Physics 2D Lecture Slides
Nov 26

Vivek Sharma
UCSD Physics

Expectation Values & Operators: More Formally

- Observable: Any particle property that can be measured
  - X,P, KE, E or some combination of them,e,g: x^2
  - How to calculate the probable value of these quantities for a QM state ?
- Operator: Associates an **operator** with each observable
  - Using these Operators, one calculates the average value of that Observable
  - The Operator acts on the Wavefunction (Operand) & extracts info about the Observable in a straightforward way→ gets Expectation value for that observable

$$< Q >= \int_{-\infty}^{+\infty} \Psi^*(x,t)\ [\hat{Q}]\ \Psi^*(x,t)dx$$

Q is the observable, $[\hat{Q}]$ is the operator

& $< Q >$ is the Expectation value

Examples: $[\mathrm{X}] = \mathrm{x}$, $\quad [\mathrm{P}] = \frac{\hbar}{\mathrm{i}} \frac{d}{dx}$

$$[\mathrm{K}] = \frac{[\mathrm{P}]^2}{2\mathrm{m}} = \frac{-\hbar^2}{2\mathrm{m}} \frac{\partial^2}{\partial x^2} \qquad [\mathrm{E}] = \mathrm{i}\hbar \frac{\partial}{\partial t}$$

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	$i\hbar\frac{\partial}{\partial t}$

Operators → Information Extractors

Plug & play form

$[p]$ or $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$ Momentum Operator

gives the value of average mometum in the following way:

$$\langle p\rangle = \int_{-\infty}^{+\infty} \psi^*(x)[p]\psi(x)dx = \int_{-\infty}^{+\infty} \psi^*(x)\left(\frac{\hbar}{i}\right)\frac{d\psi}{dx}dx$$

Similerly :

$[K]$ or $\hat{K} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ gives the value of average KE

$$\langle K\rangle = \int_{-\infty}^{+\infty} \psi^*(x)[K]\psi(x)dx = \int_{-\infty}^{+\infty} \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}\right)dx$$

Similerly

$$\langle U\rangle = \int_{-\infty}^{+\infty} \psi^*(x)[U(x)]\psi(x)dx$$: plug in the U(x) fn for that case

and $$\langle E\rangle = \int_{-\infty}^{+\infty} \psi^*(x)[K+U(x)]\psi(x)dx = \int_{-\infty}^{+\infty} \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U(x)\right)dx$$

Hamiltonian Operator **[H] = [K] +[U]**

The Energy Operator **$[E] = i\hbar\frac{\partial}{\partial t}$** informs you of the average energy

[H] & [E] Operators

- [H] is a function of x
- [E] is a function of t …….they are really different operators
- But they produce identical results when applied to any solution of the time-dependent Schrodinger Eq.

- [H]Ψ(x,t) = [E] Ψ(x,t)

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)\right]\Psi(x,t)=\left[i\hbar\frac{\partial}{\partial t}\right]\Psi(x,t)$$

- Think of S. Eq as an expression for Energy conservation for a Quantum system

Where do Operators come from ? A touchy-feely answer

Example : $[p]$ The momentum Extractor (operator):

Consider as an example: Free Particle Wavefunction

$$\Psi(x,t) = Ae^{i(kx-wt)} \quad ; \; k = \frac{2\pi}{\lambda}\,,\; \lambda = \frac{h}{p} \Rightarrow k = \frac{p}{\hbar}$$

rewrite $\Psi(x,t) = Ae^{i(\frac{p}{\hbar}x-wt)}$; $\dfrac{\partial\Psi(x,t)}{\partial x} = i\dfrac{p}{\hbar}Ae^{i(\frac{p}{\hbar}x-wt)} = i\dfrac{p}{\hbar}\Psi(x,t)$

$$\Rightarrow \left[\frac{\hbar}{i}\frac{\partial}{\partial x}\right]\Psi(x,t) = p\,\Psi(x,t)$$

So it is not unreasonable to associate $[p]=\left[\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}\right]$ with observable p

Example : Average Momentum of particle in box

- Given the symmetry of the 1D box, we argued last time that <p> = 0 : now some inglorious math to prove it !
  - Be lazy, when you can get away with a symmetry argument to solve a problem..do it & avoid the evil integration & algebra…..but be sure!

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x) \quad \& \quad \psi^*{}_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$$

$$< p >= \int_{-\infty}^{+\infty}\psi^*[p]\psi\,dx = \int_{-\infty}^{\infty}\psi^*\left[\frac{\hbar}{i}\frac{d}{dx}\right]\psi\,dx$$

$$< p >= \frac{\hbar}{i}\frac{2}{L}\frac{n\pi}{L}\int_{-\infty}^{\infty}\sin(\frac{n\pi}{L}x)\cos(\frac{n\pi}{L}x)dx$$

$$\text{Since } \int \text{sinax cosax dx} = \frac{1}{2a}\sin^2 ax \quad \text{...here a} = \frac{n\pi}{L}$$

$$\Rightarrow < p >= \frac{\hbar}{iL}\left[\sin^2(\frac{n\pi}{L}x\right]_{x=0}^{x=L} = 0 \text{ since } \mathrm{Sin}^2(0) = \mathrm{Sin}^2(n\pi) = 0$$

We knew THAT before doing any math !

Quiz 1: What is the <p> for the Quantum Oscillator in its symmetric ground state

Quiz 2: What is the <p> for the Quantum Oscillator in its asymmetric first excited state

But what about the <KE> of the Particle in Box ?

$< p >= 0$ so what about expectation value of $K = \frac{p^2}{2m}$?

$< K >= 0$ because $< p >= 0$; clearly not, since we showed $E = KE \neq 0$

Why ? What gives ?

Because $p_n = \pm\sqrt{2mE_n} = \pm\frac{n\pi\hbar}{L}$;   "±" is the key!

AVERAGE p =0 , particle is moving back & forth

$<KE> = <\frac{p^2}{2m}> \neq 0$ not $\frac{<p^2>}{2m}$!

Be careful when being "lazy"

Quiz: what about <KE> of a quantum Oscillator?

Does similar logic apply??

Schrodinger Eqn: Stationary State Form

- Recall→ when potential does not depend on time explicitly U(x,t) =U(x) only…we used separation of x,t variables to simplify Ψ(x,t) = ψ(x) ϕ(t) & broke S. Eq. into two: one with x only and another with t only

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

$$i\hbar\frac{\partial\phi(t)}{\partial t} = E\phi(t)$$

$$\Psi(x,t) = \psi(x)\phi(t)$$

How to put Humpty-Dumpty back together ? e.g to say how to go from an expression of ψ(x)→Ψ(x,t) which describes time-evolution of the overall wave function

Schrodinger Eqn: Stationary State Form

Since $\frac{\mathrm{d}}{\mathrm{dt}}[\ln f(t)] = \frac{1}{f(t)}\frac{\mathrm{d}f(t)}{\mathrm{dt}}$

In $i\hbar\frac{\partial\phi(t)}{\partial \mathrm{t}} = E\phi(t)$, rewrite as $\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial \mathrm{t}} = \frac{E}{i\hbar} = -\frac{iE}{\hbar}$

and integrate both sides w.r.t. time

$$\int_{t=0}^{t=t}\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial \mathrm{t}}dt = \int_0^t -\frac{iE}{\hbar}dt \Rightarrow \int_0^t \frac{1}{\phi(t)}\frac{\mathrm{d}\phi(t)}{\mathrm{dt}}dt = -\frac{iE}{\hbar}$$

$\therefore \ln\phi(t) - \ln\phi(0) = -\frac{iE}{\hbar}t$, now exponentiate both sides

$\Rightarrow \phi(t) = \phi(0)e^{-\frac{iE}{\hbar}t}$; $\phi(0)$ = constant= initial condition = 1 (e.g)

$\Rightarrow \phi(t) = e^{-\frac{iE}{\hbar}t}$ & Thus $\Psi(\mathrm{x,t}) = \psi(\mathrm{x})e^{-\frac{iE}{\hbar}t}$ where E = energy of system

Schrodinger Eqn: Stationary State Form

$$P(x,t) = \Psi^*\Psi = \psi^*(x)\, e^{+\frac{iE}{\hbar}t}\psi(x)\, e^{-\frac{iE}{\hbar}t} = \psi^*(x)\psi(x)e^{\frac{iE}{\hbar}t-\frac{iE}{\hbar}t} = |\psi(x)|^2$$

In such cases, P(x,t) is INDEPENDENT of time.

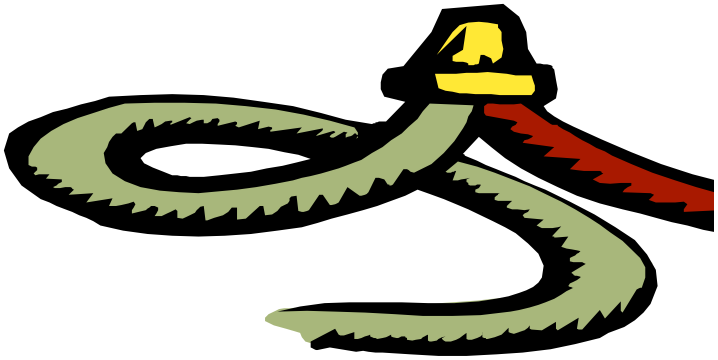
These are called "stationary" states because Prob is independent of time

Examples : Particle in a box (why?)

: Quantum Oscillator (why?)

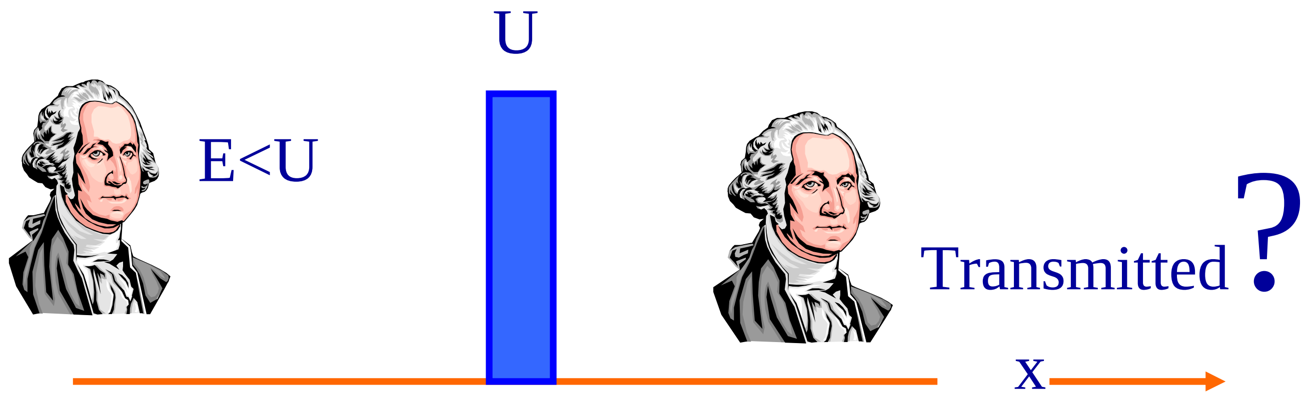
Total energy of the system depends on the spatial orientation of the system : charteristic of the potential situation !

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



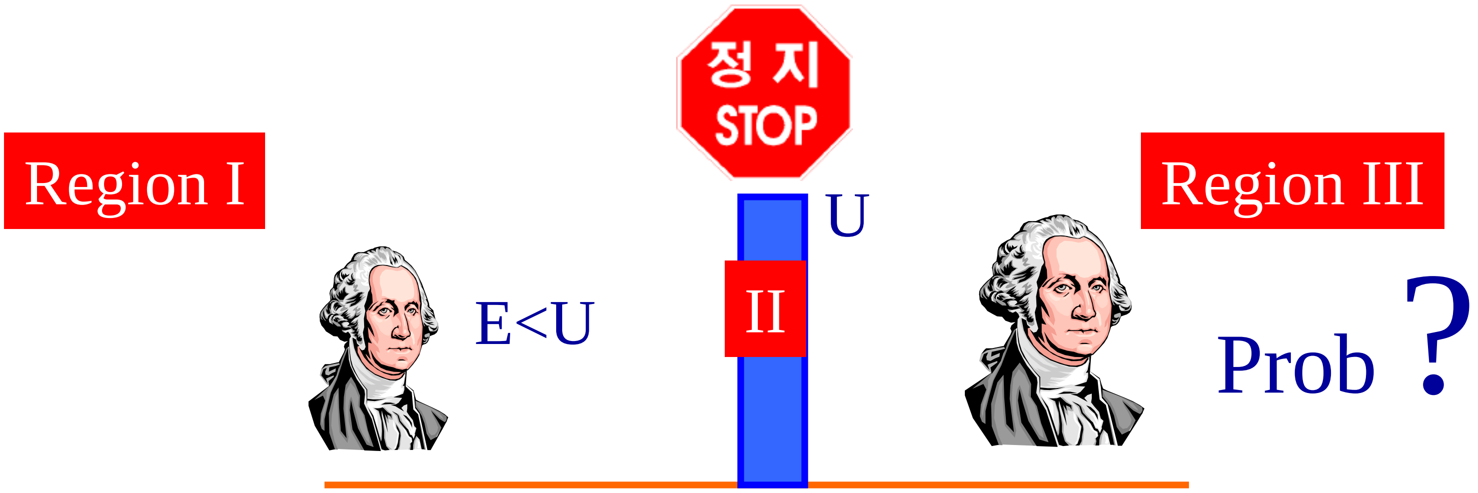
Description of Potential		
$U = 0$	$x < 0$	(Region I)
$U = U$	$0 < x < L$	(Region II)
$U = 0$	$x > L$	(Region III)

Consider George as a “free Particle/Wave” with Energy E incident from Left

Free particle are under no Force; have wavefunctions like

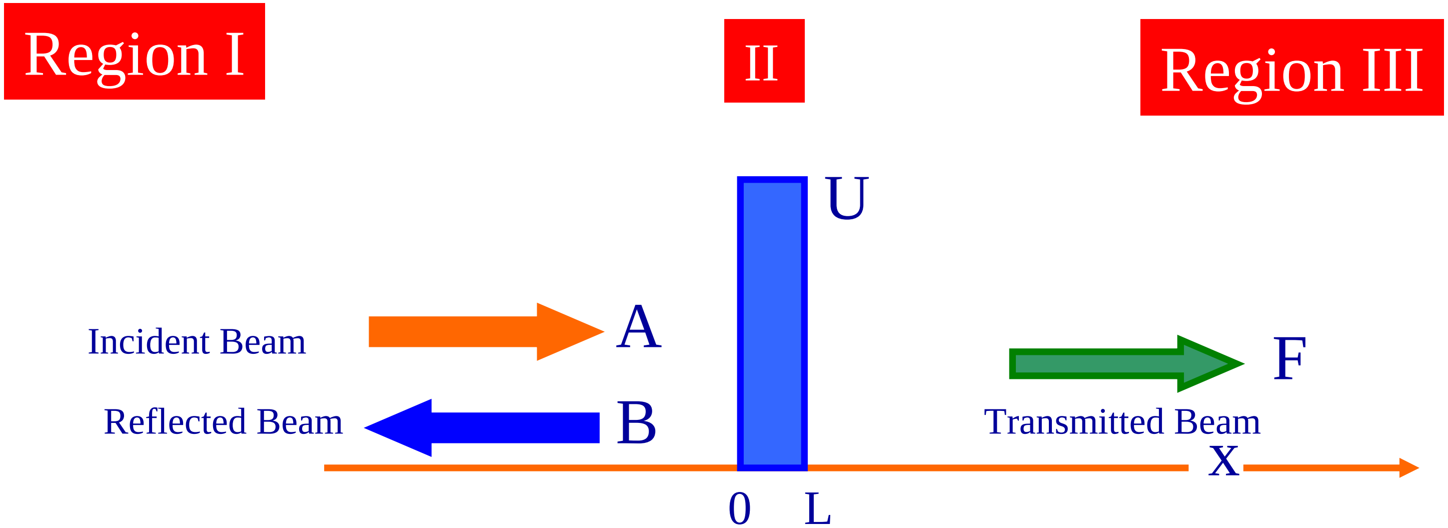
$$\Psi = A\, e^{i(kx-wt)} \text{ or } B\, e^{i(-kx-wt)}$$

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 : $\Psi_{\text{I}}(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$ = 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: $\Psi_{\text{III}}(x,t) = Fe^{i(kx-\omega t)} + Ge^{i(-kx-\omega t)} = \textit{transmitted}$

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 $\Psi_{\text{III}}(x,t) = Fe^{i(kx-\omega t)}$ 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

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

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

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

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

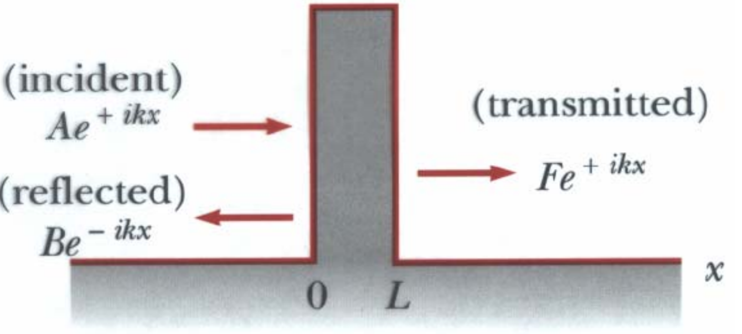
Solutions are of form $\psi(x) \propto e^{\pm\alpha x}$

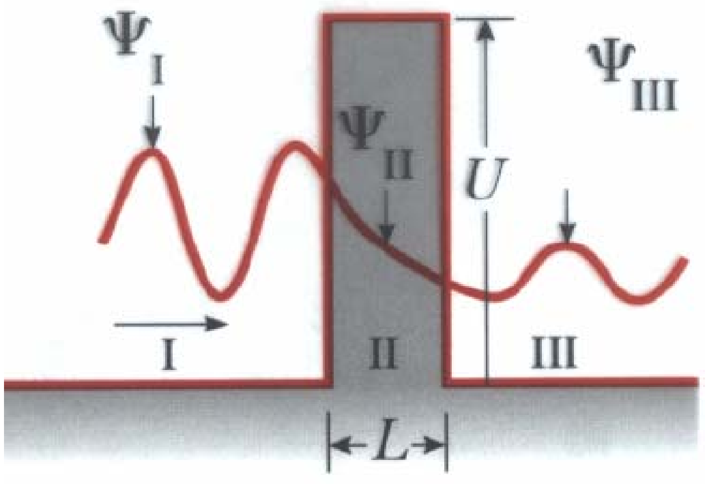
$$\boxed{\Psi_{II}(x,t) = Ce^{+\alpha x - i\omega t} + De^{-\alpha x - i\omega t}} \quad 0<x<L$$

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

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

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





Continuity Conditions Across Barrier

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

$$A+B=C+D \quad (1)$$

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

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

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

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

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

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

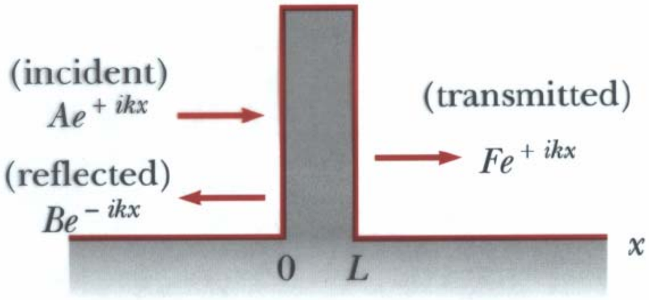
Four equations & four unknowns

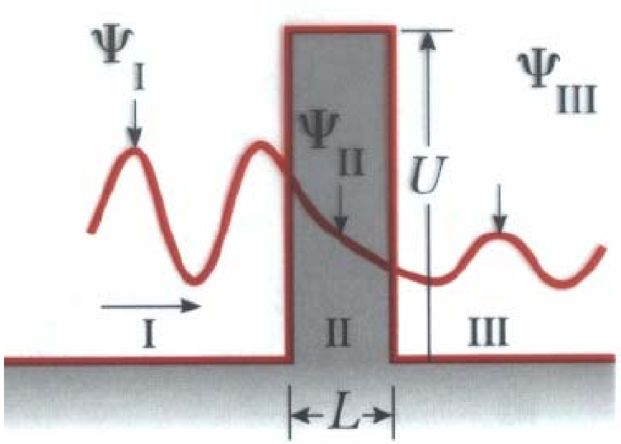
Cant determine A,B,C,D but if you

Divide thruout by A in all 4 equations :

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

That's what we need any way





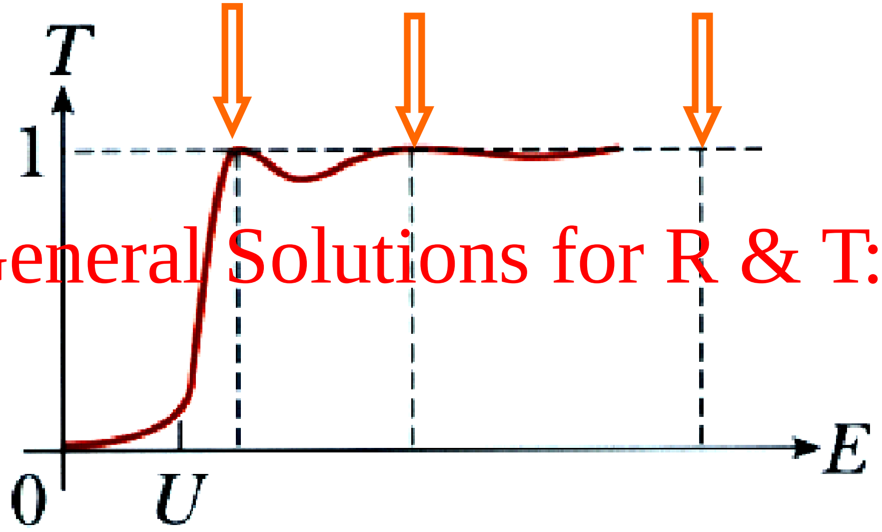
Potential Barrier when E < U

Expression for Transmission Coeff T=T(E) :

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

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

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

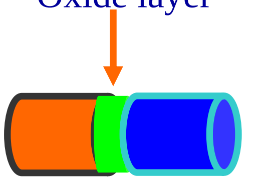
At other values of E, some particles are

reflected back ..even though E>U !!

That's the Wave nature of the

Quantum particle

Ceparated in Coppertino



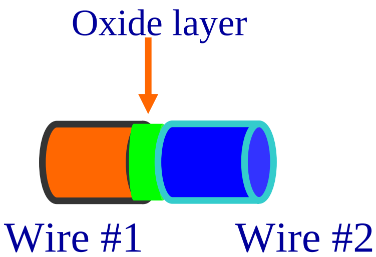
Solved Example 6.1 (...that I made such a big deal about yesterday)

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?

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

$$\alpha = \frac{\sqrt{2m(U-E)}}{\hbar}, k = \frac{\sqrt{2mE}}{\hbar}$$



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

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

$$\Rightarrow \alpha = \frac{\sqrt{2m_e(U-E)}}{\hbar} = \frac{\sqrt{2\times 511 kev/c^2(3.0\times10^{-3} keV)}}{1.973 \text{ keV.Å/c}} = 0.8875\text{Å}^{-1}$$

Substitute in expression for T=T(E)

$$T = \left[1 + \frac{1}{4}\left(\frac{10^2}{7(10-7)}\right)\sinh^2(0.8875\text{Å}^{-1})(50\text{Å})\right]^{-1} = 0.963\times10^{-38}(small)!!$$

However, for L=10Å; $T = 0.657\times10^{-7}$

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

1 mA current =I= $\frac{Q=Nq_e}{t}$ $\Rightarrow N = 6.25\times10^{15}$ *electrons*

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

$N_T = N.T = (6.25\times10^{15}\ electrons)\times \boxed{T}$;

For L=10 Å, $T=0.657\times10^{-7} \Rightarrow N_T = 4.11\times10 \Rightarrow \boxed{I_T = 65.7\ pA}$!!

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

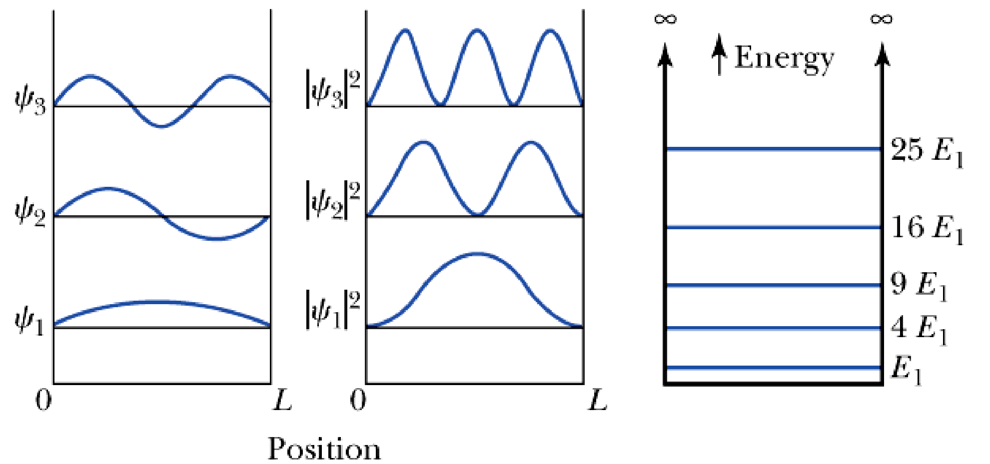
Oxide thickness makes all the difference !
That's why from time-to-time one needs to
Scrape off the green stuff off the naked wires

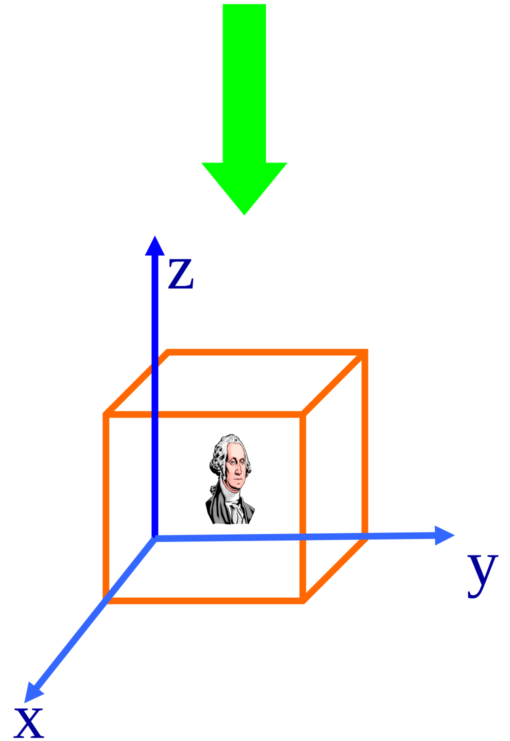
QM in 3 Dimensions

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



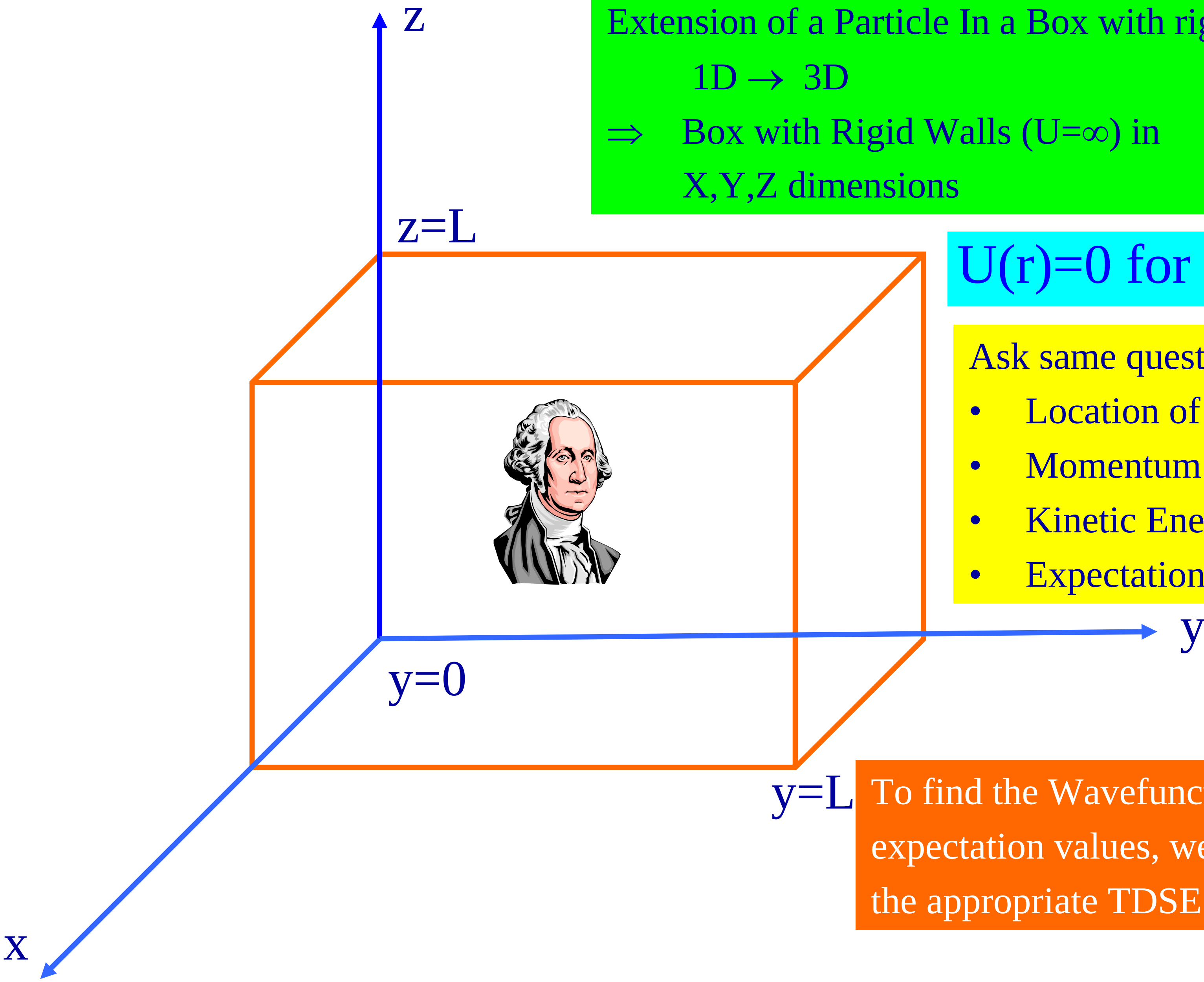


Quantum Mechanics In 3D: Particle in 3D Box

Extension of a Particle In a Box with rigid walls

1D → 3D

⇒ Box with Rigid Walls (U=∞) in X,Y,Z dimensions



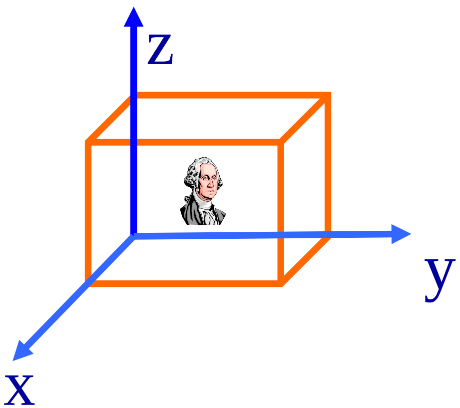
U(r)=0 for (0<x,y,z,<L)

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:

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

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

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

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

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 $\Rightarrow$

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

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

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

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

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

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

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

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

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

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

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

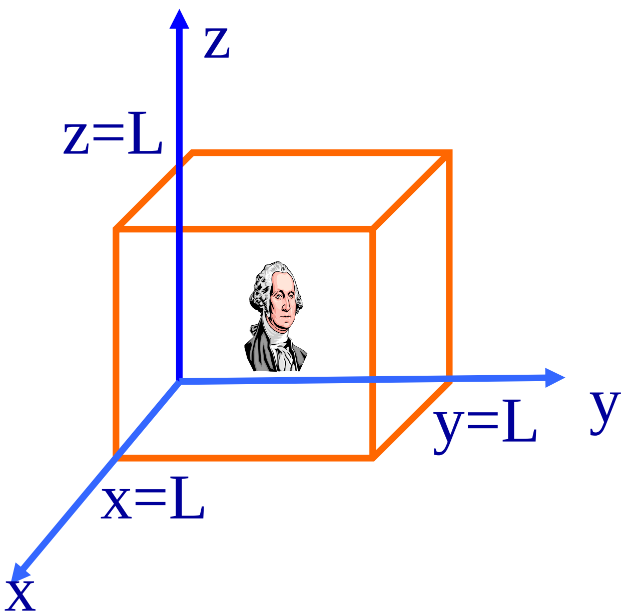
Particle in 3D Box : Energy Spectrum & Degeneracy

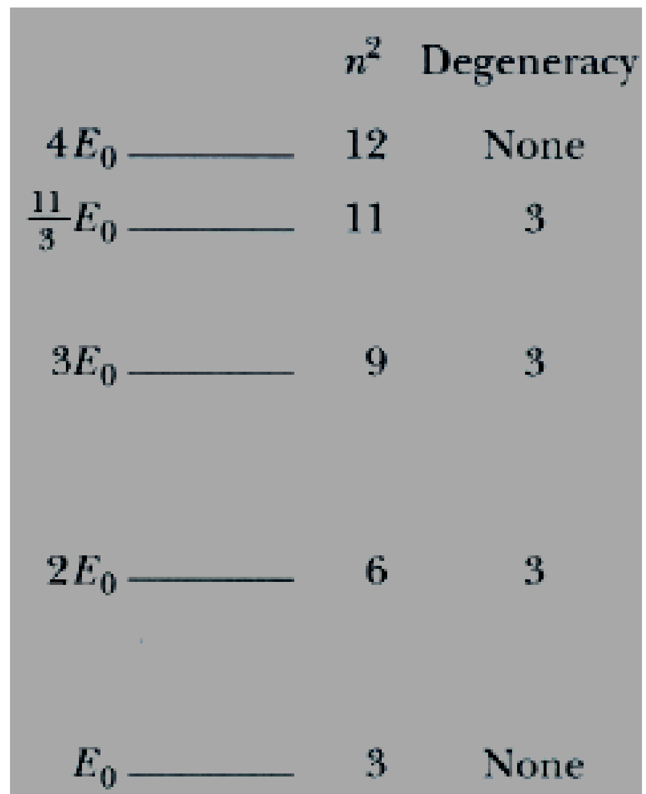
$$E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2); \quad n_i = 1,2,3\ldots\infty,\ n_i \neq 0$$

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



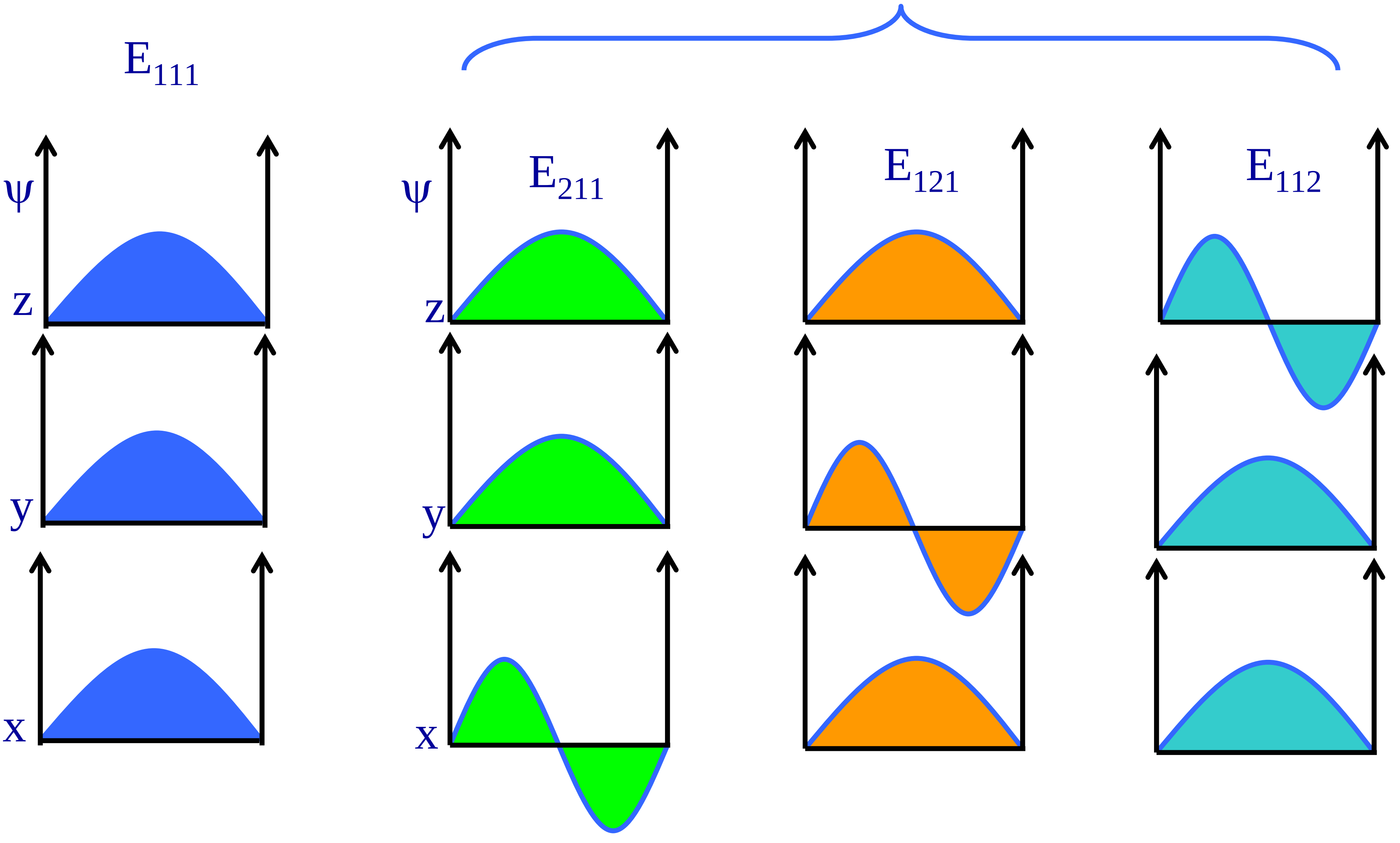


	n^2	Degeneracy
$4E_0$	12	None
$\frac{11}{3}E_0$	11	3
$3E_0$	9	3
$2E_0$	6	3
E_0	3	None

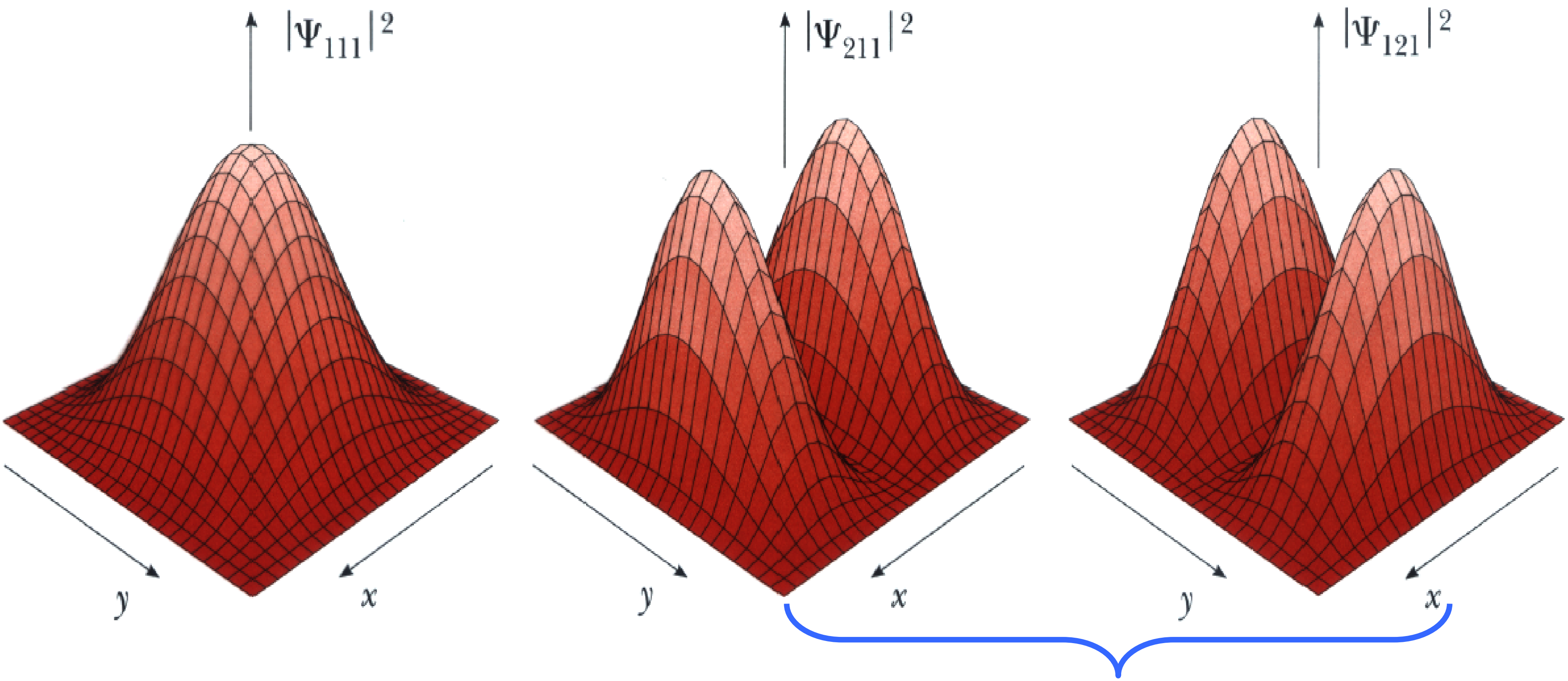
Degenerate States

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

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

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