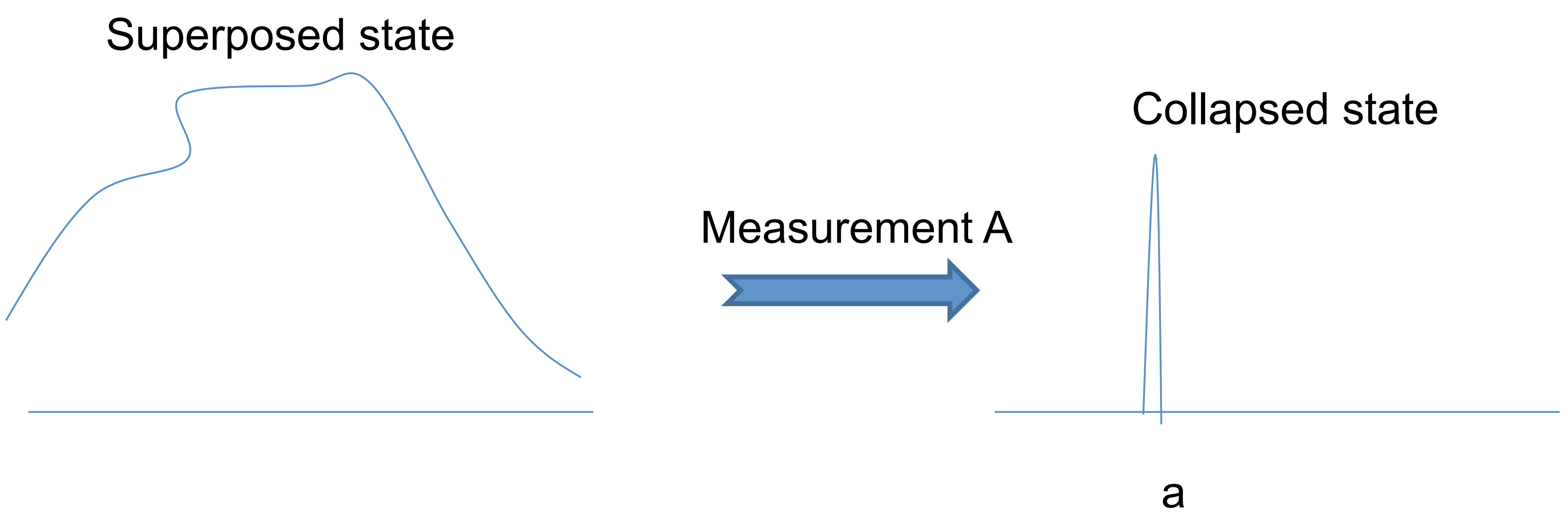
$$\sum_n \Psi_n(x,t) \xrightarrow{\text{MEASUREMENT}} \Psi_n(x,t)$$

Quantum state is fragile. Measurement causes the wave function to collapse abruptly and non-deterministically.

If the wave function is the eigen function of the operator corresponding to this measurement, then, the result will be one of the eigen values.

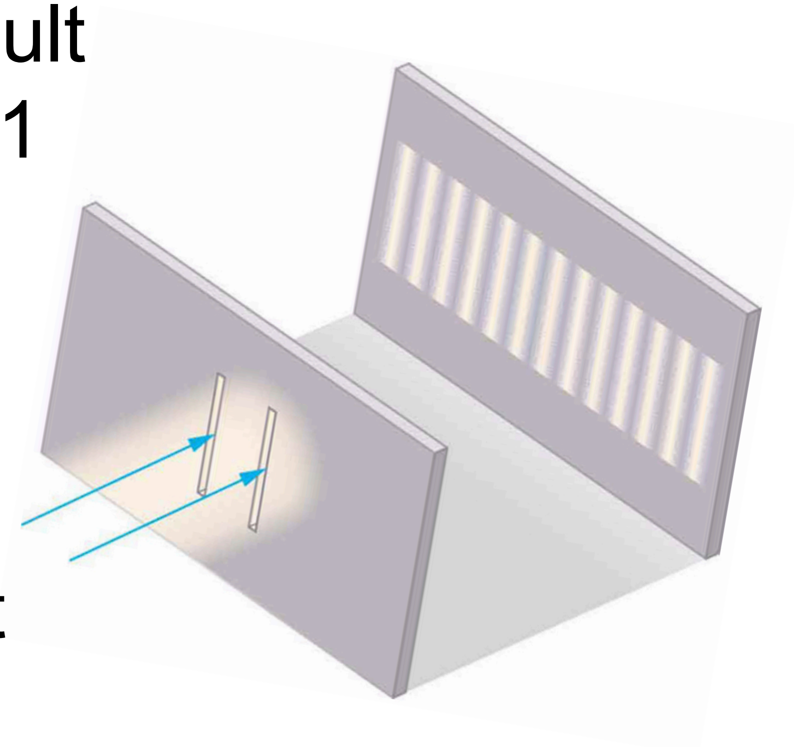
Otherwise, the result will be some value, not the expectation value.

Collapse of the wave function !!!



Going back to the Double slit expt.

Interference pattern is the result of superposed states (of slits 1 and 2).



It is the collapse of the superposed state during the detection (behind the slit) that kills the occurrence of the interference pattern.

In fact if we make measurements of two different observables in succession, the result depend on the order of the two measurements, in general.

i.e. $AB\psi \neq BA\psi$

Example: x and p_x measurements

$$Hence\,(\hat{x}+\hat{p}_x)^2 \neq \hat{x}^2 + 2\hat{x}\hat{p}_x + \hat{p}_x^2$$

$$because\,\hat{x}\hat{p}_x \neq \hat{p}_x\hat{x}$$

Very recent research work on superposition

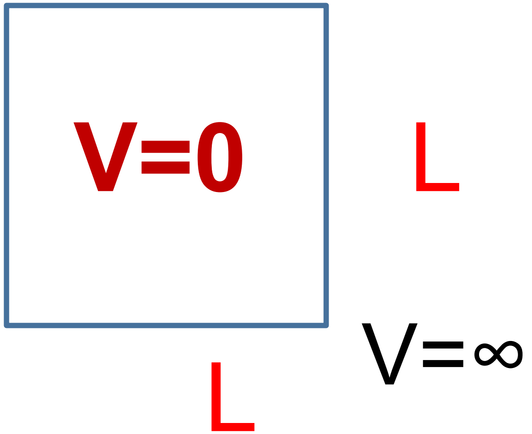
Confined a charged Be atom in a tiny electromagnetic cage and then cooled to its ground state. The researchers then stimulated the atom just enough to change its wave function corresponding to its first excited state.

It now had a 50 % probability of being in a "spin-up" state in its initial position and an equal probability of being in a "spin-down" state in a position 80 nm apart!. **In effect, the atom was in two different places, as well as two different spin states !!!!**

Higher Dimensional Problem

Particle in a 2D rigid box

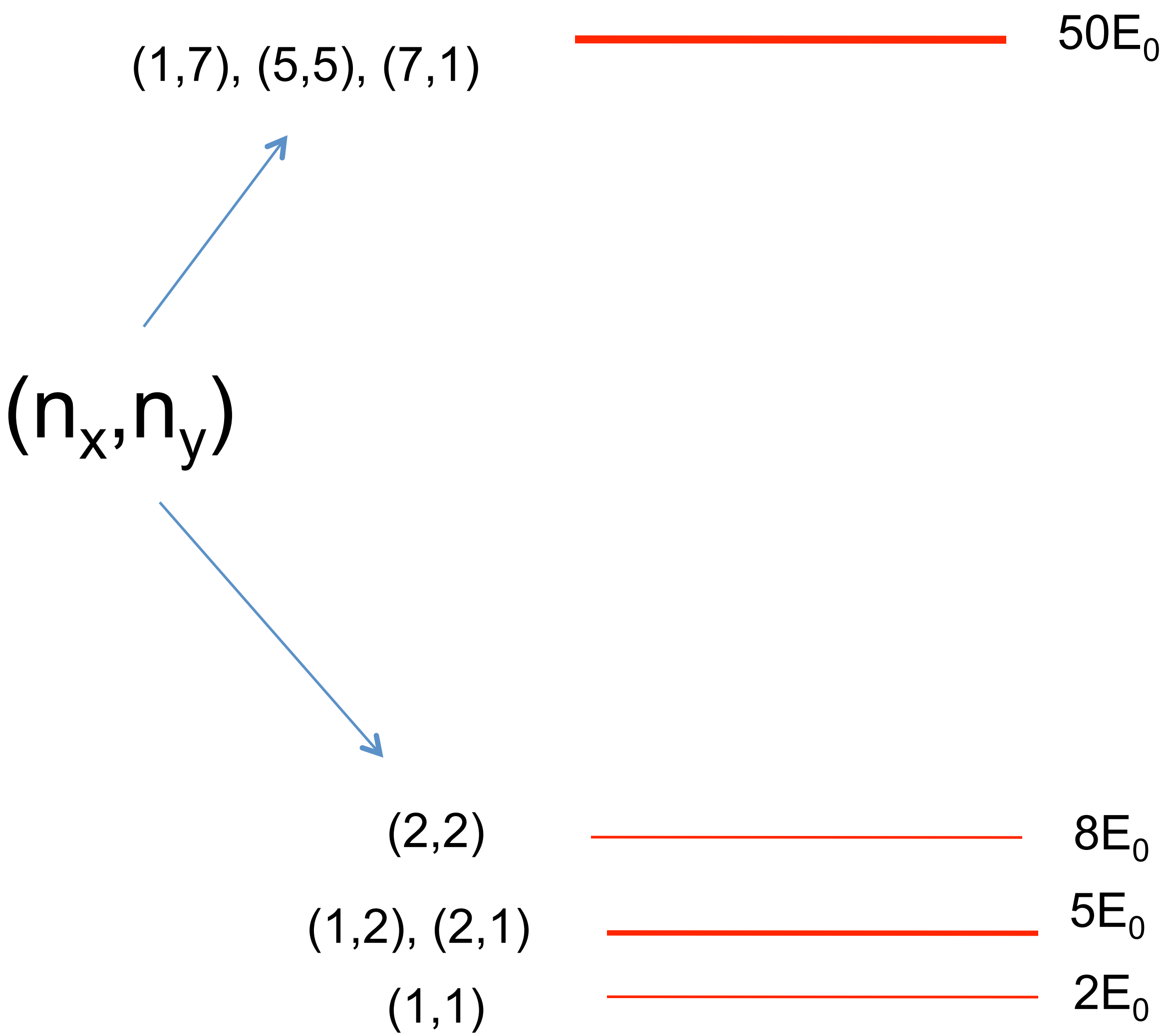
V=0 within sqaure,
V=∞, elsewhere



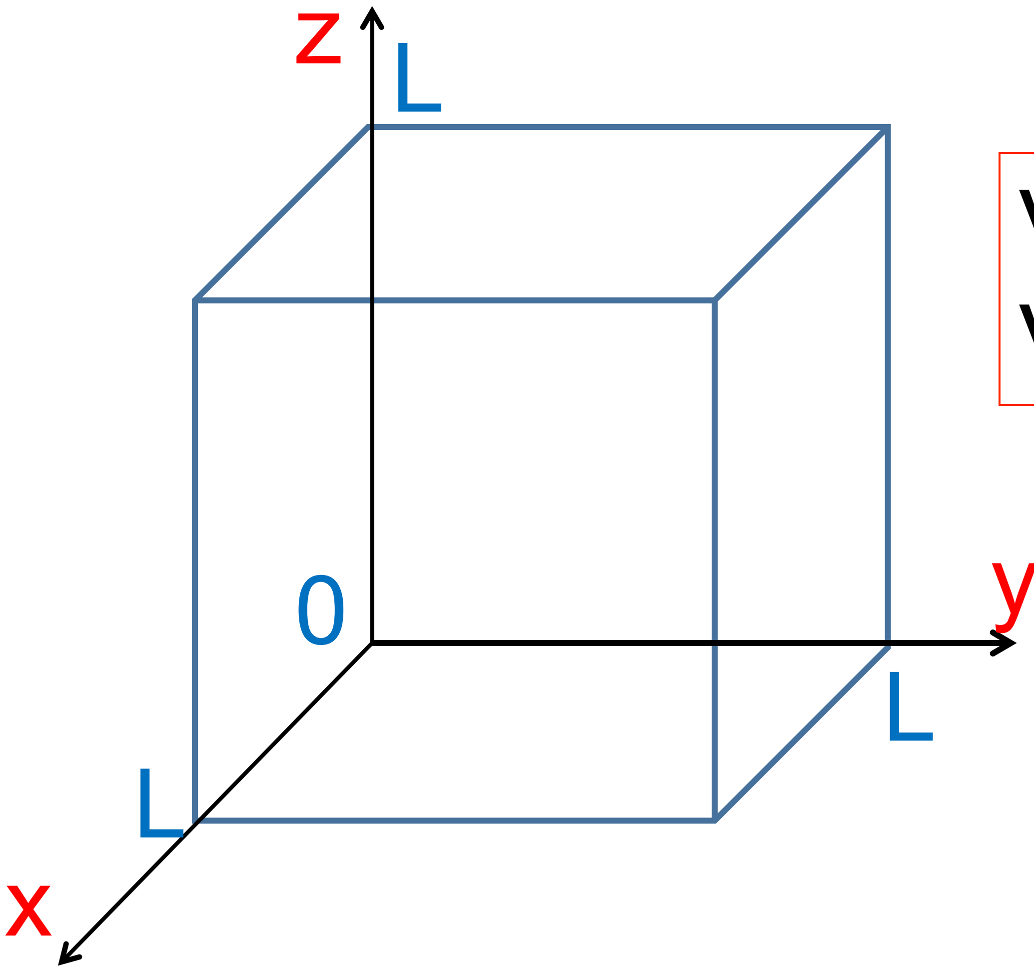
$$\psi_n(x,y) = \frac{2}{L} sin\left(\frac{n_x \pi x}{L}\right) sin\left(\frac{n_y \pi y}{L}\right)$$

$$E_n = \frac{\hbar^2 \pi^2}{2mL^2}(n_x^{\ 2} + n_y^{\ 2})$$

Degeneracy



Particle in a 3D Box



V=0 within Box,
V=∞, elsewhere

Solution of Schrodinger Eq.

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

$$= \frac{\pi^2\hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$\psi(r) = \left(\frac{2}{L}\right)^{3/2} sin\left(\frac{n_x \pi x}{L}\right) sin\left(\frac{n_y \pi y}{L}\right) sin\left(\frac{n_z \pi z}{L}\right)$$

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

Degeneracy

- Energy for $(n_x, n_y, n_z) = (2,1,1)$ $(1,2,1)$ and $(1,1,2)$ are the same though the wave functions are all different. This corresponds to a three-fold degeneracy.

Degeneracies in a 3D box

n_1	n_2	n_3	n^2	**Degeneracy**
1	1	1	3	None
1	1	2	6	
1	2	1	6	Threefold
2	1	1	6	
1	2	2	9	
2	1	2	9	Threefold
2	2	1	9	
1	1	3	11	
1	3	1	11	Threefold
3	1	1	11	
2	2	2	12	None

**Note*: $n^2 = n_1^2 + n_2^2 + n_3^2$.

Lifting the Degeneracies

What happens to the degeneracy if the sides of the cube/square are made different?