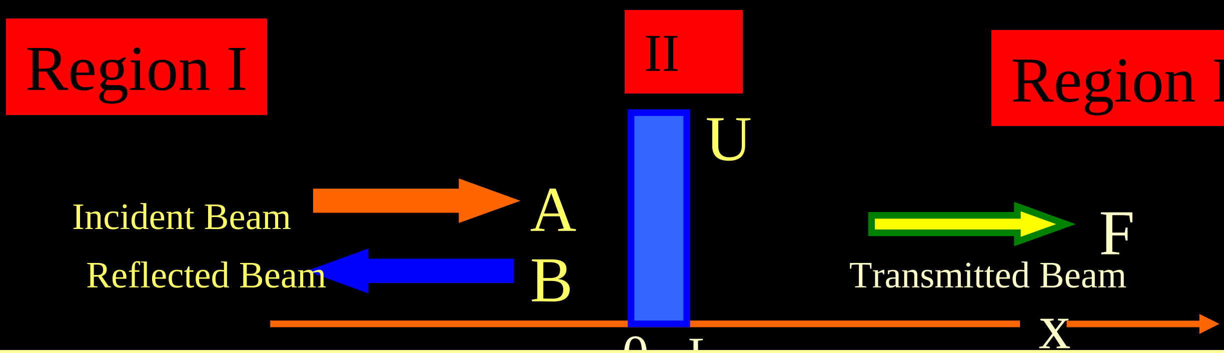
4E : The Quantum Universe

Lecture 21, May 5

Vivek Sharma
modphys@hepmail.ucsd.edu

Particle Beams and Flux Conservation



If we write the particle wavefunction for incident as $\psi_{\mathrm{I+}} = Ae^{ik_I x}$ and reflected as $\psi_{\mathrm{I-}} = Be^{-ik_I x}$

The particle flux arriving at the barrier, defined as number of particles per unit length per unit time

$$S_{\mathrm{I+}} = |\psi_{\mathrm{I+}}{}^{*}\psi_{\mathrm{I+}}| V_{I+} = |\psi_{\mathrm{I+}}{}^{*}\psi_{\mathrm{I+}}| \left(\frac{p}{m}\right) \text{ and } S_{\mathrm{I-}} = |\psi_{\mathrm{I-}}{}^{*}\psi_{\mathrm{I-}}| \left(\frac{p}{m}\right);$$ (for non-relativistic case)

Since the wavefunction in region III $\psi_{\mathrm{III+}} = \psi_{\mathrm{III}} = Fe^{ik_{III} x}$ and $S_{\mathrm{III+}} = |\psi_{\mathrm{III+}}{}^{*}\psi_{\mathrm{III+}}| \left(\frac{p_{III}}{m}\right)$

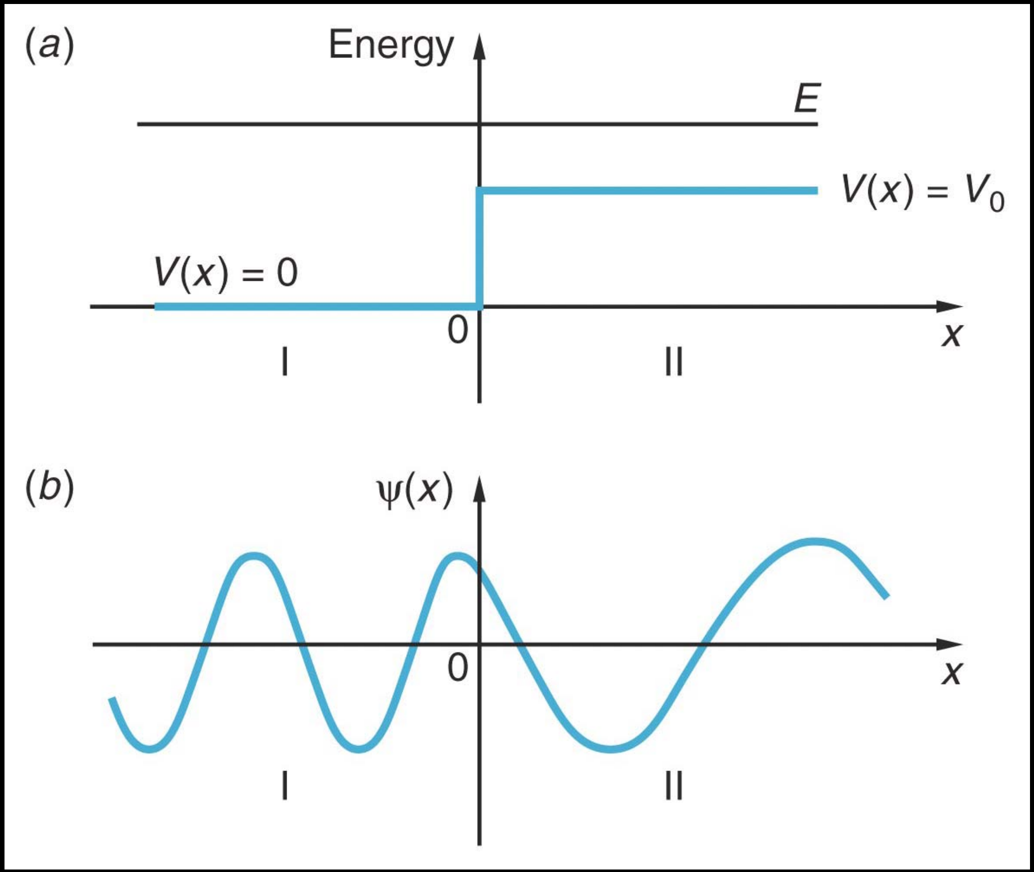
The general expression for flux probabilities : number of particles passing by any point per unit time:

$$\text{Transmission Probability } T = \frac{|\psi_{\mathrm{III+}}{}^{*}\psi_{\mathrm{III+}}| V_{III+}}{|\psi_{\mathrm{I+}}{}^{*}\psi_{\mathrm{I+}}| V_{I+}} = \left(\frac{F}{A}\right)^{*}\left(\frac{F}{A}\right)\left(\frac{V_{III+}}{V_{I+}}\right)$$

$$\text{Reflection Probability } R = \frac{|\psi_{\mathrm{I-}}{}^{*}\psi_{\mathrm{I-}}| V_{I-}}{|\psi_{\mathrm{I+}}{}^{*}\psi_{\mathrm{I+}}| V_{I+}} = \left(\frac{B}{A}\right)^{*}\left(\frac{B}{A}\right)\left(\frac{V_{I-}}{V_{I+}}\right)$$

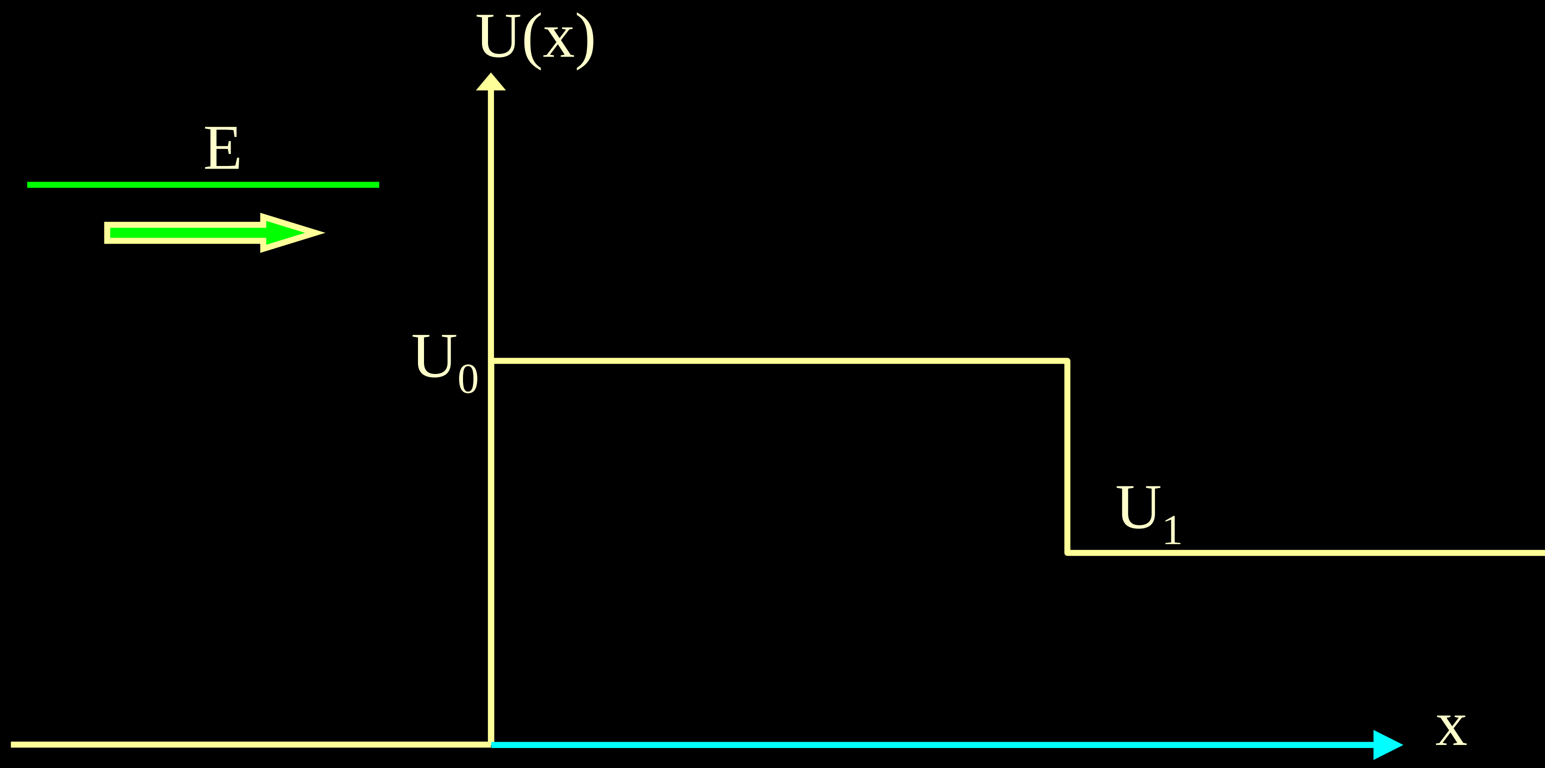
The general expression for conservation of particle flux remains: $\boxed{1 = T + R}$

Where does this generalization become important?



- Particle with energy E incident from left on a potential step U, with E>U
- Particle momentum, wavelength and velocities are different in region I and II
- Is the reflection probability = 0 ?

Where does this generalization become important?

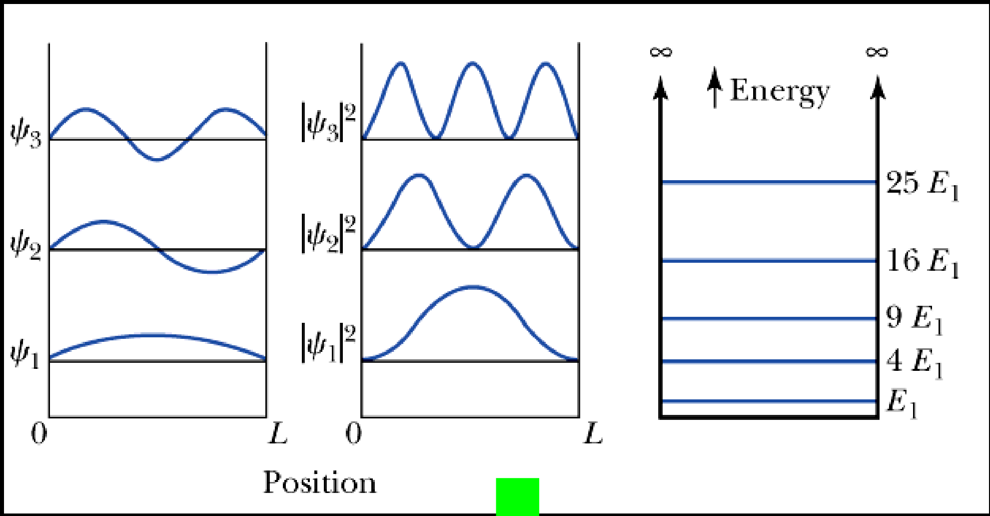


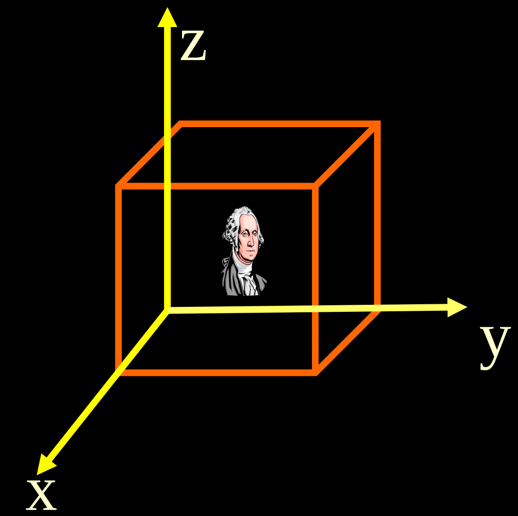
QM in 3 Dimensions

- Learn to extend S. Eq and its solutions from "toy" examples in 1-Dimension (x) → three orthogonal dimensions (r ≡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)



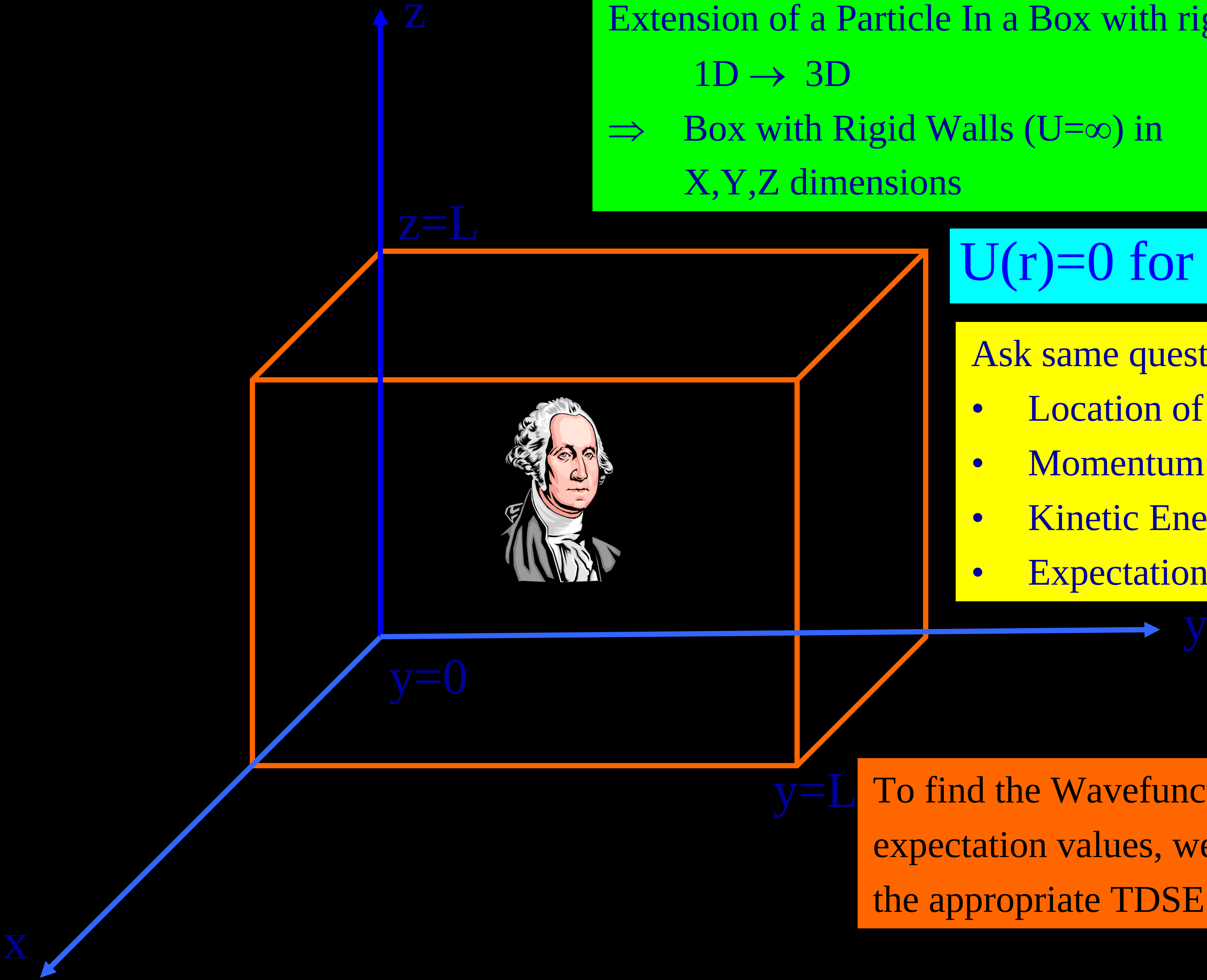


Quantum Mechanics In 3D: Particle in 3D Box

Extension of a Particle In a Box with rigid walls

1D $\rightarrow$ 3D

$\Rightarrow$ Box with Rigid Walls (U=∞) in X,Y,Z dimensions



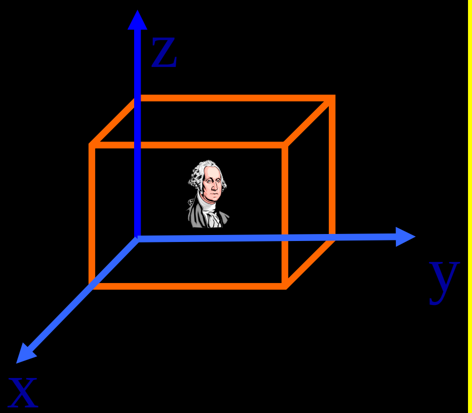
U(r)=0 for (0<x,y,z,<L)

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:

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

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

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

$$= \quad [\mathrm{K_x}] \quad + \quad [\mathrm{K_x}] \quad + \quad [\mathrm{K_x}]$$

$so\ \ [H]\Psi(x,t)=[E]\Psi(x,t)$ 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:

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

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 $\Rightarrow$

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

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 $\psi_1(x) \propto \sin k_1 x$, $\psi_2(y) \propto \sin k_2 y$, $\psi_3(z) \propto \sin k_3 z$

Continuity Conditions for ψ_i and its first spatial derivatives $\Rightarrow$ $n_i \pi = k_i L$

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

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

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

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

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

and $\psi(\vec{r}) = A \sin k_1 x \sin k_2 y \sin k_3 z$ (A = Overall Normalization Constant)

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

Particle in 3D Box :Wave function Normalization Condition

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

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

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

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

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

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

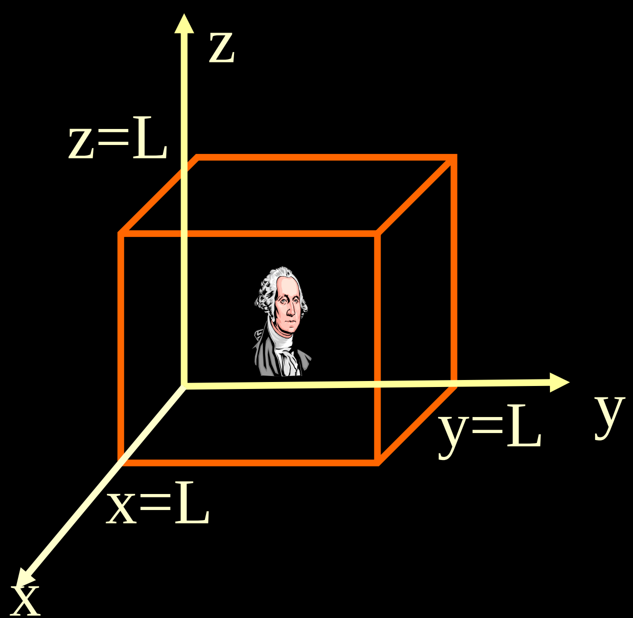
Particle in 3D Box : Energy Spectrum & Degeneracy

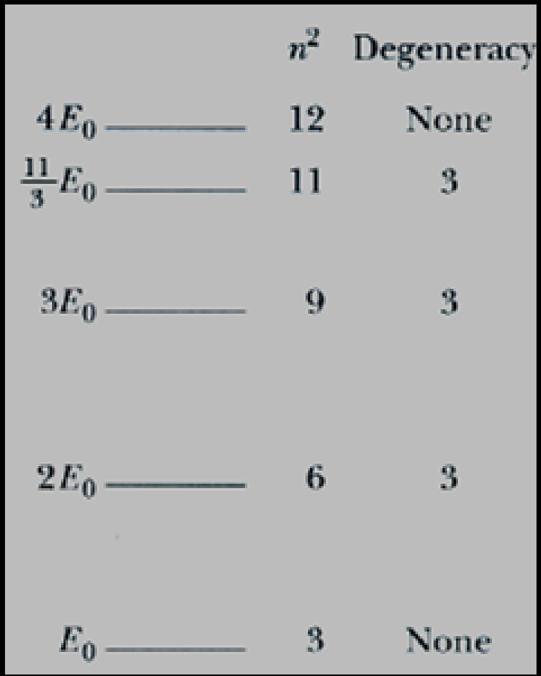
$$E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2mL^2}(n_1^2+n_2^2+n_3^2); \quad n_i = 1,2,3\ldots\infty, n_i \neq 0$$

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



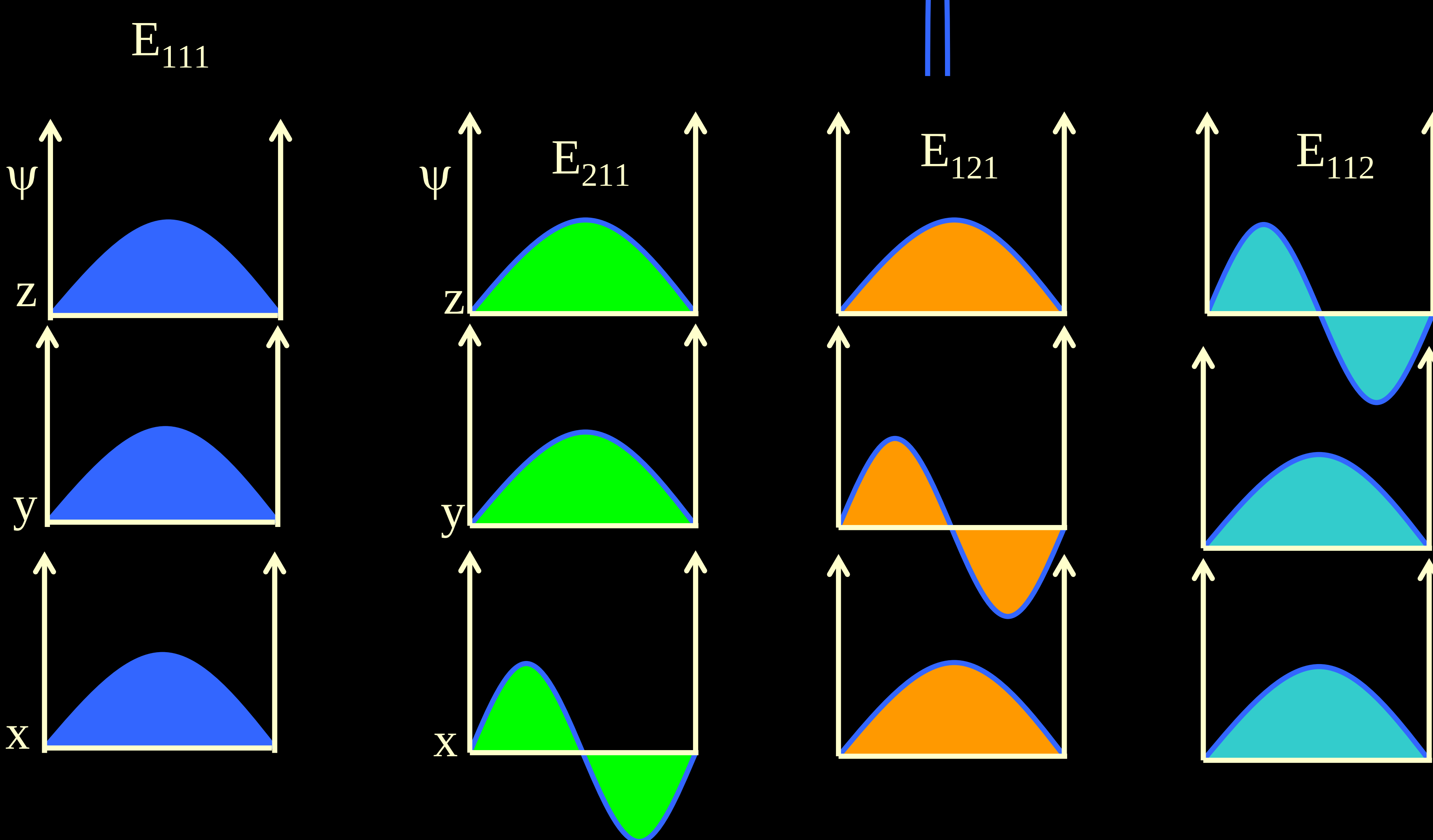


	n^2	Degeneracy
$4E_0$	12	None
$\frac{11}{3}E_0$	11	3
$3E_0$	9	3
$2E_0$	6	3
E_0	3	None

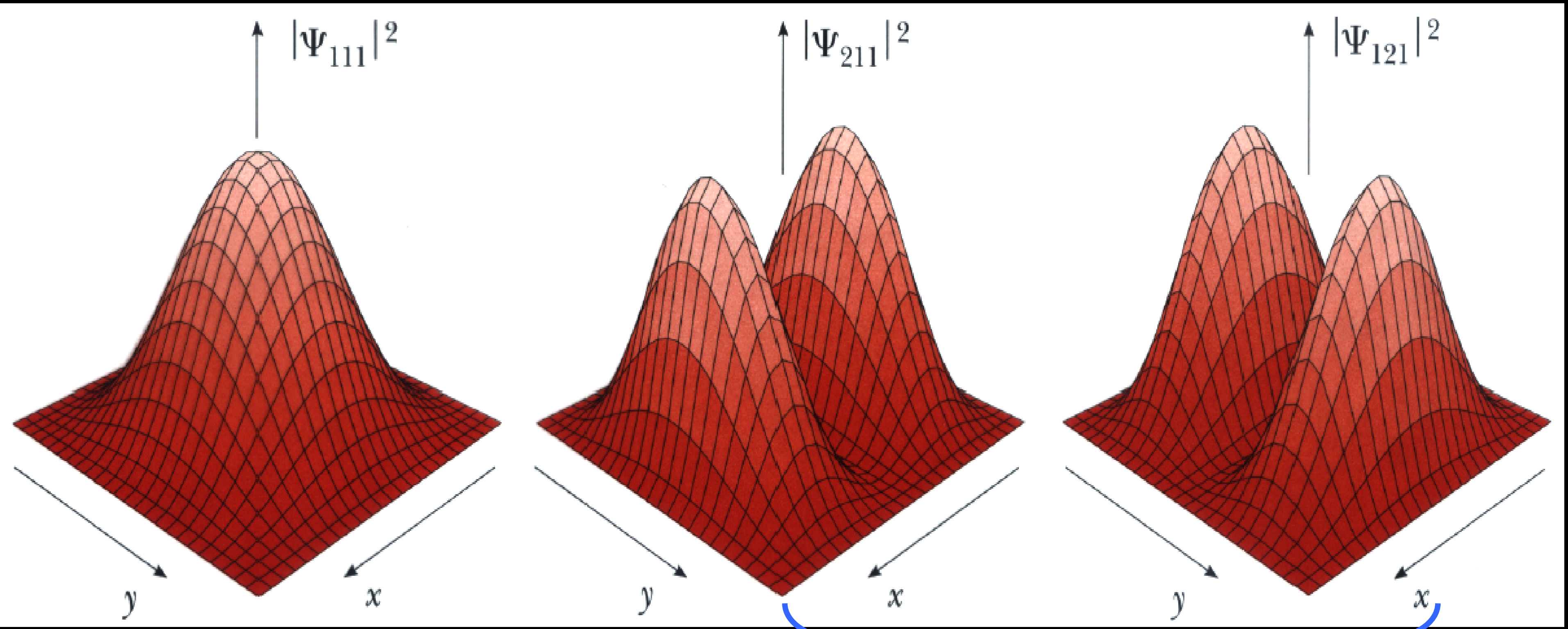
Degenerate States

$$E_{211} = E_{121} = E_{112} = \frac{6\pi^2\hbar^2}{2mL^2}$$

Ground State



Probability Density Functions for Particle in 3D Box



Same Energy → Degenerate States

Cant tell by measuring energy if particle is in 211, 121, 112 quantum State

Source of Degeneracy: How to "Lift" Degeneracy

- Degeneracy came from the threefold symmetry of a CUBICAL Box ($L_x = L_y = L_z = L$)

- To Lift (remove) degeneracy → change each dimension such that CUBICAL box → Rectangular Box
  - ($L_x \neq L_y \neq L_z$)
  - Then

$$E = \left(\frac{n_1^2 \pi^2}{2mL_x^2}\right) + \left(\frac{n_2^2 \pi^2}{2mL_y^2}\right) + \left(\frac{n_3^2 \pi^2}{2mL_z^2}\right)$$