

**Confirmed: 2D Final Exam:  
Thursday 18<sup>th</sup> March 11:30-2:30 PM WLH 2005**

**Course Review 14<sup>th</sup> March 10am WLH 2005 (TBC)**

Date	Time	Read	Topic	HW problems for the week	Location
Monday	11:00 am	Ch 5	Quantum Mechanics in 1 Dimension		WLH 2005
Tuesday	8:00 pm	Ch 5	Quantum Mechanics in 1 Dimension	Ch 5 :20, 21, 25, 30, 33, 34, 35, 39, 40	WLH 2005
Wednesday	11:00 am	Ch 6	Tunneling Phenomenan	Read Section 6.1	WLH 2005
Wednesday	3:00 pm	Ch 5	Discussion	-	WLH 2005
Thursday	5:00-6:20 pm	-	Problem Session		Peterson 108
Friday	11:00am	-	Quiz	Ch 5	WLH 2005



**Physics 2D Lecture Slides  
Lecture 26: Mar 3<sup>rd</sup>**

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# Measurement Expectation: Statistics Lesson

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

$$\langle x \rangle = \frac{n_1 x_1 + n_2 x_2 + n_3 x_3 + \dots + n_i x_i}{n_1 + n_2 + n_3 + \dots + n_i} = \frac{\sum_{i=1}^n n_i x_i}{N} = \frac{\int_{-\infty}^{\infty} x P(x) dx}{\int_{-\infty}^{\infty} P(x) dx}$$

For a general Fn f(x)

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

Sharpness of A Distr:

Scatter around average

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

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

$\sigma = \text{small} \rightarrow \text{Sharp distr.}$

Uncertainty  $\Delta X = \sigma$

## Particle in the Box, n=1, find $\langle x \rangle$ & $\Delta x$ ?

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

$$\begin{aligned} \langle x \rangle &= \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L} x\right) x \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L} x\right) dx \\ &= \frac{2}{L} \int_0^L x \sin^2\left(\frac{\pi}{L} x\right) dx, \text{ change variable } \theta = \left(\frac{\pi}{L} x\right) \end{aligned}$$

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

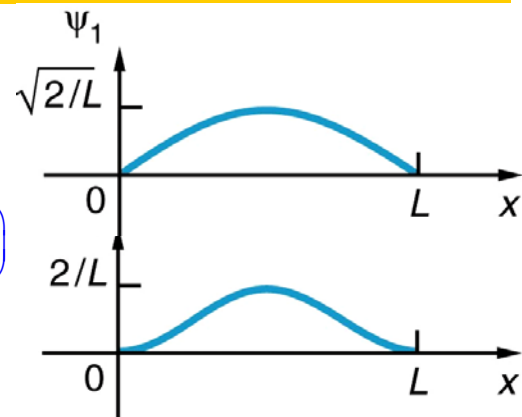
$$\Rightarrow \langle x \rangle = \frac{2L}{2\pi^2} \left[ \int_0^{\pi} \theta d\theta - \int_0^{\pi} \theta \cos 2\theta d\theta \right] \text{ use } \int u dv = uv - \int v du$$

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

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

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

$\Delta X = 20\%$  of L, Particle not sharply confined in Box



## 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

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

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

&  $\langle Q \rangle$  is the Expectation value

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

$$[K] = \frac{[P]^2}{2m} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$[E] = i\hbar \frac{\partial}{\partial t}$$

**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

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

gives the value of average momentum in the following way:

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

Similarly :

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

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

Similarly

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

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

$$\text{Hamiltonian Operator } [H] = [K] + [U]$$

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

## [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.

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

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

- 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

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

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

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

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

## Example : Average Momentum of particle in box

- Given the symmetry of the 1D box, we argued last time that  $\langle p \rangle = 0$   
: 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!

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

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

$$\langle p \rangle = \frac{\hbar}{i} \frac{2}{L} \frac{n\pi}{L} \int_{-\infty}^{+\infty} \sin\left(\frac{n\pi}{L}x\right) \cos\left(\frac{n\pi}{L}x\right) dx$$

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

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

We knew THAT before doing any math !

Quiz 1: What is the  $\langle p \rangle$  for the Quantum Oscillator in its symmetric ground state

Quiz 2: What is the  $\langle p \rangle$  for the Quantum Oscillator in its asymmetric first excited state

## But what about the $\langle KE \rangle$ of the Particle in Box ?

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

$\langle K \rangle = 0$  because  $\langle p \rangle = 0$ ; 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!

The AVERAGE  $p = 0$ , since particle is moving back & forth

$\langle KE \rangle = \langle \frac{p^2}{2m} \rangle \neq 0$ ; not  $\frac{\langle p^2 \rangle}{2m}$  !

Be careful when being "lazy"

Quiz: what about  $\langle KE \rangle$  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  $\Psi(x,t) = \psi(x)\phi(t)$  & broke S. Eq. into two: one with  $x$  only and another with  $t$  only

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

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

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

How to put **Humpty-Dumpty** back together ? e.g to say how to go from an expression of  $\psi(x) \rightarrow \Psi(x,t)$  which describes time-evolution of the overall wave function

## Schrodinger Eqn: Stationary State Form

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

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

and integrate both sides w.r.t. time

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

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

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

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

## 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.

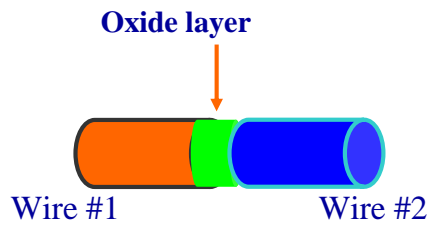
These are called "stationary" states because Prob is independent of time

**Examples : Particle in a box (why?)**

**: Quantum Oscillator (why?)**

Total energy of the system depends on the spatial orientation of the system : characteristic of the potential U(x,t) !

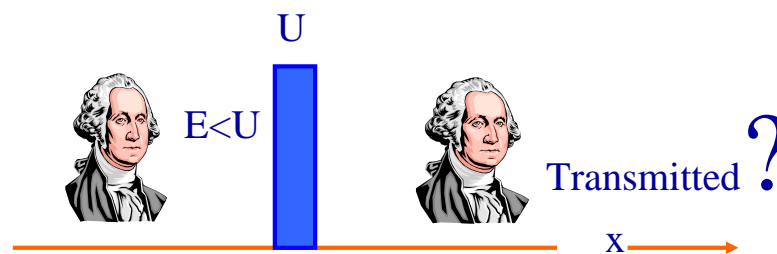
# The Case of a Rusty “Twisted Pair” of Naked Wires & How Quantum Mechanics Saved ECE Majors !



- 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  $\text{Cu} \rightarrow \text{Cu}_2\text{O}$
  - In wet air  $\text{Cu} \rightarrow \text{Cu}(\text{OH})_2$  (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  $\rightarrow$  no EE, no ECE !!
- All ECE majors must now switch to Chemistry instead & play with benzene !!! Bad news !



## Potential Barrier

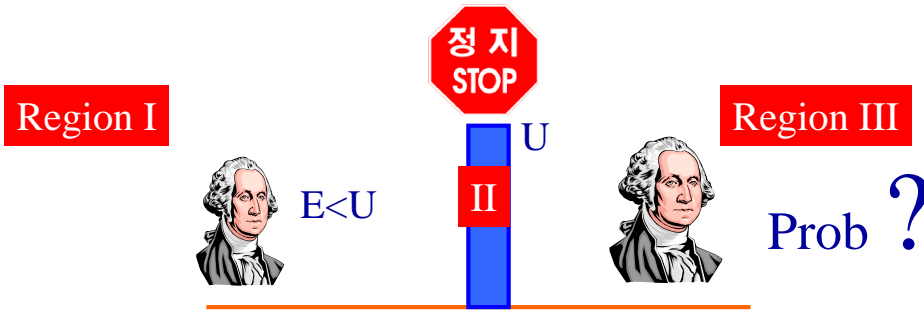


Description of Potential		
$U = 0$	$x < 0$	(Region I)
$U = U$	$0 < x < L$	(Region II)
$U = 0$	$x > L$	(Region III)

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

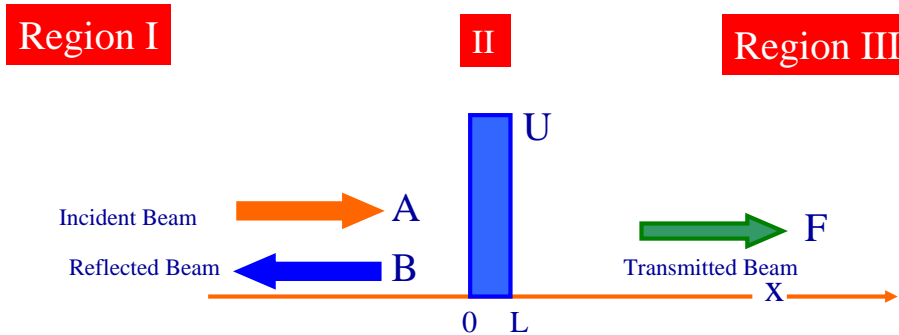
$$\Psi = A e^{i(kx - \omega t)} \text{ or } B e^{i(-kx - \omega t)}$$

# 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  $E > U \rightarrow$  Particle just goes over the barrier (gets transmitted)
  - When  $E < U \rightarrow$  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:  $R = \frac{|B|^2}{|A|^2}$  = 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  $T = \frac{|F|^2}{|A|^2}$

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

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

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

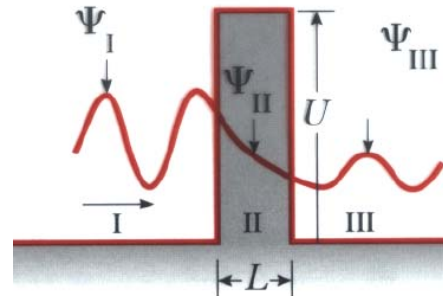
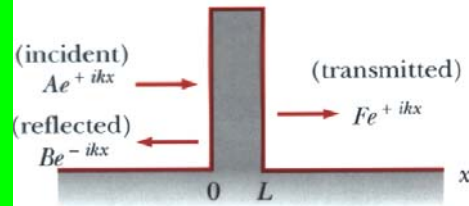
Solutions are of form  $\psi(x) \propto e^{\pm\alpha x}$

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

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

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

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



# 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  $\frac{d\psi(x)}{dx} \Rightarrow$

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

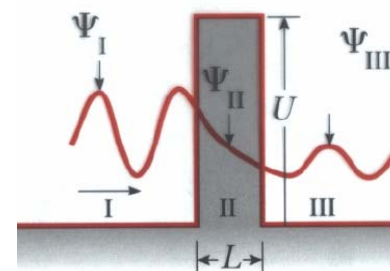
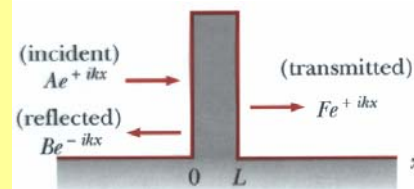
Four equations & four unknowns

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 anyway



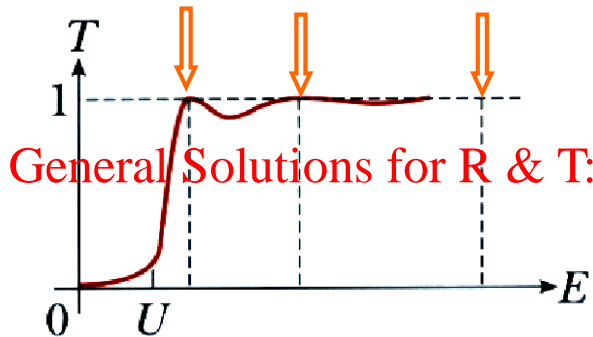
## Potential Barrier when $E < U$

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



Above equation holds only for  $E < U$

For  $E > U$ ,  $\alpha = \text{imaginary}$

$\sinh(\alpha L)$  becomes oscillatory

This leads to an Oscillatory  $T(E)$  and

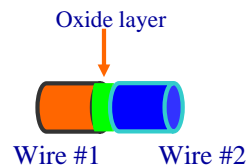
Transmission resonances occur where

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

## Ceprated in Coppertino

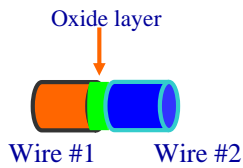


Solved Example 6.1 (...that I made such a big deal about yesterday)

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

Q: If a  $1.0\text{mA}$  current in one of the intertwined 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  $1.0\text{nm}$ ? What becomes of the remaining current?

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



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

Use  $\hbar = 1.973 \text{ keV} \cdot \text{\AA} / c$ ,  $m_e = 511 \text{ keV} / c^2$

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

Substitute in expression for  $T = T(E)$

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

However, for  $L = 10 \text{\AA}$ ;  $T = 0.657 \times 10^{-7}$

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

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

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

$$N_T = N \cdot T = (6.25 \times 10^{15} \text{ electrons}) \times [T];$$

$$\text{For } L = 10 \text{\AA}, T = 0.657 \times 10^{-7} \Rightarrow N_T = 4.11 \times 10 \Rightarrow [I_T = 65.7 \text{ pA}]!!$$

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

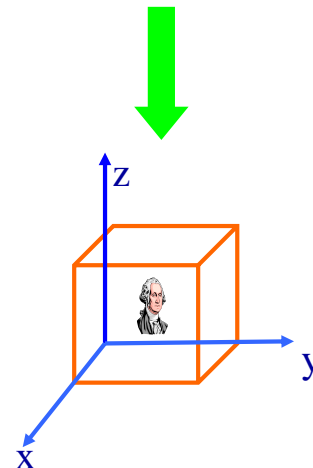
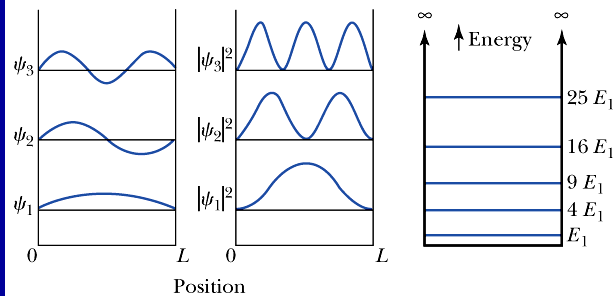
Oxide thickness makes all the difference !  
That's why from time-to-time one needs to Scrape off the green stuff off the naked wires

## 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  $\rightarrow$  3D rigid box
  - 1D Harmonic Oscillator  $\rightarrow$  3D Harmonic Oscillator
    - Keep an eye on the number of different integers needed to specify system  $1 \rightarrow 3$  (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

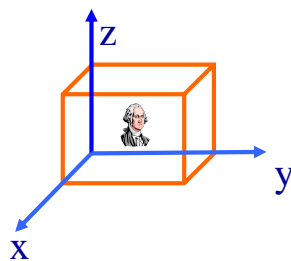
$U(r)=0$  for  $(0 < x, y, z, < L)$

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:

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

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

$$\begin{aligned} \text{So } -\frac{\hbar^2}{2m} \nabla^2 &= \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) + \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} \right) + \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \right) = [K] \\ &= [K_x] + [K_y] + [K_z] \end{aligned}$$

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 separable form:

$$\Psi(x, y, z, t) = \Psi(\vec{r}, t) = \psi(\vec{r}) e^{-iEt/\hbar}$$

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

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

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  $(0 < x, y, z, < L) \Rightarrow$

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

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

Continuity Conditions for  $\psi_i$  and its first spatial derivatives  $\Rightarrow \boxed{n_i \pi = k_i L}$

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

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

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

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

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

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

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

## Particle in 3D Box : Wave function Normalization Condition

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

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

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

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

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

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

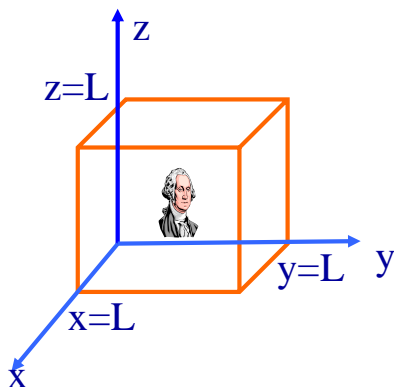
## Particle in 3D Box : Energy Spectrum & Degeneracy

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

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  $\psi(\vec{r}) = \psi(x, y, z)$  have same energy  $\Rightarrow$  degeneracy



Energy	$n^2$	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

$E_{111}$

