4E : The Quantum Universe

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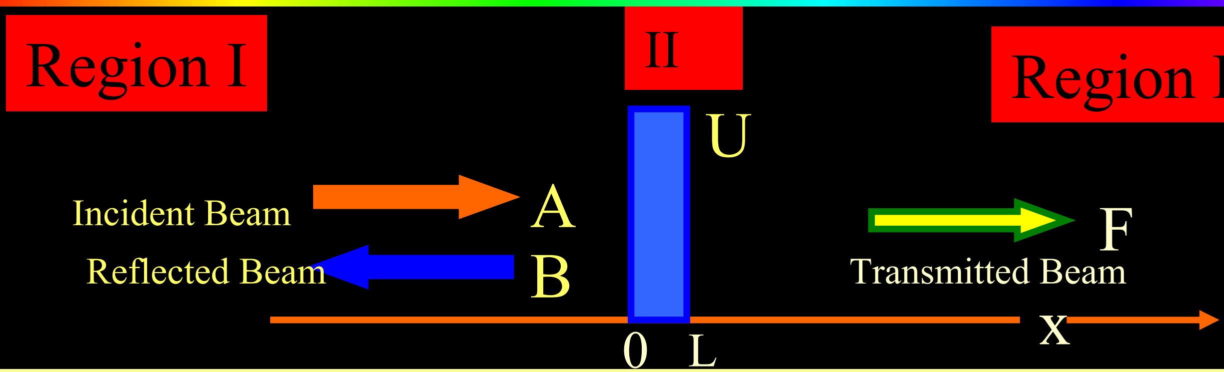
Potential Barrier : An Unintuitive Result When E>U



Description Of WaveFunctions in Various regions: Simple Ones first

In Region I : $\Psi_{I}(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$; In Region III: $\Psi_{III}(x,t) = Fe^{i(kx-\omega t)}$

In Region II of Potential U:

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

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

Define $\alpha = ik'; \alpha^2 = -(k')^2; k' = \sqrt{\frac{2m(E-U)}{\hbar^2}}$

$\Rightarrow \Psi_{II} = Ce^{i(-k'x-\omega t)} + De^{i(k'x-\omega t)} \Rightarrow$ Oscillatory Wavefunction

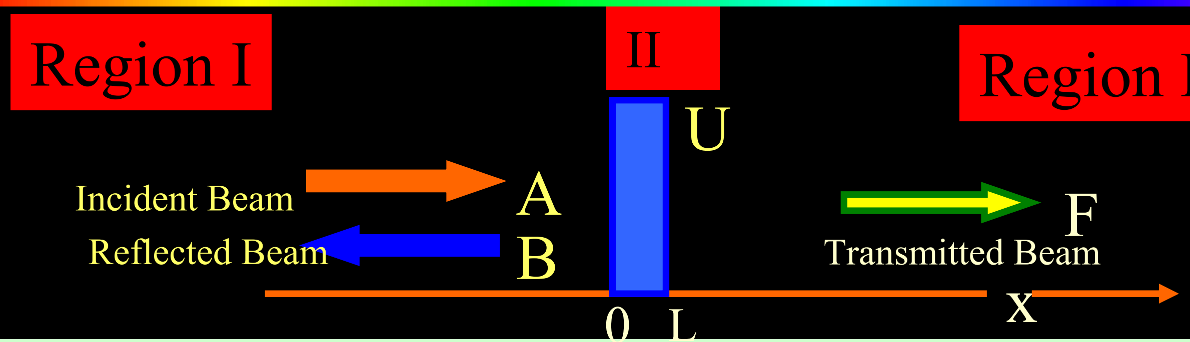
Apply continuity condition at x=0 & x=L

$$\boxed{A+B=C+D};\quad \boxed{kA - kB = k'D - k'C};\quad \boxed{Ce^{-ik'L} + De^{ik'L} = Fe^{ikL}};\quad \boxed{k'De^{ik'L} - k'Ce^{-ik'L} = kFe^{ikL}}$$

Eliminate B, C,D and write every thing in terms of A and F $\Rightarrow$

$$A = \frac{1}{4}Fe^{ikL}\left\{\left[2-\left(\frac{k'}{k}+\frac{k}{k'}\right)\right]e^{ik'L} + \left[2+\left(\frac{k'}{k}+\frac{k}{k'}\right)\right]e^{-ik'L}\right\}$$

Potential Barrier : An Unintuitive Result When E>U



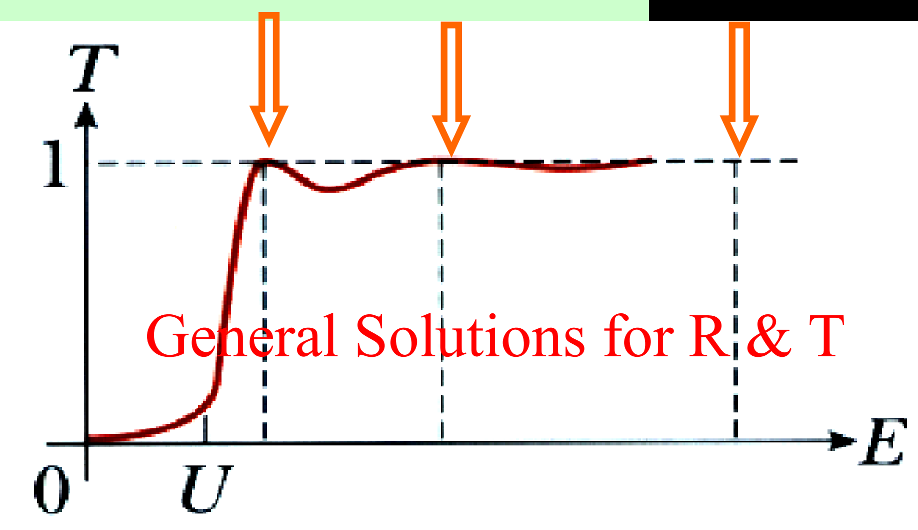
$$\Rightarrow \frac{1}{T} = \frac{A^{*}A}{F^{*}F} = \frac{1}{4}\left[2\cos k'L - i\left(\frac{k'}{k}+\frac{k}{k'}\right)\sin k'L\right]^{2} = 1+\frac{1}{4}\left[\frac{U^{2}}{E(E-U)}\right]\sin^{2}k'L > 1$$

Only when $\sin k'L = 0, T = 1$; this happens when $\boxed{k'L = n\pi}$

Since $k' = \sqrt{\frac{2m(E-U)}{\hbar^{2}}} \Rightarrow \sqrt{\frac{2m(E-U)}{\hbar^{2}}} = n\pi$

$$\Rightarrow \boxed{E_n = U + n^{2}\left(\frac{\pi^{2}\hbar^{2}}{2mL^{2}}\right)}$$ is the condition

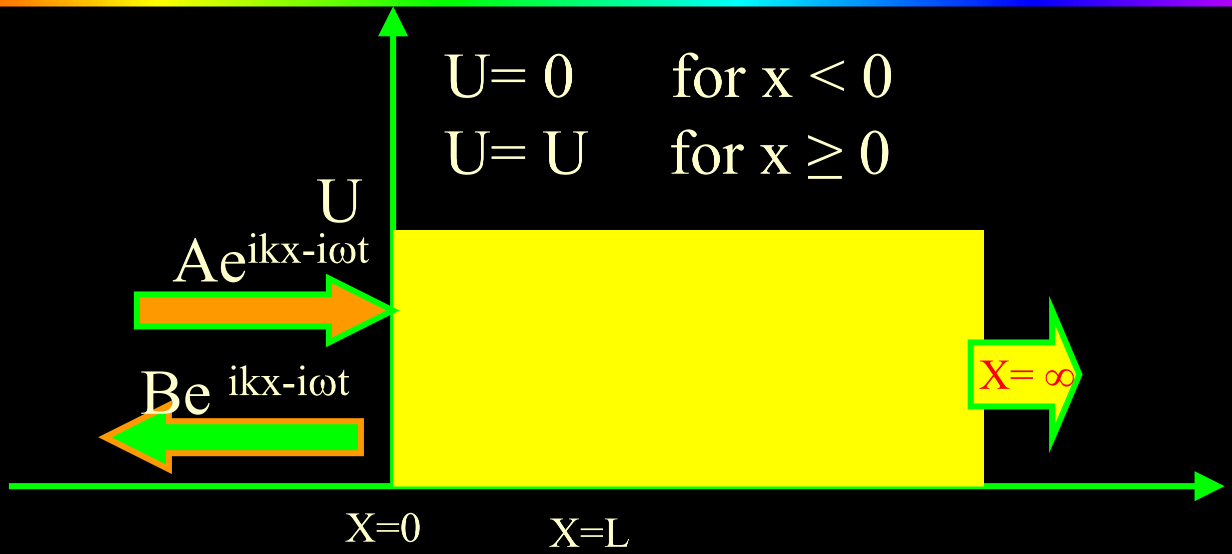
for particle to be completely transmitted



For all other energies, T<1 and R>0 !!!

This is Quantum Mechanics in your face !

Special Case: A Potential Step



In region I (X<0) : $\Psi_{\mathrm{I}}(x,t) = Ae^{ikx-i\omega t} + Be^{-ikx-i\omega t}$

In region II (X ≥ 0) : $\Psi_{\mathrm{II}}(x,t) = Ce^{-\alpha x-i\omega t}$ $\boxed{+De^{\alpha x-i\omega t}}$

Applying Continuity conditions of Ψ and $\dfrac{d\Psi}{dx}$ at x=0

$\mathrm{A+B=C}$ & $\mathrm{ikA - ikB = -}\alpha\mathrm{C}$; Eliminating C $\Rightarrow \mathrm{ikA - ikB} = -\alpha(A+B)$

Defining Penetration Depth $\delta = \dfrac{1}{\alpha} \Rightarrow \dfrac{\hbar}{\sqrt{2m(U-E)}}$,

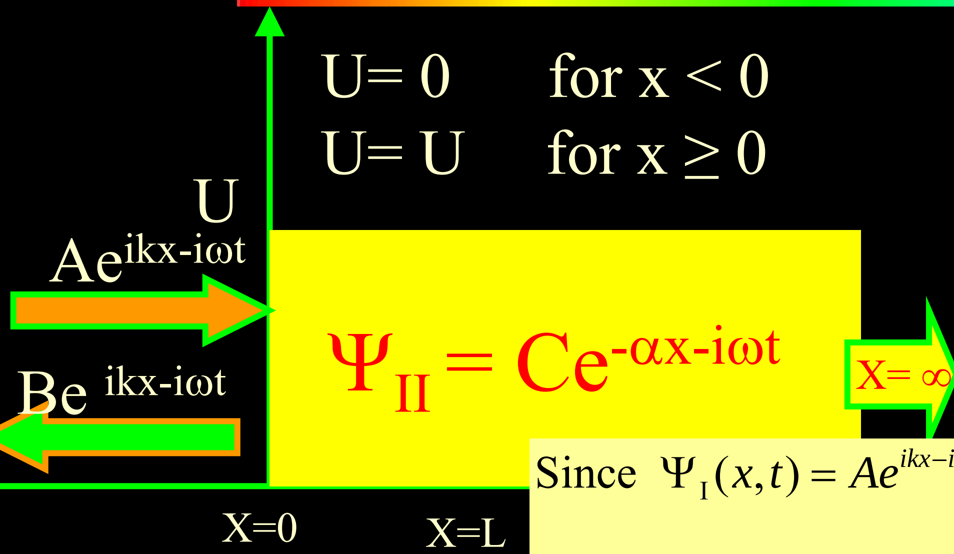
rewrite as $\mathrm{ik}\delta\mathrm{A} - \mathrm{ik}\delta\mathrm{B} = -(\mathrm{A+B}) \Rightarrow \mathrm{A}(1+\mathrm{ik}\delta) = -\mathrm{B}(1-\mathrm{ik}\delta)$

$\Rightarrow \dfrac{\mathrm{B}}{\mathrm{A}} = -\dfrac{(1+\mathrm{ik}\delta)}{(1-\mathrm{ik}\delta)} \Rightarrow$ Reflection Coeff $\mathrm{R} = \dfrac{\mathrm{B^*B}}{\mathrm{A^*A}} = 1$; as expected

Transmission Probability in A Potential Step

U= 0 for x < 0

U= U for x ≥ 0



Since $\Psi_{I}(x,t) = Ae^{ikx-i\omega t} + Be^{-ikx-i\omega t}$; $\Psi_{II}(x,t) = Ce^{-\alpha x-i\omega t}$

Applying Continuity conditions of Ψ and $\frac{d\Psi}{dx}$ at x=0 :

$$A + B = C \Rightarrow \frac{C}{A} = 1 + \frac{B}{A} = 1 - \frac{(1+ik\delta)}{(1-ik\delta)}$$

$$\Rightarrow \frac{C}{A} = -\frac{2ik\delta}{1-ik\delta} \neq 0 \quad \Rightarrow \boxed{T = \left(\frac{C}{A}\right)\left(\frac{C}{A}\right)^{*} > 0!!!}$$

The particle burrows into the skin of the step barrier. If one has a barrier of width L=δ, particle escapes thru the barrier.

penetration distance Δx= distance for which prob. drops by 1/e.

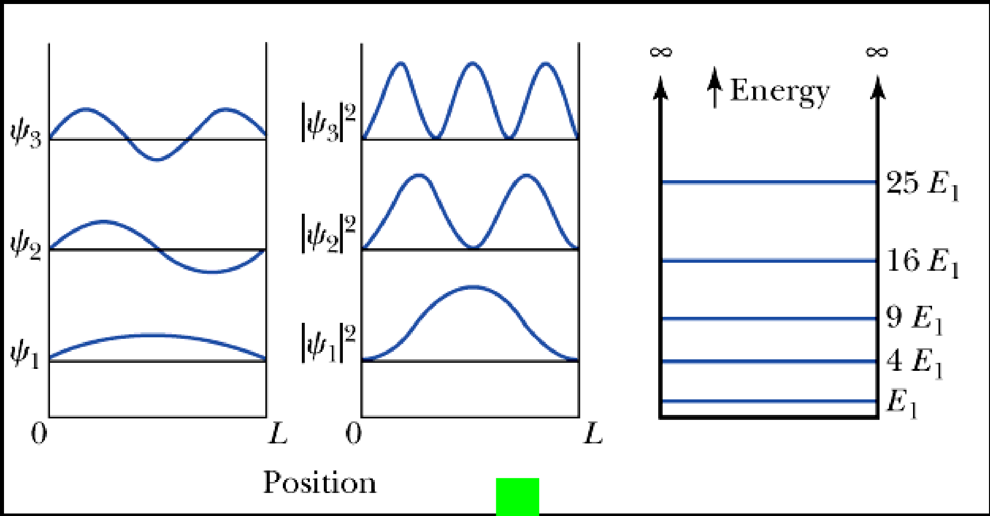
$|\psi(x=\Delta x)|^2 = C^2 e^{-2\alpha\Delta x} = C^2 e^{-1}$; happens when $2\alpha\Delta x = 1$ or $\boxed{\Delta x = \frac{1}{2}\ \frac{\hbar}{\sqrt{2m(U-E)}}}$

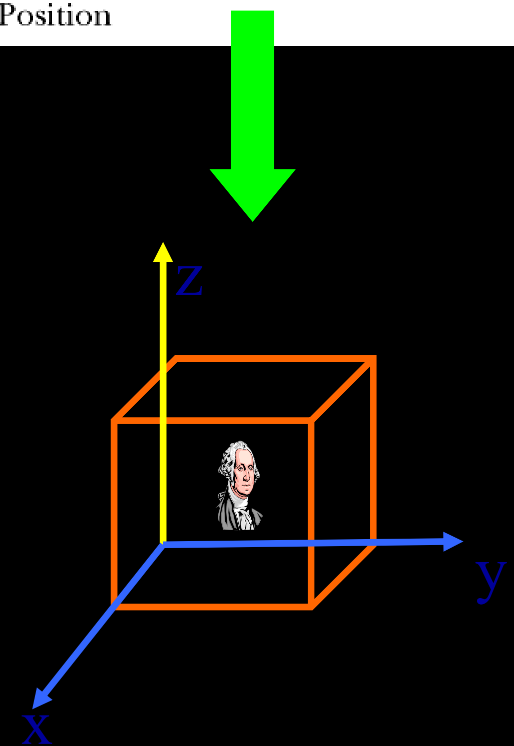
QM in 3 Dimensions

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

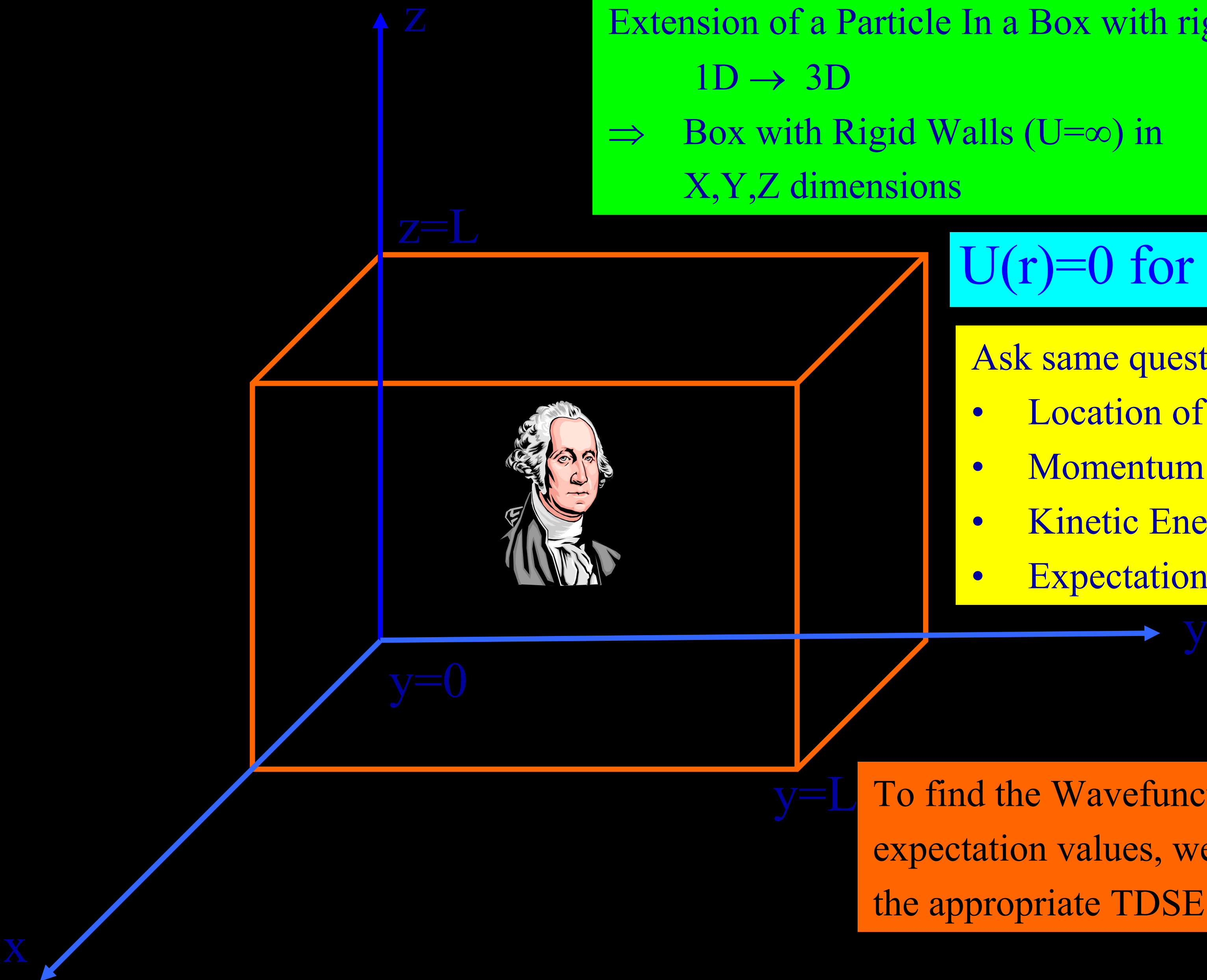
$$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z$$

- 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 ($U=\infty$) in X,Y,Z dimensions

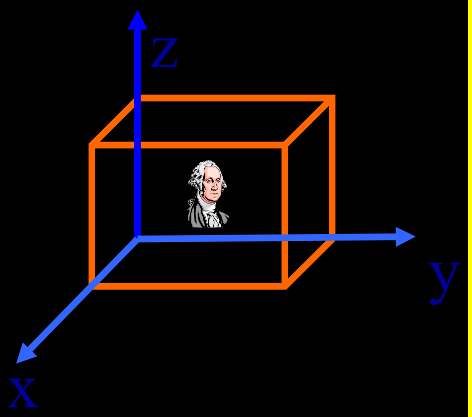
$U(r)=0$ for $(0<x,y,z,<L)$

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:

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

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

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

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

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

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

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

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 $n_1, n_2, n_3 = 0!$ $(why?)$

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

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

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

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

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

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

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

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

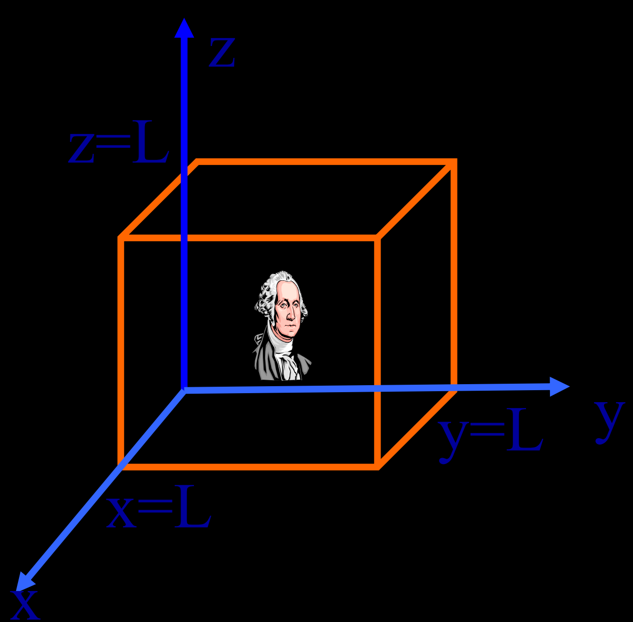
Particle in 3D Box : Energy Spectrum & Degeneracy

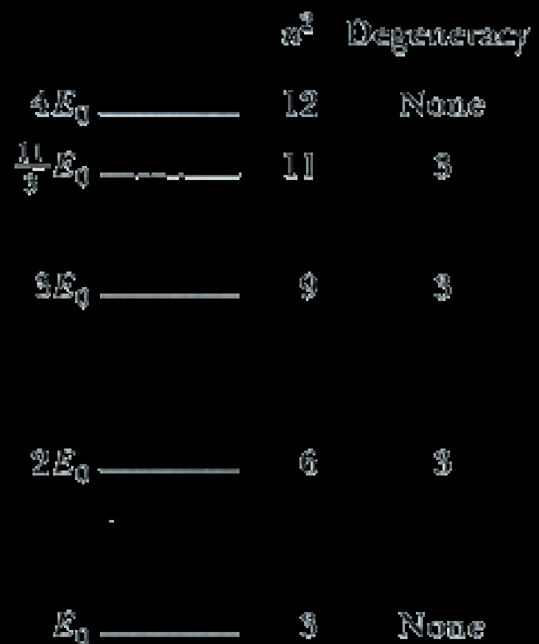
$$E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2); \quad n_i = 1,2,3\ldots\infty,\ n_i \neq 0$$

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

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

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

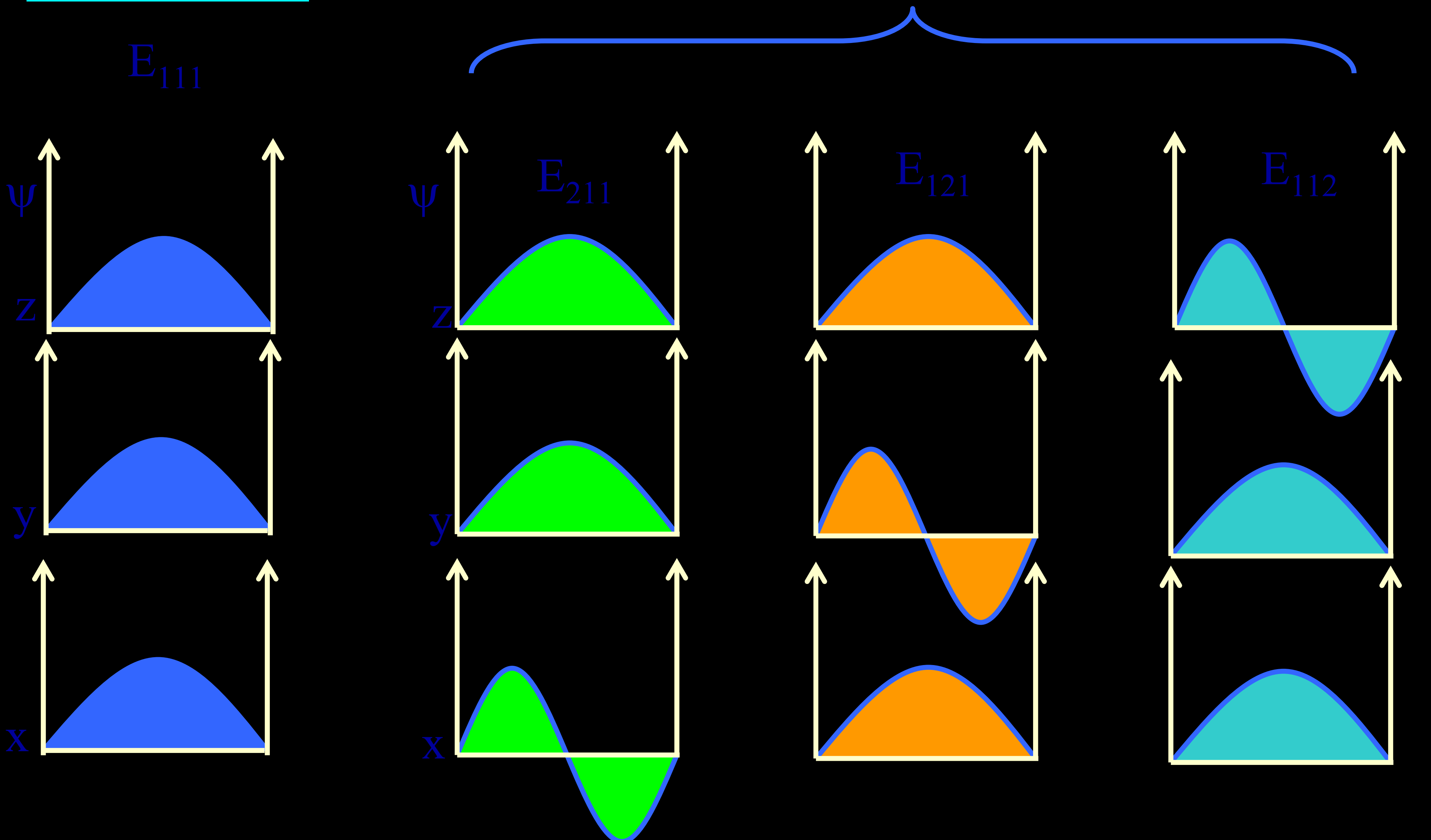




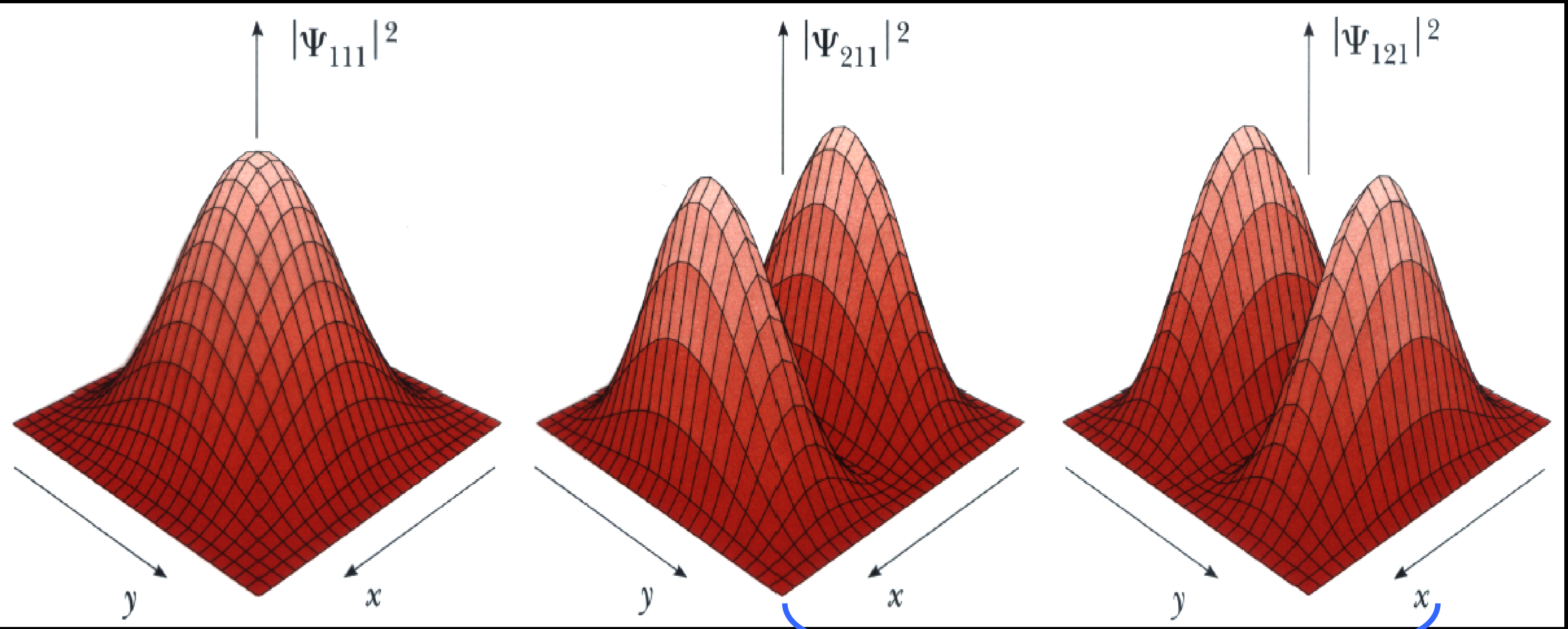
Degenerate States

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

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

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