Physics 2D Lecture Slides
Lecture 26: March 2nd 2005

Vivek Sharma
UCSD Physics

Measurement Expectation: Statistics Lesson

- Ensemble & probable outcome of a single measurement or the average outcome of a large # of measurements

$$< x >= \frac{n_1 x_1 + n_2 x_2 + n_3 x_3 + \ldots . n_i x_i}{n_1 + n_2 + n_3 + \ldots n_i} = \frac{\sum_{i=1}^{n} n_i x_i}{N} = \frac{\int_{-\infty}^{\infty} xP(x)dx}{\int_{-\infty}^{\infty} P(x)dx}$$

For a general Fn f(x)

$$< f(x) >= \frac{\sum_{i=1}^{n} n_i f(x_i)}{N} = \frac{\int_{-\infty}^{\infty} \psi^*(x) f(x) \psi(x) dx}{\int_{-\infty}^{\infty} P(x)dx}$$

Sharpness of a distribution:
= scatter around the average

$$\sigma = \sqrt{\frac{\sum (x_i - \bar{x})^2}{N}}$$

$$\sigma = \sqrt{(\overline{x^2}) - (\bar{x})^2}$$

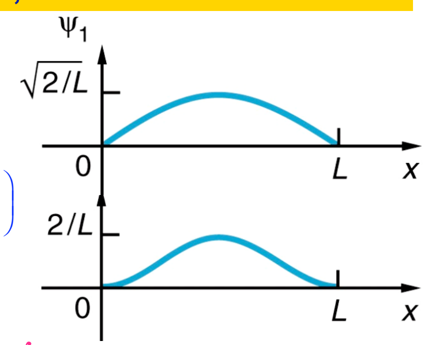
σ = small $\rightarrow$ Sharp distr.

Uncertainty $\Delta X = \sigma$

Table 5.2 Common Observables and Associated Operators

Observable	Symbol	Associated Operator
position	x	x
momentum	p	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
potential energy	U	$U(x)$
kinetic energy	K	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
hamiltonian	H	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$
total energy	E	$i\hbar\frac{\partial}{\partial t}$

Particle in the Box, n=1, find <x> & Δx ?



$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right)$

$\langle x\rangle = \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right)\, x\, \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right)dx$

$= \frac{2}{L}\int_0^L x\sin^2\left(\frac{\pi}{L}x\right)dx$, change variable $\theta = \left(\frac{\pi}{L}x\right)$

$\Rightarrow \langle x\rangle = \frac{2}{L\pi^2}\int_0^\pi \theta\sin^2\theta$, use $\sin^2\theta = \frac{1}{2}(1-\cos 2\theta)$

$\Rightarrow \langle x\rangle = \frac{2L}{2\pi^2}\left[\int_0^\pi \theta d\theta - \int_0^\pi \theta\cos 2\theta d\theta\right]$ use $\int udv = uv - \int vdu$

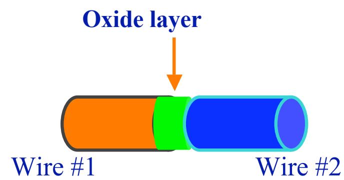
$\Rightarrow \langle x\rangle = \frac{L}{\pi^2}\left(\frac{\pi^2}{2}\right) = \frac{L}{2}$ (same result as from graphing $\psi^2(x)$)

Similarly $\langle x^2\rangle = \int_0^L x^2\sin^2\left(\frac{\pi}{L}x\right)dx = \frac{L^2}{3} - \frac{L^2}{2\pi^2}$

and $\Delta X = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{L^2}{3} - \frac{L^2}{2\pi^2} - \frac{L^2}{4}} = 0.18L$

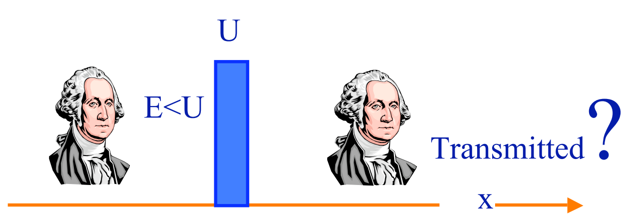
ΔX= 20% of L, Particle not sharply confined in Box

The Case of a Rusty "Twisted Pair" of Naked Wires & How Quantum Mechanics Saved ECE Majors !



- Twisted pair of Cu Wire (metal) in virgin form
- Does not stay that way for long in the atmosphere
  - Gets oxidized in dry air quickly Cu → Cu_2O
  - In wet air Cu → $Cu(OH)_2$ (the green stuff on wires)
- Oxides or Hydride are non-conducting ..so no current can flow across the junction between two metal wires
- No current means no circuits → no EE, no ECE !!
- All ECE majors must now switch to Chemistry instead & play with benzene !!! Bad news !

Potential Barrier

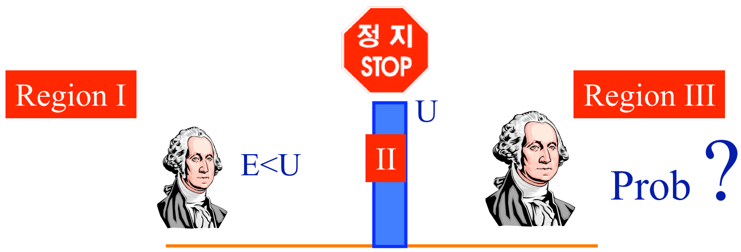


Description of Potential		
U = 0	x < 0	(Region I)
U = U	0 < x < L	(Region II)
U = 0	x > L	(Region III)

Consider George as a "free Particle/Wave" with Energy E incident from Left
Free particle are under no Force; have wavefunctions like

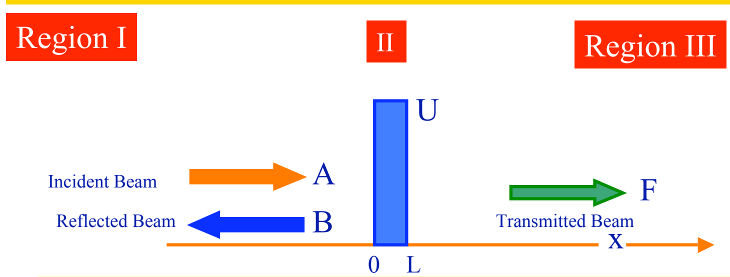
$$\Psi = A\, e^{i(kx-wt)} \text{ or } B\, e^{i(-kx-wt)}$$

Tunneling Through A Potential Barrier



- Classical & Quantum Pictures compared: When E>U & when E<U
- Classically , an particle or a beam of particles incident from left encounters barrier:
  - when E > U → Particle just goes over the barrier (gets transmitted)
  - When E<U → particle is stuck in region I, gets entirely reflected, no transmission (T)
- What happens in a Quantum Mechanical barrier ? No region is inaccessible for particle since the potential is (sometimes small) but finite

Beam Of Particles With E < U Incident On Barrier From Left



Description Of WaveFunctions in Various regions: Simple Ones first

In Region I : $\Psi_I(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$ = incident + reflected Waves

$$\text{with } E = \hbar\omega = \frac{\hbar^2 k^2}{2m}$$

define Reflection Coefficient : $\boxed{R = \frac{|B|^2}{|A|^2}}$ = *frac* of incident wave intensity reflected back

In Region III: $\Psi_{III}(x,t) = Fe^{i(kx-\omega t)} + Ge^{i(-kx-\omega t)}$ = *transmitted*

Note : $Ge^{i(-kx-\omega t)}$ corresponds to wave incident from right !

This piece does not exist in the scattering picture we are thinking of now (G=0)

So $\Psi_{III}(x,t) = Fe^{i(kx-\omega t)}$ represents transmitted beam. Define $\boxed{T = \frac{|F|^2}{|A|^2}}$

Unitarity Condition $\Rightarrow$ R + T= 1 (particle is either reflected or transmitted)

Wave Function Across The Potential Barrier

In Region II of Potential U

TISE: $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi(x)}{dx^2}+U\psi(x)=E\psi(x)$

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

$$=\alpha^2\psi(x)$$

with $\alpha^2=\dfrac{\sqrt{2m(U-E)}}{\hbar}$; U>E $\Rightarrow \alpha^2>0$

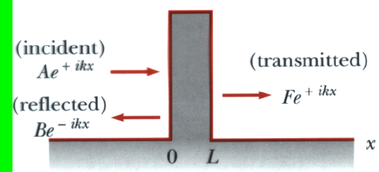
Solutions are of form $\psi(x)\propto e^{\pm\alpha x}$

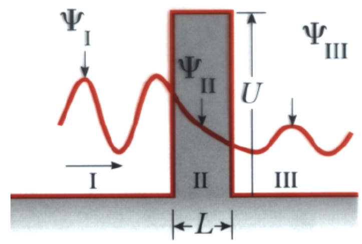
$\boxed{\Psi_{II}(x,t)=Ce^{+\alpha x-i\omega t}+De^{-\alpha x-i\omega t}}$ 0<x<L

To determine C & D $\Rightarrow$ apply matching cond.

$\Psi_{II}(x,t)=\mathit{continuous}$ across barrier (x=0,L)

$\dfrac{d\Psi_{II}(x,t)}{dx}=\mathit{continuous}$ across barrier (x=0,L)





Continuity Conditions Across Barrier

At x = 0 , continuity of $\psi(x)$ $\Rightarrow$

A+B=C+D (1)

At x = 0 , continuity of $\dfrac{d\psi(x)}{dx}$ $\Rightarrow$

$$ikA-ikB=\alpha C-\alpha D \quad (2)$$

Similarly at x=L continuity of $\psi(x)$ $\Rightarrow$

$$Ce^{-\alpha L}+De^{+\alpha L}=Fe^{ikL} \quad (3)$$

at x=L, continuity of $\dfrac{d\psi(x)}{dx}$ $\Rightarrow$

$$-(\alpha C)e^{-\alpha L}+(\alpha D)e^{\alpha L}=ikFe^{ikL} \quad (4)$$

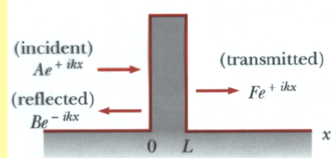
Four equations & four unknowns

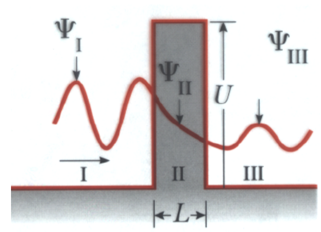
Cant determine A,B,C,D but if you

Divide thruout by A in all 4 equations :

$\Rightarrow$ ratio of amplitudes $\rightarrow$ relations for R & T

That's what we need any way





Potential Barrier when E < U

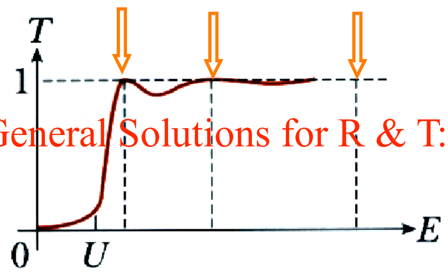
Expression for Transmission Coeff T=T(E) :

Depends on barrier Height U, barrier Width L and particle Energy E

$$\boxed{T(E) = \left[1+\frac{1}{4}\left(\frac{U^2}{E(U-E)}\right)\sinh^2(\alpha L)\right]^{-1}}; \quad \alpha = \frac{\sqrt{2m(U-E)}}{\hbar}$$

and R(E)=1- T(E).........what's not transmitted is reflected

General Solutions for R & T:



Above equation holds only for E < U

For E>U, α=imaginary#

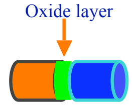
Sinh(αL) becomes oscillatory

This leads to an Oscillatory T(E) and Transmission resonances occur where For some specific energy ONLY, T(E) =1

At other values of E, some particles are reflected back ..even though E>U !!

That's the Wave nature of the Quantum particle

Ceparated in Coppertino

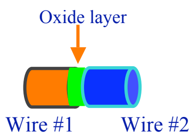


Solved Example 6.1 (...that I made such a big deal about yesterday)

Q: 2 Cu wires are seperated by insulating Oxide layer. Modeling the Oxide layer as a square barrier of height U=10.0eV, estimate the transmission coeff for an incident beam of electrons of E=7.0 eV when the layer thickness is (a) 5.0 nm (b) 1.0nm

Q: If a 1.0 mA current in one of the intwined wires is incident on Oxide layer, how much of this current passes thru the Oxide layer on to the adjacent wire if the layer thickness is 1.0nm? What becomes of the remaining current?

$$\boxed{T(E) = \left[1+\frac{1}{4}\left(\frac{U^2}{E(U-E)}\right)\sinh^2(\alpha L)\right]^{-1}} \quad \alpha=\frac{\sqrt{2m(U-E)}}{\hbar}, k = \frac{\sqrt{2mE}}{\hbar}$$



$$T(E) = \left[1+\frac{1}{4}\left(\frac{U^2}{E(U-E)}\right)\sinh^2(\alpha L)\right]^{-1}$$

Use $\hbar$=1.973 keV.Å/c , m_e = 511 keV/c^2

$$\Rightarrow \alpha = \frac{\sqrt{2m_e(U-E)}}{\hbar} = \frac{\sqrt{2\times 511 kev/c^2 (3.0\times 10^{-3} keV)}}{1.973 \text{ keV.Å/c}} = 0.8875\text{Å}^{-1}$$

Substitute in expression for T=T(E)

$$T= \left[1+\frac{1}{4}\left(\frac{10^2}{7(10-7)}\right)\sinh^2(0.8875\text{Å}^{-1})(50\text{Å})\right]^{-1} = 0.963\times 10^{-38}(small)!!$$

However, for L=10Å; T=0.657×10^{-7}

Reducing barrier width by $\times 5$ leads to Trans. Coeff enhancement by 31 orders of magnitude !!!

1 mA current =I=$\frac{Q=Nq_e}{t}$ $\Rightarrow N=6.25\times 10^{15}$ *electrons*

N_T=# of electrons that escape to the adjacent wire (past oxide layer)

$N_T = N.T = (6.25\times 10^{15}\ electrons)\times \boxed{T}$;

For L=10 Å, T=0.657×10^{-7} $\Rightarrow N_T = 4.11\times 10 \Rightarrow \boxed{I_T = 65.7\,pA}$!!

Current Measured on the first wire is sum of incident+reflected currents and current measured on "adjacent" wire is the I_T

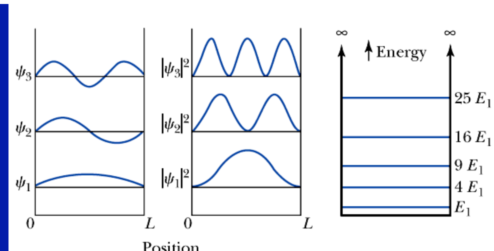
Oxide thickness makes all the difference ! That's why from time-to-time one needs to Scrape off the green stuff off the naked wires

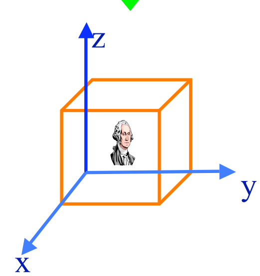
QM in 3 Dimensions

- Learn to extend S. Eq and its solutions from "toy" examples in 1-Dimension (x) $\rightarrow$ three orthogonal dimensions (r$\equiv$ x,y,z)

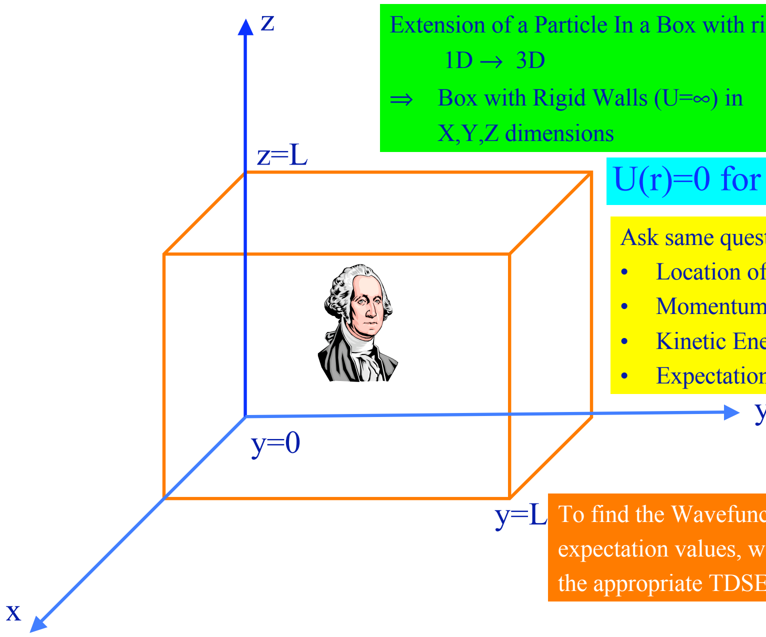
$$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z$$

- Then transform the systems
  - Particle in 1D rigid box → 3D rigid box
  - 1D Harmonic Oscillator → 3D Harmonic Oscillator
    - Keep an eye on the number of different integers needed to specify system 1→ 3 (corresponding to 3 available degrees of freedom x,y,z)





Quantum Mechanics In 3D: Particle in 3D Box



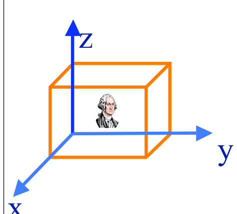
Extension of a Particle In a Box with rigid walls
1D → 3D
⇒ Box with Rigid Walls ($U=\infty$) in X,Y,Z dimensions

$U(r)=0$ for $(0<x,y,z,<L)$

Ask same questions:
- Location of particle in 3d Box
- Momentum
- Kinetic Energy, Total Energy
- Expectation values in 3D

To find the Wavefunction and various expectation values, we must first set up the appropriate TDSE & TISE

The Schrodinger Equation in 3 Dimensions: Cartesian Coordinates



Time Dependent Schrodinger Eqn:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(x,y,z,t)+U(x,y,z)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,y,z,t)}{\partial t} \quad \text{.....In 3D}$$

$$\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

$$So\ -\frac{\hbar^2}{2m}\nabla^2=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)+\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}\right)+\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\right)=[K]$$

$$= \quad [K_x] \quad + \quad [K_x] \quad + \quad [K_x]$$

$so\ [H]\Psi(x,t)=[E]\Psi(x,t)$ is still the Energy Conservation Eq

Stationary states are those for which all probabilities are constant in time and are given by the solution of the TDSE in seperable form:

$$\Psi(x,y,z,t)=\Psi(\vec{r},t)=\psi(\vec{r})e^{-i\omega t}$$

This statement is simply an extension of what we derived in case of 1D time-independent potential

Particle in 3D Rigid Box : Separation of Orthogonal Spatial (x,y,z) Variables

TISE in 3D: $-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z)+U(x,y,z)\psi(x,y,z)=E\psi(x,y,z)$

x,y,z independent of each other , write $\psi(x,y,z)=\psi_1(x)\psi_2(y)\psi_3(z)$

and substitute in the master TISE, after dividing thruout by $\psi=\psi_1(x)\psi_2(y)\psi_3(z)$

and noting that U(r)=0 for (0<x,y,z,<L) $\Rightarrow$

$$\left(-\frac{\hbar^2}{2m}\frac{1}{\psi_1(x)}\frac{\partial^2\psi_1(x)}{\partial x^2}\right)+\left(-\frac{\hbar^2}{2m}\frac{1}{\psi_2(y)}\frac{\partial^2\psi_2(y)}{\partial y^2}\right)+\left(-\frac{\hbar^2}{2m}\frac{1}{\psi_3(z)}\frac{\partial^2\psi_3(z)}{\partial z^2}\right)=E=Const$$

This can only be true if each term is constant for all x,y,z $\Rightarrow$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi_1(x)}{\partial x^2}=E_1\psi_1(x)};\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi_2(y)}{\partial y^2}=E_2\psi_2(y)};\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi_3(z)}{\partial z^2}=E_3\psi_3(z)}$$

With $\boxed{E_1+E_2+E_3=E=\text{Constant}}$ (Total Energy of 3D system)

Each term looks like particle in 1D box (just a different dimension)

So wavefunctions must be like $\boxed{\psi_1(x)\propto\sin k_1x}$, $\boxed{\psi_2(y)\propto\sin k_2y}$, $\boxed{\psi_3(z)\propto\sin k_3z}$

Particle in 3D Rigid Box : Separation of Orthogonal Variables

Wavefunctions are like $\boxed{\psi_1(x)\propto\sin k_1x}$, $\boxed{\psi_2(y)\propto\sin k_2y}$, $\boxed{\psi_3(z)\propto\sin k_3z}$

Continuity Conditions for ψ_i and its first spatial derivatives $\Rightarrow$ $\boxed{n_i\pi=k_iL}$

Leads to usual Quantization of Linear Momentum $\boxed{\vec{p}=\hbar\vec{k}}$.....in 3D

$$\boxed{p_x=\left(\frac{\pi\hbar}{L}\right)n_1};\ \boxed{p_y=\left(\frac{\pi\hbar}{L}\right)n_2};\ \boxed{p_z=\left(\frac{\pi\hbar}{L}\right)n_3}\ (n_1,n_2,n_3=1,2,3,..\infty)$$

Note: by usual Uncertainty Principle argument neither of $n_1,n_2,n_3=0$! (*why*?)

Particle Energy $E=K+U=K+0=\frac{1}{2m}(p_x^2+p_y^2+p_z^2)=\boxed{\frac{\pi^2\hbar^2}{2mL^2}(n_1^2+n_2^2+n_3^2)}$

Energy is again quantized and brought to you by integers n_1,n_2,n_3 (independent)

and $\psi(\vec{r})=A\sin k_1x\sin k_2y\sin k_3z$ (A = Overall Normalization Constant)

$$\Psi(\vec{r},t)=\psi(\vec{r})\,e^{-i\frac{E}{\hbar}t}=\boxed{A\,[\sin k_1x\sin k_2y\sin k_3z]\,e^{-i\frac{E}{\hbar}t}}$$

Particle in 3D Box :Wave function Normalization Condition

$$\Psi(\vec{r},t)=\psi(\vec{r})\, e^{-i\frac{E}{\hbar}t} = \boxed{A\,[\sin k_1 x \sin k_2 y \sin k_3 z]\, e^{-i\frac{E}{\hbar}t}}$$

$$\Psi^*(\vec{r},t)=\psi^*(\vec{r})\, e^{i\frac{E}{\hbar}t} = \boxed{A\,[\sin k_1 x \sin k_2 y \sin k_3 z]\, e^{i\frac{E}{\hbar}t}}$$

$$\Psi^*(\vec{r},t)\Psi(\vec{r},t)=A^2\,[\sin^2 k_1 x \sin^2 k_2 y \sin^2 k_3 z]$$

$$\text{Normalization Condition : } 1 = \iiint_{x,y,z} P(r)\,dx\,dy\,dz \;\Rightarrow$$

$$1 = A^2 \int_{x=0}^{L} \sin^2 k_1 x\, dx \int_{y=0}^{L} \sin^2 k_2 y\, dy \int_{z=0}^{L} \sin^2 k_3 z\, dz = A^2 \left(\sqrt{\frac{L}{2}}\right)\left(\sqrt{\frac{L}{2}}\right)\left(\sqrt{\frac{L}{2}}\right)$$

$$\Rightarrow A = \left[\frac{2}{L}\right]^{\frac{3}{2}} \text{ and } \boxed{\Psi(\vec{r},t) = \left[\frac{2}{L}\right]^{\frac{3}{2}} [\sin k_1 x \sin k_2 y \sin k_3 z]\, e^{-i\frac{E}{\hbar}t}}$$

Particle in 3D Box : Energy Spectrum & Degeneracy

$$\boxed{E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2mL^2}(n_1^2+n_2^2+n_3^2);\quad n_i = 1,2,3\ldots\infty, n_i \neq 0}$$

Ground State Energy $E_{111} = \dfrac{3\pi^2\hbar^2}{2mL^2}$

Next level $\Rightarrow$ 3 Excited states $E_{211} = E_{121} = E_{112} = \dfrac{6\pi^2\hbar^2}{2mL^2}$

Different configurations of $\psi(r)=\psi(x,y,z)$ have same energy $\Rightarrow$ degeneracy