4E : The Quantum Universe

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4E : A Course on the Quantum Universe

- Quantum physics is the most exciting advance in the history of science. Its firestorm like birth and development makes it an excellent example of the symbiosis between theory and experimentation
- It is the fountainhead of Modern Chemistry, Biology and many fields of Engineering
- What to expect in this course:
  - You will see Quantum mechanics a few times as UCSD UG
    - For Example, 130 A,B,C series will be a formal and mathematical account of the methods of quantum Mechanics
  - This course will be a more conceptual and "intuitive" introduction to quantum physics
  - The last part of this course will be a survey of some interesting examples of the Quantum Universe:
    - Particle Physics
    - Astrophysics and Cosmology

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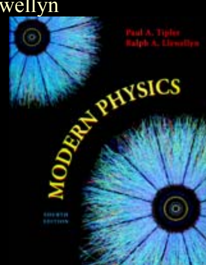
Some Bookkeeping Issues Related to This Course

- Course text: Modern Physics by Tipler, Llewellyn
  - 4th edition, Published by WH Freeman



- Instructor :
  - Vivek Sharma: modphys@ucsd.edu
  - 3314 Mayer Hall, Ph: (858) 534 1943
  - Office Hours:
    - Mon: 1:30-2:30pm, Tue: 2:30-3:30pm
- Teaching Assistant:
  - Jason Wright: jwright@physics.ucsd.edu
  - 5116 Mayer Hall
  - Office Hour: Thursday 3:00-4:00pm in Mayer 2101 (Tutorial Center)
- Class Web Site: http://modphys.ucsd.edu/4es05
  - Web page is important tool for this class, make sure you can access it

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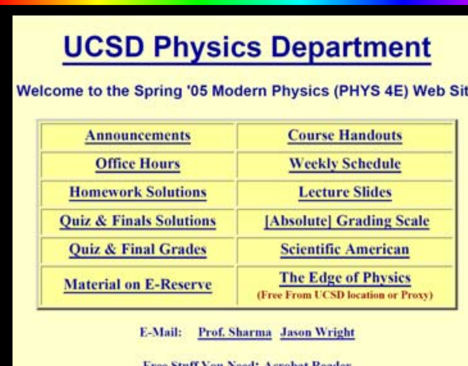
4E Website: http://modphys.ucsd.edu/4es05/



Pl. try to access this website and let me know if you have problems viewing any content.

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Weekly Schedule

Pl. attend discussion session on Wednesday and problem session on Thursday if you plan to do well in this course

General Class Schedule

Lecture	Monday	11:00-11:50 am	CNTR 217A	Prof. Sharma
Prof. Office Hour	Monday	1:30 - 2:30 pm	Mayer 3314	Prof. Sharma
Lecture	Tuesday	9:00-9:50 am	SOLIS 109	Prof. Sharma
Prof. Office Hour	Tuesday	2:30-3:30 pm	Mayer 3314	Prof. Sharma
Lecture	Wednesday	11:00-11:50 am	CNTR 217A	Prof. Sharma
Discussion	Wednesday	12:00-12:50 pm	SOLIS 109	Prof. Sharma/Jason Wright
TA Office Hour	Thursday	3:00-4:00 pm	Mayer 2101	Jason Wright
Problem Solving	Thursday	7:00-8:50 pm	SOLIS 111	Jason Wright
Lecture	Friday	11:00-11:50 am	CNTR 217A	Announce Quiz/Midterm Dates
Prof. Office Hour	Weekend	By Appointment	Mayer 3314	Prof. Sharma

Check the announcements page for important schedule changes

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Week 1 Schedule & HW

Date	Time	Read	Topic	HW problems for the week	Location
Monday	11:00 am	Ch. 3	Quantization of Charge, Light & Energy	Read Section 3.1	CNTR 217A
Tuesday	9:00 am	Ch. 3	Quantization of Charge, Light & Energy	Ch 3: 2,6,11,15,21,22	SOLIS 109
Wednesday	11:00 am	Ch. 3	Quantization of Charge, Light & Energy	Ch 3: 25,32,34,38,41	CNTR 217A
Wednesday	12:00 pm	-----	Discussion	-	SOLIS 109
Thursday	7:00-8:50 pm	-	Problem Session	Attempt problems before PS	SOLIS 111
Friday	11:00am	Ch..3	Quantization of Charge, Light & Energy	Ch. 3: 42,46	CNTR 217A

Check the announcements page for important schedule changes

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Quizzes, Final and Grades

- Course score = 60% Quiz + 40% Final Exam
  - 5 quizzes if I can schedule them, best 4 (=n-1) scores used
    - Two problems in each quiz, 45 minutes to do it
      - One problem HW like, other more interesting
    - Closed book exam, but you can bring one page "CHEAT SHEET"
    - Blue Book required, Code numbers will be given at the 1st quiz. Bring calculator, check battery !
    - **No makeup quizzes**
    - See handout for **Quiz regrade protocol**
- Final Exam : TBA, but in Week of June 6-10
  - Inform me of possible conflict within 2 weeks of course
  - Don't plan travel/vacation before finals schedule is confirmed !
    - No makeup finals for any reason

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All Quizzes During My Research Related Travel

Tentative Schedule, TBC next week

- Quiz 1 on Monday April 11
- Quiz 2 on Friday April 29
- Quiz 3 Friday May 13
- Quiz 4 Friday 20 or 27th (TBC)
- Quiz 5 Friday June 3

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Course Grade

- Our wish is that every body gets an A ! …So no curve
- Grading is on an absolute scale. Roughly it looks like this :

Total Score	Grade
> 85	A+
> 75	A
> 60	B
> 45	C
< 30	F

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How To Do Well In This Course

- Read the assigned text BEFORE lecture to get a feel of the topic
- Don't rely on your intuition ! The concepts are quite abstract.
- Attend lecture (ask questions during/before/after lecture) and discussion.
- Do not just accept a concept without understanding the logic
- Attempt all homework problems ***yourself***
  - Before looking at the problem solutions (available on web by Tuesday afternoon) & before attending Problem Solving session
- The textbook, the lectures and the discussions are all integral to this course. Just following lectures is not sufficient (I won't cover every thing)
- Quarter goes fast, don't leave every thing for the week before exam !!
- Don't hesitate to show up at Prof. or TA office hour (they don't bite !)

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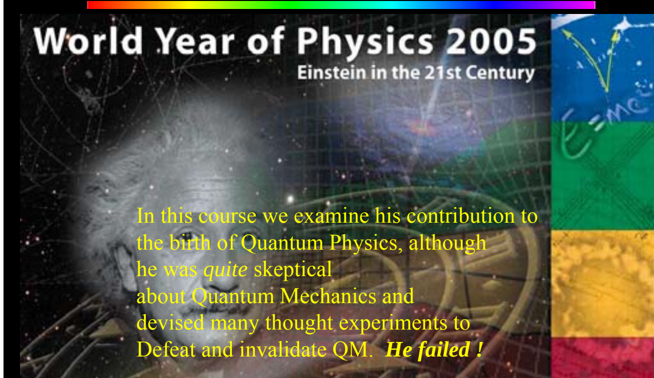
2005 is World Year of Physics: Celebrating Einstein



In this course we examine his contribution to the birth of Quantum Physics, although he was *quite* skeptical about Quantum Mechanics and devised many thought experiments to Defeat and invalidate QM. ***He failed !***

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Constituents of Nature: The Ancient View

Every civilization has speculated about the constitution of the Universe. The Greek philosophers thought that the universe was made up of just four elements: Earth, air, Fire and Water

This was a great "scientific" theory because it was simple but it had one drawback: It was wrong! There was no experimental proof for it.

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Concept of An Atom

- Around 6^{th}-5^{th} century BC, Indians and more famously the Greeks speculated on "indivisible" constituents of matter
- In 5^{th} BC, Leucippus and his follower Democritus set the scene for modern physics by asking " what would happen if you chopped up matter into ever smaller pieces. There would be a limit beyond which you could chop no more!"
- They called this indivisible piece an *Atom (or Anu in Sanskrit)*

Some Highlights in Understanding Matter

- Lavosier's measurement of conservation of matter in chemical reactions
- Faraday's Electrolysis experiment (1833) : Same amount of charge F is required to decompose 1 gram-ionic weight of monovalent ions
  - 1 F passed thru NaCl leads to 23gm of Na at cathode and 35.5gm Cl at anode but it takes 2F to disassociate $CuSO_4$
  - → Mass of element liberated at an electrode is directly proportional to charge transferred and inversely prop. to the valence of the freed element
- Avagadro postulated that pure gases at same temprature and pressure have same number of molecules per unit volume.
  - → N_A=6.023x 10^{23}
- Dalton & Mendeleev's theory that all elementary atoms differing in mass and chemical properties
- Discovery of cathode rays and measurement of their properties ……

Quantum Nature of Matter

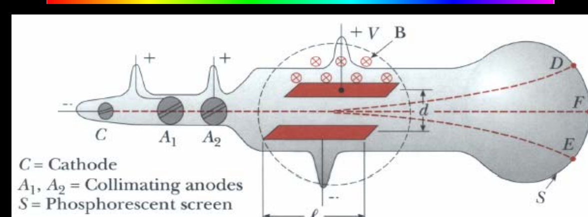
- Fundamental Characteristics of different forms of matter
  - Mass
  - Charge
    - Experimentally measurable
      - using some combination of **E** & **B**

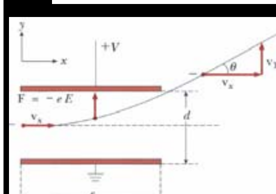
$$\vec{F} = q(\vec{E} + \vec{v} \times \vec{B})$$

      - **Or E/B and some other macroscopic force**

e.g. Drag Force

Thomson's Determination of e/m of Electron

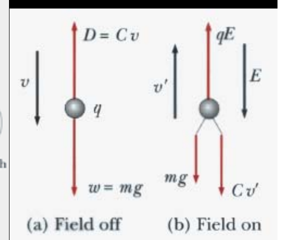




- In E Field alone, electron lands at D
- In B field alone, electron lands at E
- When E and B field adjusted to cancel each other's force → electron lands at F

→ e/m = 1.7588 x 10^{11} C/Kg

Millikan's Measurement of Electron Charge



Find charge on oil drop is always in integral multiple of some Q

$Q_e = 1.688 \times 10^{-19}$ Coulombs

→ $M_e = 9.1093 \times 10^{-31}$ Kg

→ Fundamental properties (finger print) of electron

(similarly can measure proton properties etc)

Necessary Homework Reading

- Pl. read Section 3.1, including the discussion detailing the Millikan's oil drop experiment (download from www.freeman.com/modphys4e)
- This is straightforward reading. HW problems are assigned on this and the material may show up in the quiz

Ch 3 : Quantum Theory Of Light

- What is the nature of light ?
  - When it propagates ?
  - When it interacts with Matter?
- What is Nature of Matter ?
  - When it interacts with light ?
  - As it propagates ?
- Revolution in Scientific Thought
  - A firestorm of new ideas (NOT steady dragged out progress)
    - Old concepts violently demolished , new ideas born
      - Rich interplay of experimental findings & scientific reason
- One such revolution happened at the turn of 20th Century
  - Led to the birth of Quantum Theory & Modern Physics

Classical Picture of Light : Maxwell's Equations

Maxwell's Equations:

$$\oint_S \mathbf{E}\cdot d\mathbf{A} = \frac{Q}{\epsilon_0}$$

$$\oint_S \mathbf{B}\cdot d\mathbf{A} = 0$$

$$\oint \mathbf{E}\cdot d\mathbf{s} = -\frac{d\Phi_B}{dt}$$

$$\oint \mathbf{B}\cdot d\mathbf{s} = \mu_0 I + \mu_0\epsilon_0 \frac{d\Phi_E}{dt}$$

$$\frac{\partial^2 E}{\partial x^2} = \mu_0\epsilon_0 \frac{\partial^2 E}{\partial t^2}$$

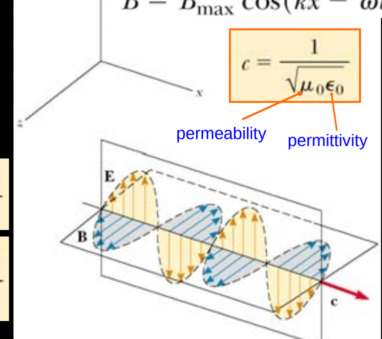
$$\frac{\partial^2 B}{\partial x^2} = \mu_0\epsilon_0 \frac{\partial^2 B}{\partial t^2}$$

$$E = E_{max}\cos(kx - \omega t)$$

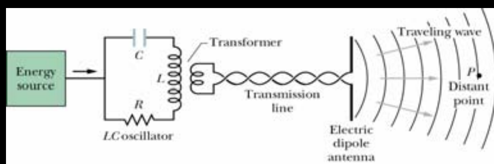
$$B = B_{max}\cos(kx - \omega t)$$

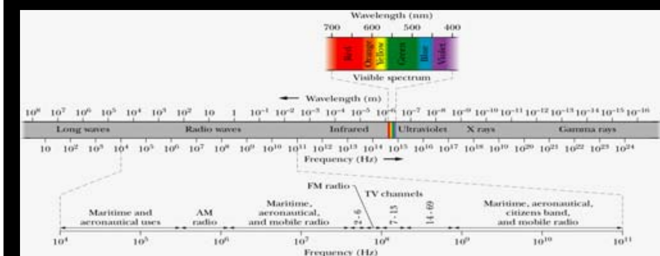
$$c = \frac{1}{\sqrt{\mu_0\epsilon_0}}$$

permeability   permittivity



Hertz & Experimental Demonstration of Light as EM Wave





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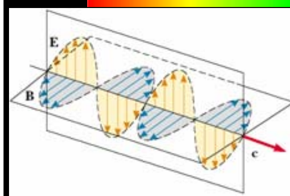
Properties of EM Waves: Maxwell's Equations



Energy Flow in EM Waves

Poynting Vector $\vec{S} = \dfrac{1}{\mu_0}(\vec{E} \times \vec{B})$

Power incident on an area A $= \vec{S}.\vec{A} = \dfrac{1}{\mu_0}\left(AE_0B_0Sin^2(kx-\omega t)\right)$

Intensity of Radiation $I = \dfrac{1}{2\mu_0 c}E_0^2$

Larger the amplitude of Oscillation More intense is the radiation

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Disasters in Classical Physics (1899-1922)

Disaster ➔ Experimental observation that could not be explained by Classical theory

- Disaster # 1 : Nature of Blackbody Radiation from your BBQ grill
- Disaster # 2: Photo Electric Effect
- Disaster # 3: Scattering light off electrons (Compton Effect)

Resolution of Experimental Observation will require radical changes in how we think about nature

– ➔ QUANTUM PHYSICS: The Art of Conversation with Subatomic Particles

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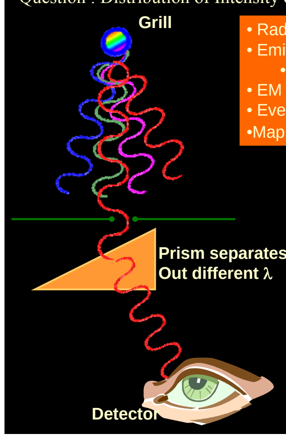
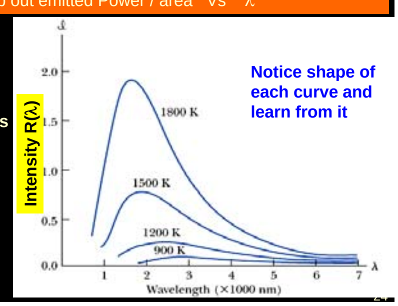
Nature of Radiation: An Expt with BBQ Grill

Question : Distribution of Intensity of EM radiation Vs T & λ

- Radiator (BBQ grill) at some temp T
- Emits variety of wavelengths
  - Some with more intensity than others
- EM waves of diff. λ bend differently within prism
- Eventually recorded by a detector (eye)
- Map out emitted Power / area Vs λ





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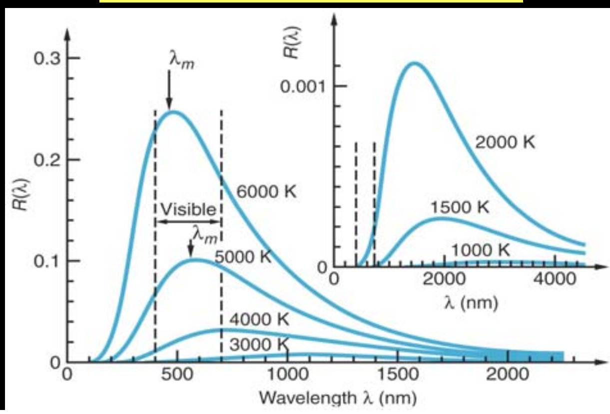
Radiation From a Blackbody at Different Temperatures

Radiancy is Radiation intensity per unit λ



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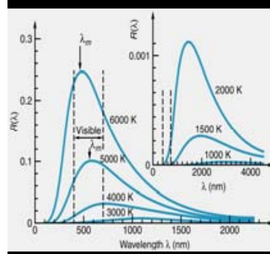
(a) Intensity of Radiation $I = \int R(\lambda)d\lambda \propto T^4$

$I = \sigma\ T^4$ (Area under curve)

Stephan-Boltzmann Constant $\sigma = 5.67\ 10^{-8}\ W / m^2 K^4$



(b) Higher the temperature of BBQ, Lower is the λ of PEAK intensity

$I_{MAX} \propto 1 / T$

$\lambda_{MAX}\ T = \text{const}$
$= 2.898\ 10^{-3}$ mK

As a body gets hotter it gets more RED then White : Wein's Law

Reason for different shape of R(λ) Vs λ for different temperature?
Can one explain in on basis of Classical Physics ??

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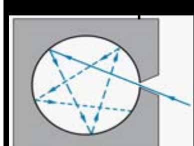
Blackbody Radiator: An Idealization



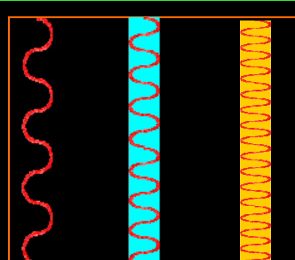
Classical Thought:
- **Box is filled with EM standing waves**
- **Radiation reflected back-and-forth between walls**
- **Radiation in thermal equilibrium with walls of Box**
- **How may waves of wavelength λ can fit inside the box ?**

Blackbody Absorbs everything
Reflects nothing
All light entering opening gets absorbed (ultimately) by the cavity wall

Cavity in equilibrium T w.r.t. surrounding. So it radiates everything It absorbs

Emerging radiation is a sample of radiation inside box at temp T

Predict nature of radiation inside Box ?



less **more** **Even more**

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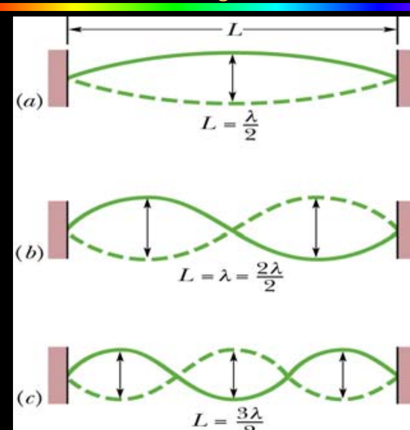
Standing Waves



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The Beginning of The End ! How BBQ Broke Physics

Classical Calculation

# of standing waves between Wavelengths λ and λ+dλ are

$$N(\lambda)d\lambda = \frac{8\pi V}{\lambda^4} \bullet d\lambda \; ; \; V = \text{Volume of box} = L^3$$

Each standing wave contributes energy E= kT to radiation in Box

Energy density $u(\lambda)$= [# of standing waves/volume]× Energy/Standing Wave

$$= \frac{8\pi V}{\lambda^4} \times \frac{1}{V} \times kT = \frac{8\pi}{\lambda^4} kT$$

$$\text{Radiancy } R(\lambda) = \frac{c}{4} u(\lambda) = \frac{c}{4}\frac{8\pi}{\lambda^4} kT = \frac{2\pi c}{\lambda^4} kT$$

Radiancy is Radiation intensity per unit λ interval: Lets plot it

Prediction : as λ → 0 (high frequency f), R(λ) → Infinity ! Oops !

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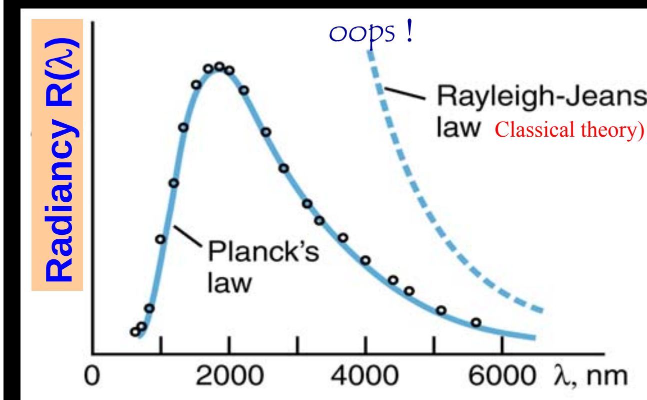
Ultra Violet (Frequency) Catastrophe



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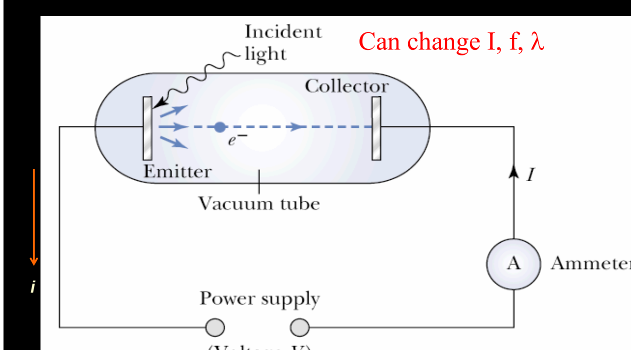
That was a Disaster !

(#1)

Disaster # 2 : Photo-Electric Effect

Light of intensity I, wavelength λ and frequency f incident on a photo-cathode



Measure characteristics of current in the circuit as a fn of I, f, λ

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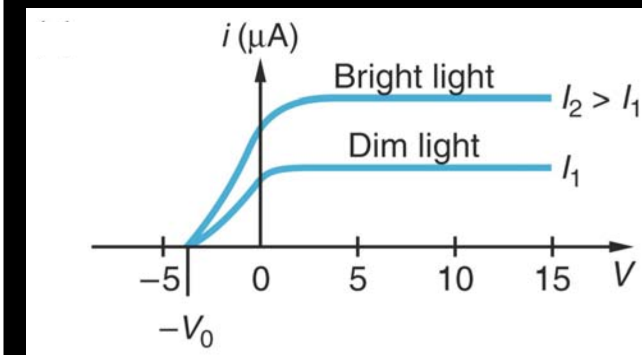
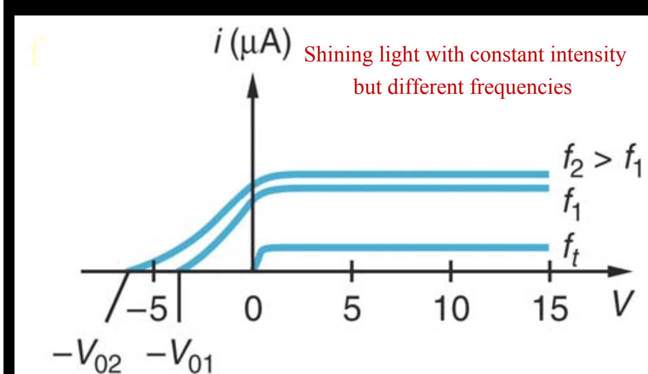
Photo Electric Effect: Measurable Properties

- Rate of electron emission from cathode
  - From current *i* seen in ammeter in the circuit. More photoelectrons → more current registered in ammeter
- Maximum kinetic energy of emitted electron
  - By applying retarding potential on electron moving left to tright towards Collector plate
    - **$K_{MAX} = eV_0$ (V_0 = Stopping voltage)**
    - **Stopping potential → no current flows**
- Photoelectric Effect on different types of photo-cathode metal surface
- Time between shining light and first sign of photo-current in the circuit

Observations:PhotoCurrent Vs Intensity of Incident Light

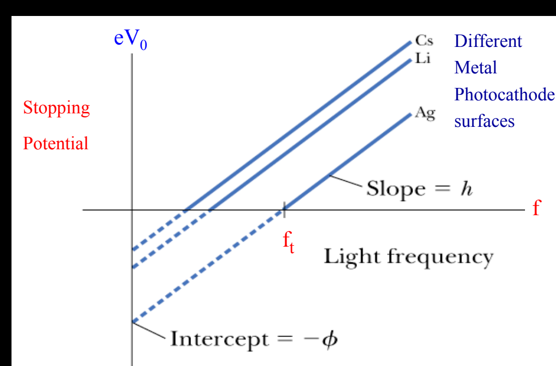


Observations: Photocurrent Vs frequency of incident light



Stopping Voltage (V_0) Vs Incident Light Frequency (f)

Try different photocathode materials…..see what happens



Conclusions from the Experimental Observations

- Max Kinetic energy K_{MAX} independent of Intensity I for light of same frequency
- No photoelectric effect occurs if light frequency f is below a threshold no matter how high the intensity of light
- For a particular metal, light with $f > f_t$ causes photoelectric effect IRRESPECTIVE of light intensity.
  - f_t is characteristic of that metal
- Photoelectric effect is instantaneous !...not time delay

Can one Explain all this Classically !

Classical Explanation of Photo Electric Effect

- As light Intensity increased ⇒ $\vec{E}$ field amplitude larger
  - E field and electrical force seen by the "charged subatomic oscillators" Larger
    - $\vec{F} = e\vec{E}$
    - More force acting on the subatomic charged oscillator
    - ⇒ More (work done) ➔ more energy transferred to it
    - ⇒ Charged particle "hooked to the atom" should leave the surface with more Kinetic Energy KE !! The intensity of light (EM Wave) shining rules !
- As long as light is <u>intense enough</u> , light of ANY frequency f should cause photoelectric effect
- Because the Energy in a Wave is uniformly distributed over the Spherical wavefront incident on cathode, should be a noticeable time lag ΔT between time is incident & the time a photo-electron is ejected : Energy absorption time
  - How much time for electron ejection ? Lets calculate it classically

Classical Physics: Time Lag in Photo-Electric Effect ?

- Electron absorbs energy incident on a surface area where the electron is confined ≅ size of atom in cathode metal
- Electron is "bound" by attractive Coulomb force in the atom, so it must absorb a minimum amount of radiation before its stripped off
- Example : Laser light Intensity I = 120W/m² on Na metal
  - Binding energy = 2.3 eV= "Work Function Φ "
  - Electron confined in Na atom, size ≅ 0.1nm; how long before ejection ?
  - Average Power Delivered $P_{AV} = \mathbf{I} \cdot \mathbf{A}$, $A = \pi r^2 \cong 3.1 \times 10^{-20}$ m²
  - If all energy absorbed then $\Delta E = P_{AV} \cdot \Delta T \Rightarrow \Delta T = \Delta E / P_{AV}$

$$\Delta T = \frac{(2.3eV)(1.6\times10^{-19}\,J/eV)}{(120W/m^2)(3.1\times10^{-20}\,m^2)} = 0.10\ S$$

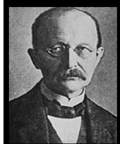
  - Classical Physics predicts <u>measurable delay</u> even by the primitive clocks of 1900
  - But in experiment, the effect was observed to be instantaneous !!
  - Classical Physics fails in explaining all results

That was a Disaster !

(# 2)

Beginning of a search for a new hero or an explanation or both !

Max Planck & Birth of Quantum Physics



Back to Blackbody Radiation Discrepancy

Planck noted the Ultraviolet catastrophe at high frequency

"Cooked" calculation with new "ideas" so as bring:

$R(\lambda) \rightarrow 0$ as $\lambda \rightarrow 0$

$f \rightarrow \infty$

- Cavity radiation as equilibrium exchange of energy between EM radiation & "atomic" oscillators present on walls of cavity
- Oscillators can have any frequency f
- But the Energy exchange between radiation and oscillator NOT continuous, it is discrete …in packets of same amount
- E = n hf , with n = 1,2, 3, 4,…. ∞

  h = constant he invented, a number he made up !

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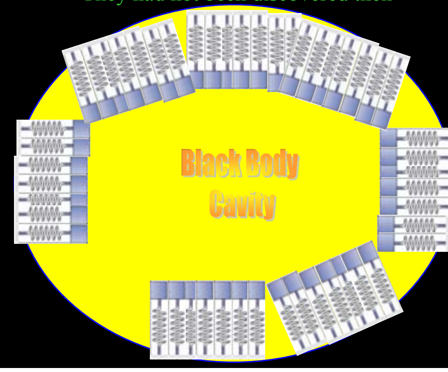
Planck's "Charged Oscillators" in a Black Body Cavity

Planck did not know about electrons, Nucleus etc:

They had not been discovered then



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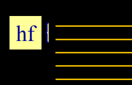
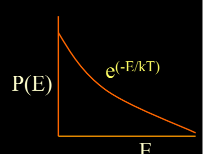
Planck, Quantization of Energy & BlackBody Radiation

- Keep the rule of counting how many waves fit in a BB Volume
- Radiation Energy in cavity is quantized
- EM standing waves of frequency f have energy

  E = n hf (n = 1,2 ,3 …10 ….1000…)



- Probability Distribution: At an equilibrium temp T, possible energy of oscillators is distributed over a spectrum of states: $P(E) = e^{(-E/kT)}$
- Modes of Oscillation with :
  - •Less energy E=hf = favored
  - •More energy E=hf = disfavored



By this discrete statistics, large energy = high f modes of EM disfavored

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Planck's Calculation: A preview to keep the story going

$$R(\lambda) = \left(\frac{c}{4}\right)\left(\frac{8\pi}{\lambda^4}\right)\left[\frac{hc}{\lambda}\left(\frac{1}{e^{\frac{hc}{\lambda kT}} - 1}\right)\right]$$

Odd looking form

When $\lambda \rightarrow$ large $\Rightarrow \frac{hc}{\lambda kT} \rightarrow$ small

Recall $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + ...$

$$\Rightarrow e^{\frac{hc}{\lambda kT}} - 1 = (1 + \frac{hc}{\lambda kT} + \frac{1}{2}\left(\frac{hc}{\lambda kT}\right)^2 + ...] - 1$$

$$= \frac{hc}{\lambda kT}$$ plugging this in $R(\lambda)$ eq:

$$R(\lambda) = \left(\frac{c}{4}\right)\left(\frac{8\pi}{\lambda^4}\right)\frac{hc}{\lambda kT}$$

Graph & Compare With BBQ data

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Planck's Formula and Small λ

When λ is small (large f)

$$\frac{1}{e^{\frac{hc}{\lambda kT}}-1} \cong \frac{1}{e^{\frac{hc}{\lambda kT}}} = e^{-\frac{hc}{\lambda kT}}$$

Substituting in R(λ) eqn:

$$R(\lambda) = \left(\frac{c}{4}\right)\left(\frac{8\pi}{\lambda^4}\right)e^{-\frac{hc}{\lambda kT}}$$

$$\text{As } \lambda \to 0,\ e^{-\frac{hc}{\lambda kT}} \to 0$$

$$\Rightarrow R(\lambda) \to 0$$

Just as seen in the experimental data !

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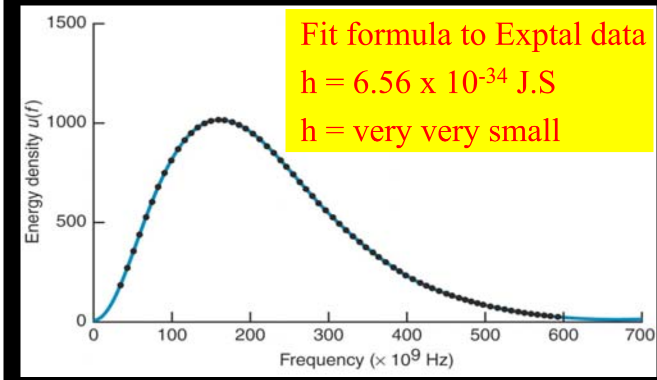
Planck's Explanation of Black Body Radiation



Fit formula to Exptal data

$h = 6.56 \times 10^{-34}$ J.S

h = very very small

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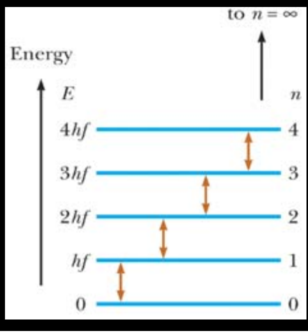
Major Consequence of Planck's Energy Postulate

Quantization of Energy !



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Judging Planck's Postulate : Visionary or just a Wonk?

Einstein Provided the "warmth & feeling" to Planck's Wonky idea

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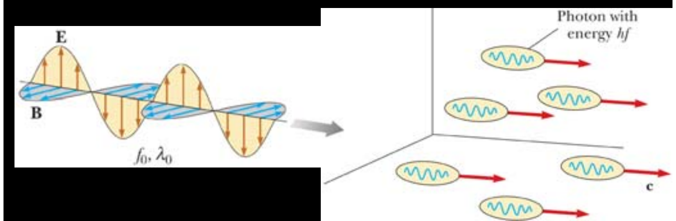
Einstein's Explanation of Photoelectric Effect

What Maxwell Saw of EM Waves

What Einstein Saw of EM Waves



Light as bullets of "photons"
Energy concentrated in photons
Energy exchanged instantly
Energy of EM Wave E= hf

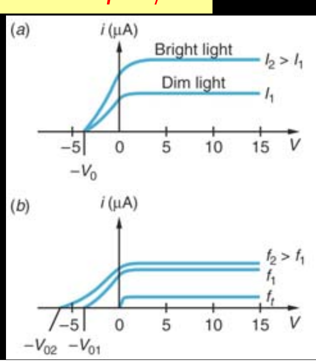
Einstein's Explanation of Photoelectric Effect

- Energy associated with EM waves not uniformly distributed over wavefront, rather is contained in packets of energy ⇒ PHOTON
- E= hf = hc/λ [but is it the same h as in Planck's th.?]
- Light shining on metal emitter/cathode is a *stream of photons* of energy E which depends on frequency f
- Photons knock off electron from metal instantaneously
  - Transfer all energy to electron
  - Energy gets used up to pay for Work Function Φ. Remaining energy shows up as KE of electron KE = hf- Φ
- Cutoff Frequency hf_0 = Φ (pops an electron, KE = 0)
- Larger intensity I → more photons incident
- Low frequency light f → not energetic enough to overcome work function of electron in atom

Einstein's Interpretation of Photoelectric Effect (1905)

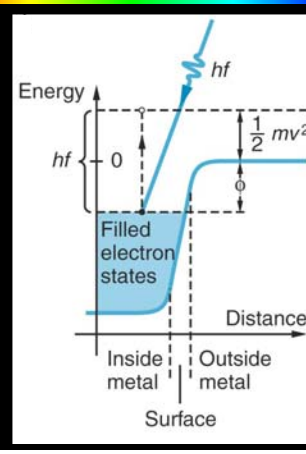
$$E = hf = \varphi + KE_{electron}$$
$$eV_0 = KE = hf - \varphi$$

Now interpret the experimental data
Under the "single bullet" theory



Makes Sense !

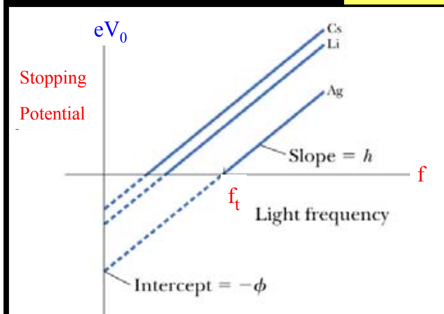
Modern View of Photoelectric Effect



Is "h" same in Photoelectric Effect as BB Radiation?

Slope h $= 6.626 \times 10^{-34}$ JS

Einstein → Nobel Prize!



NOBEL PRIZE FOR PLANCK !

Work Function (Binding Energy) In Metals

TABLE 3-1 Photoelectric work functions

Element	φ (eV)
Na	2.28
C	4.81
Cd	4.07
Al	4.08
Ag	4.73
Pt	6.35
Mg	3.68
Ni	5.01
Se	5.11
Pb	4.14

Reinterpreting Photoelectric Effect With Light as Photons

Photoelectric Effect on An Iron Surface

Light of Intensity $I = 1.0\ \mu W/cm^2$ incident on $1.0 cm^2$ surface of Fe

Assume Fe reflects 96% of light

further *only* 3% *of incident light* is Violet region ($\lambda = 250$nm)

barely above threshold frequency for Photoelectric effect

(a) Intensity available for Ph. El effect $I = 3\% \times 4\% \times (1.0\ \mu W/cm^2)$

(b) how many photo-electrons emitted per second ?

$$\#\text{ of photoelectrons} = \frac{\text{Power}}{\text{h f}} = \frac{3\% \times 4\% \times (1.0\ \mu W/cm^2)\ \lambda}{hc}$$

$$= \frac{(250 \times 10^{-9} m)(1.2 \times 10^{-9} J/s)}{(6.6 \times 10^{-34} J \cdot s)(3.0 \times 10^{8} m/s)}$$

$$1.5 \times 10^{9}$$

(c) Current in Ammeter : $i = (1.6 \times 10^{-19} C)(1.5 \times 10^{9}) = 2.4 \times 10^{-10} A$

(d) Work Function $\Phi = hf_0 = (4.14 \times 10^{-15} eV \cdot s)(1.1 \times 10^{15} s^{-1})$

$= 4.5$ eV

Facts about Light Quantum

- The human eye is a sensitive photon detector at visible wavelengths: Need >5 photons of ≅ 550nm to register on your optical sensor
- The Photographic process :
  - Energy to Dissociate an AgBr molecule = 0.6eV
- Photosynthesis Process : 9 sunlight photon per reaction cycle of converting CO_2 and water to carbohydrate & O_2
  - chlorophyll absorbs best at $\lambda \cong$ 650-700 nm
- Designing Space Shuttle "skin" : Why Platinum is a good thing
- designing Solar cells : picking your metal cathode

Photon & Relativity: Wave or a Particle ?

- Photon associated with EM waves, travel with speed =c
- For light (m =0) : Relativity says $E^2 = (pc)^2 + (mc^2)^2$
- $\Rightarrow E = pc$
- But Planck tells us : $E = hf = h (c/\lambda)$
- Put them together : $hc/\lambda = pc$
  - $\Rightarrow$ $p = h/\lambda$
  - Momentum of the photon (light) is inversely proportional to λ
- But we associate λ with waves & p with particles ….what is going on??
  - Quantum Physics !

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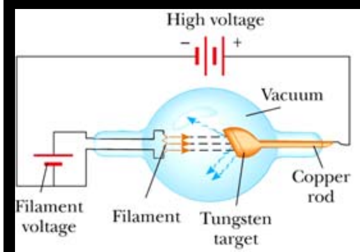
X Rays "Bremsstrahlung": The Braking Radiation

- EM radiation, produced by bombarding a metal target with energetic electrons.
- Produced in general by ALL decelerating charged particles
- X rays : very short $\lambda \cong$ 60-100 pm (10^{-12}m), large frequency f
- Very penetrating because very energetic $E = hf$!!



Useful for probing structure of sub-atomic Particles (and your teeth !)

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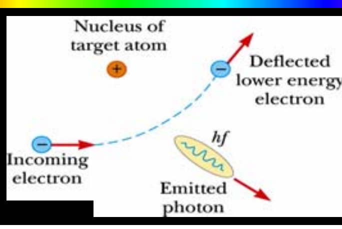
X Ray Production Mechanism



When electron passes near a positively charged target nucleus contained in target material, its deflected from its path because of Coulomb attraction, experiences acceleration.

E&M ➔ that any charged particle will emit radiation when accelerated.
This EM radiation "appears" as photons. Since photo carries energy and momentum, the electron must lose same amount. If all of electron's energy is lost in just one single collision then:

$$e\,\Delta V = hf_{max} = \frac{hc}{\lambda_{min}} \quad \text{or} \quad \lambda_{min} = \frac{hc}{e\,\Delta V}$$

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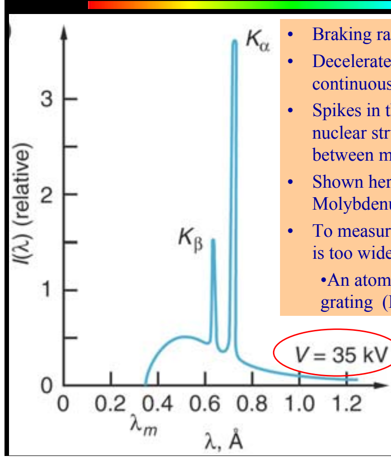
X Ray Spectrum in Molybdenum (Mo)



- Braking radiation predicted by Maxwell's eqn
- Decelerated charged particle will radiate continuously
- Spikes in the spectrum are characteristic of the nuclear structure of target material and varies between materials
- Shown here are the α and β lines for Molybdenum (Mo)
- To measure the wavelength, diffraction grating is too wide, need smaller slits
  - An atomic crystal lattice as diffraction grating (Bragg)

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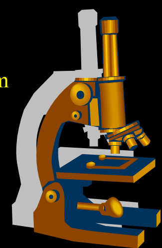
X rays As Subatomic Probes

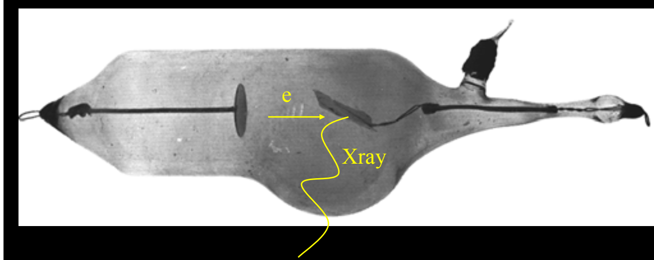
X rays are EM waves of low wavelength, high frequency (and energy) and demonstrate characteristic features of a wave

- Interference &Diffraction

- To probe into a structure size ΔX you need a light source with wavelength much smaller than the features of the object being probed
  - Good Resolution → $\lambda_{SOURCE} << \Delta X$
  - X rays allows one probe at atomic size (10^{-10})m



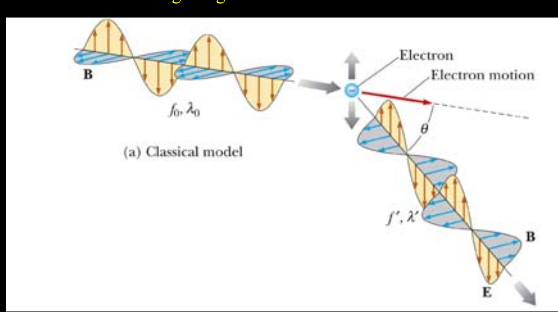
An X-ray Tube from 20th Century



The "High Energy Accelerator" of 1900s: produced energetic light : X –Ray , gave new optic to subatomic world

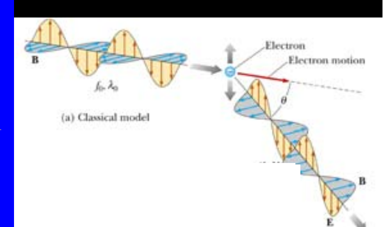
Compton Scattering : Quantum Pool !

- Arthur Compton (USA) proves that X-rays (EM Waves) have particle like properties (acts like photons)
  - Showed that classical theory failed to explain the scattering effect of X rays on to free (not bound, barely bound electrons)
- Experiment : shine X ray on to a surface with "almost" free electrons
  - Watch the scattering of light off electron : measure time + λ of scattered X-ray

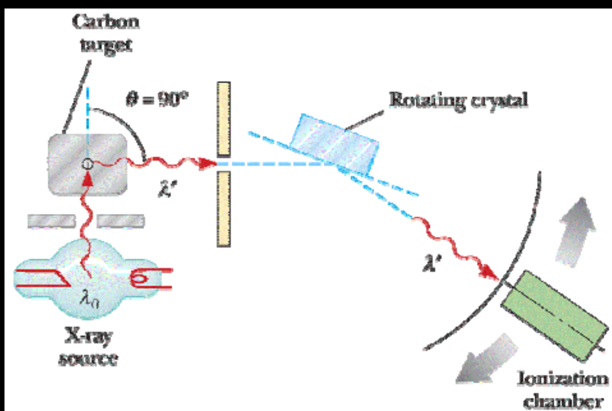


Compton Effect: what should Happen Classically?

- Plane wave $[f,\lambda]$ incident on a surface with loosely bound electrons → interaction of E field of EM wave with electron: $\mathbf{F} = e\mathbf{E}$
- Electron oscillates with $f = f_{incident}$
- Eventually radiates spherical waves with $f_{radiated} = f_{incident}$
  - At all scattering angles, Δf & $\Delta\lambda$ must be zero
- Time delay while the electron gets a "tan": soaks in radiation



Compton Scattering : Experimental Setup & Results



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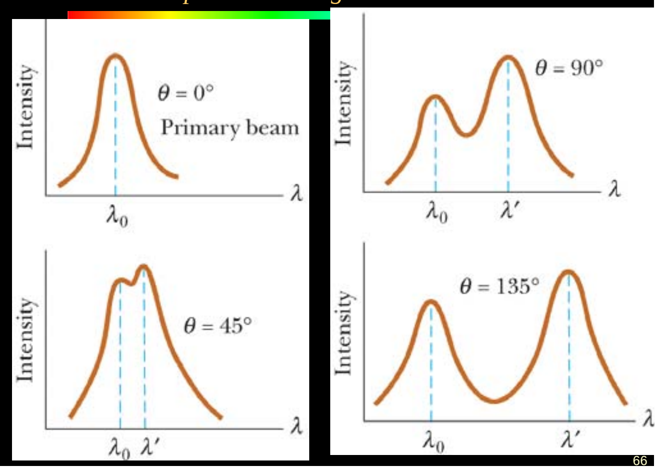
Compton Scattering : Observations



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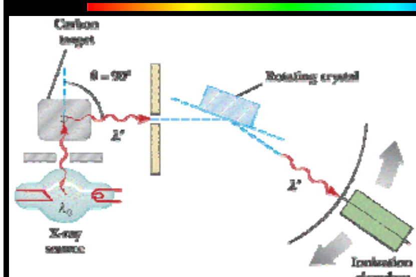
Compton Scattering : Summary of Observations



$\Delta\lambda = (\lambda' - \lambda) \propto (1 - \cos\theta)$!

Not isotropy in distribution of scattered radiation

How does one explain this startling anisotropy?

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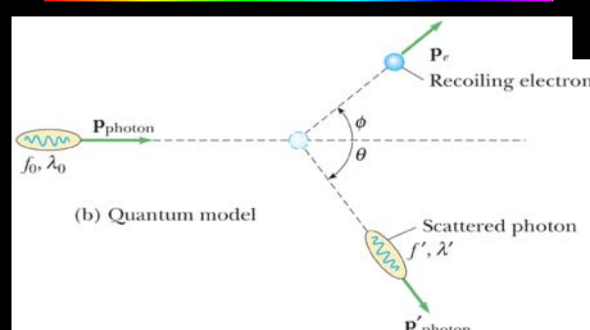
Compton Effect : Quantum (Relativistic) Pool



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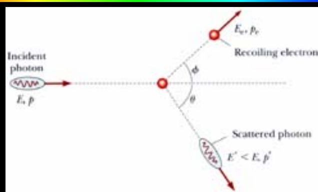
Compton Scattering: The Quantum Picture



Energy Conservation:

$E + m_e c^2 = E' + E_e$

Momentum Conserv:

$p = p'\cos\theta + p_e \cos\phi$

$0 = p'\sin\theta - p_e \sin\phi$

Use these to eliminate electron deflection angle (not measured)

$p_e \cos\phi = p - p'\cos\theta$

$p_e \sin\phi = p'\sin\theta$

Square and add $\Rightarrow$

$p_e^2 = p^2 - 2pp'\cos\theta + p'^2$

Eliminate p_e & E_e using

$E_e^2 = p_e^2 c^2 + m_e^2 c^4$ &

$E_e = (E - E') + m_e c^2$

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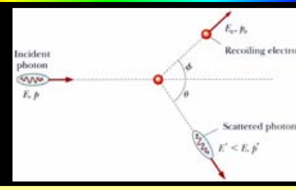
Compton Scattering: The Quantum Picture



$$\left((E - E') + m_e c^2\right)^2 = \left[p^2 - 2pp'\cos\theta + p'^2\right] + (m_e c^2)^2$$

For light $p = \frac{E}{c} \Rightarrow$

$$E^2 + E'^2 - 2EE' + 2(E - E')mc^2 = \left[\frac{E^2}{c^2} - 2\frac{EE'}{c^2}\cos\theta + \frac{E'^2}{c^2}\right]c^2$$

$$\Rightarrow -EE' + (E - E')mc^2 = -EE'\cos\theta$$

$$\Rightarrow \frac{E - E'}{EE'} = -\frac{1}{m_e c^2}(1 - \cos\theta) \Rightarrow (\lambda' - \lambda) = \left(\frac{h}{m_e c}\right)(1 - \cos\theta)$$

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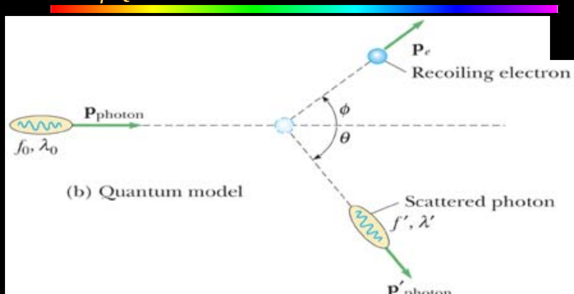
Rules of Quantum Pool between Photon and Electron



$$(\lambda' - \lambda) = \left(\frac{h}{m_e c}\right)(1 - \cos\theta)$$

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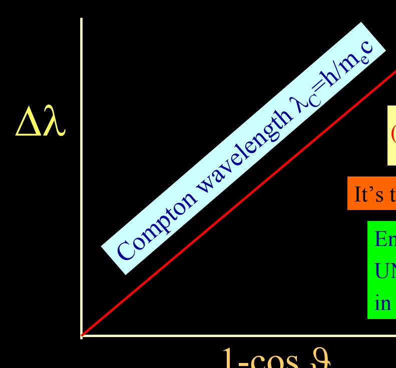
Checking for "h" in Compton Scattering

From scattered photon λ, plot Δλ, calculate slope and measure "h"



$(\lambda' - \lambda) = \left(\frac{h}{m_e c}\right)(1 - \cos\theta)$

It's the same value for h again !

Energy Quantization is a UNIVERSAL characteristic in energy transactions !

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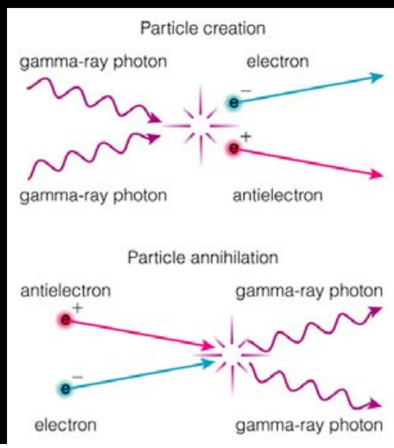
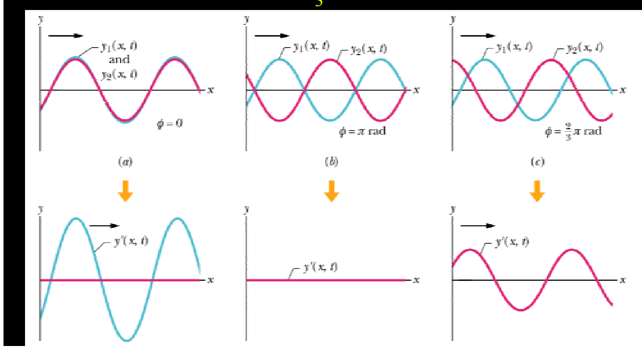
Other Forms of Energy Exchange between Radiation and Matter

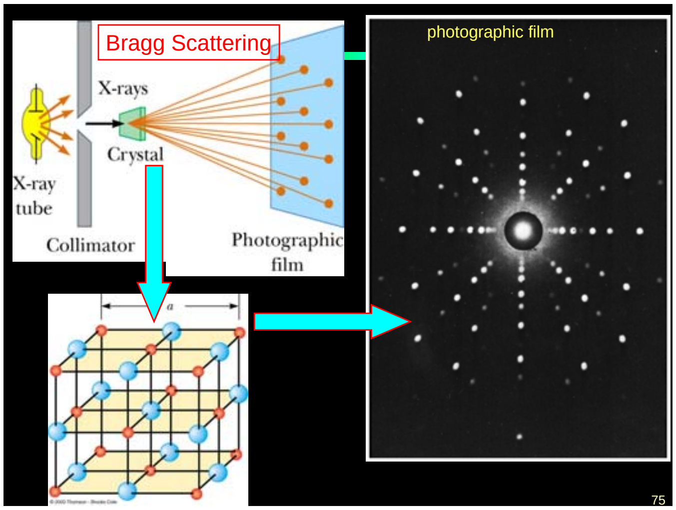
$E \rightleftharpoons mc^2 + mc^2$
same kind of
matter & antimatter
produced or destroyed
in pairs



Constructive Interference depends on Path (or phase) diff. Traversed

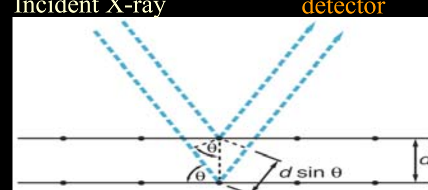
Two Identical waves $y_i(x,t) = y_{max}\sin(k_i x - \omega_i t + \phi_i)$ travel along +x and interefere to give a resulting wave $y'(x,t)$. The resulting wave form depends on relative phase difference between 2 waves. Shown for $\Delta\phi = 0, \pi, \frac{2}{3}\pi$





Bragg Scattering: Probing Atoms With X-Rays

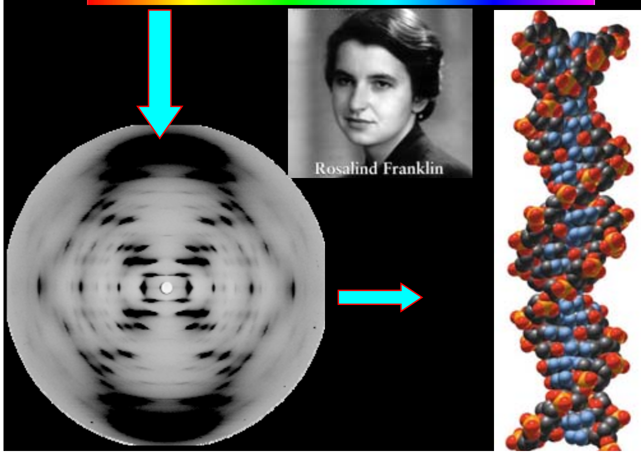
Incident X-ray detector



Constructive Interference when net phase difference is 0, 2π etc
This implied path difference traveled by two waves must be integral multiple of wavelength : **$n\lambda = 2d\sin\vartheta$**

From X Ray (EM Wave) Scattering data,
size of atoms was known to be about 10^{-10} m

X-Ray Picture of a DNA Crystal and Discovery of DNA Structure !



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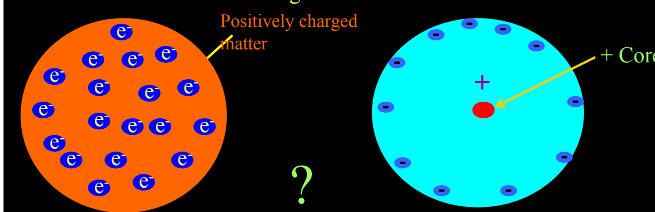
Where are the electrons inside the atom?

Early Thought: "Plum pudding" model→ Atom has a homogenous distribution of Positive charge with electrons embedded in them



- How to test these hypotheses? → Shoot "bullets" at the atom and watch their trajectory. What Kind of bullets ?
  - •Indestructible charged bullets → Ionized He^{++} atom = α^{++} particles
  - •Q = +2e , Mass M_α=4amu >> m_e , V_α= 2 x 10 ^{7} m/s (non-relavistic) [charged to probe charge & mass distribution inside atom]

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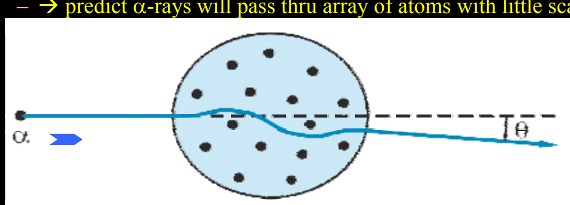
Plum Pudding Model of Atom

- Non-relativistic mechanics ($V_\alpha/c = 0.1$)
- In Plum-pudding model, α-rays hardly scatter because
  - Positive charge distributed over size of atom (10^{-10}m)
  - $M_\alpha >> M_e$ (like moving truck hits a bicycle)
  - → predict α-rays will pass thru array of atoms with little scatter



Need to test this hypothesis → Ernest Rutherford

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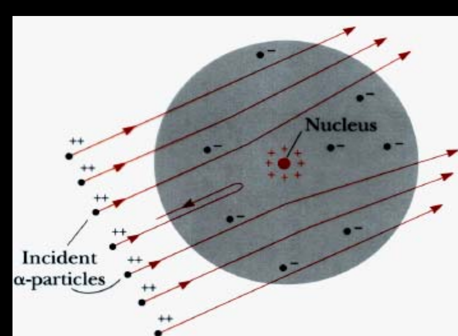
"Rutherford Scattering" discovered by his PhD Student (Marsden)



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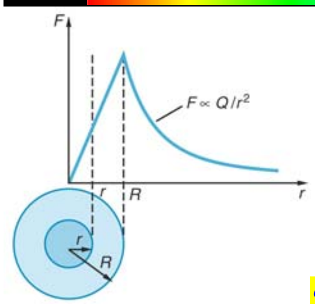
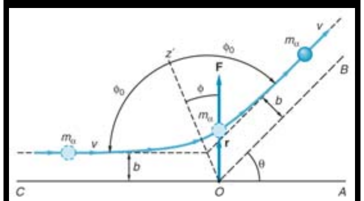
Force on α-particle due to heavy Nucleus





α particle trajectory is hyperbolic

Scattering angle is related to impact par.

Impact Parameter $b = \left(\frac{kq_\alpha Q}{m_\alpha v_\alpha^2}\right)\left(\cot\frac{\theta}{2}\right)$

- Outside radius r = R, $F \propto Q/r^2$
- Inside radius r < R, $F \propto q/r^2 = Qr/R^2$
- Maximum force at radius r = R

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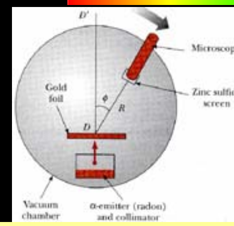
Rutherford Scattering: Prediction and Experimental Result



$$\Delta n = \frac{k^2 Z^2 e^4 NnA}{4R^2\left(\frac{1}{2}m_\alpha v_\alpha^2\right)^2 Sin^4(\varphi/2)}$$

scattered Vs ϕ depends on :

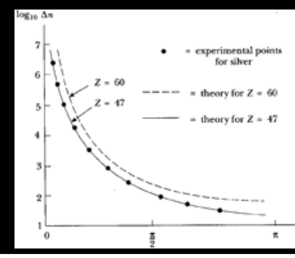
n = # of incident alpha particles

N = # of nuclei/area of foil

Ze = Nuclear charge

K_α of incident alpha beam

A= detector area



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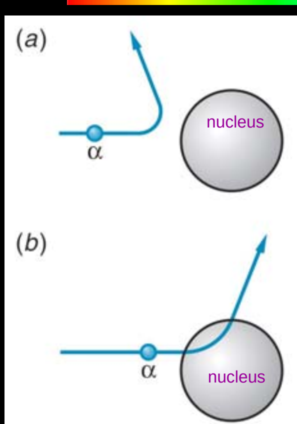
Rutherford Scattering & Size of Nucleus



distance of closest appoach $\propto$ r size of nucleus

Kinetic energy of α = $K_\alpha = \frac{1}{2}m_\alpha v_\alpha^2$

α particle will penetrate thru a radius r until all its kinetic energy is used up to do work AGAINST the Coulomb potential of the Nucleus:

$$K_\alpha = \frac{1}{2}m_\alpha v_\alpha^2 = 8MeV = k\frac{(Ze)(2e)}{r}$$

$$\Rightarrow \quad r = \frac{2kZe^2}{K_\alpha}$$

For K_α =7.7.MeV, Z_{Al} =13

$$\Rightarrow \quad r = \frac{2kZe^2}{K_\alpha} = 4.9\times10^{-15}m$$

Size of Nucleus = $10^{-15}m$

Size of Atom = $10^{-10}m$

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Dimension Matters !

Size of Nucleus = $10^{-15}m$

Size of Atom = $10^{-10}m$

How are the electrons located inside an atom ?

How are they held in a stable fashion ?

necessary condition for us to exist !

All these discoveries will require new experiments and observations

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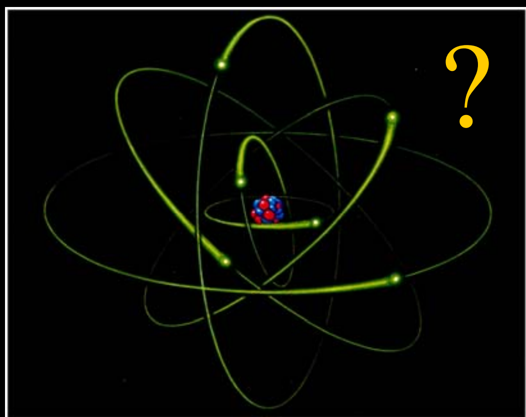
Where are the Electrons in an Atom ?



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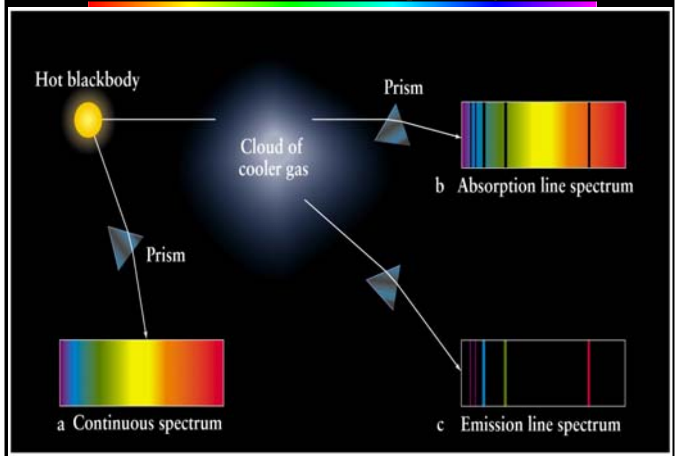
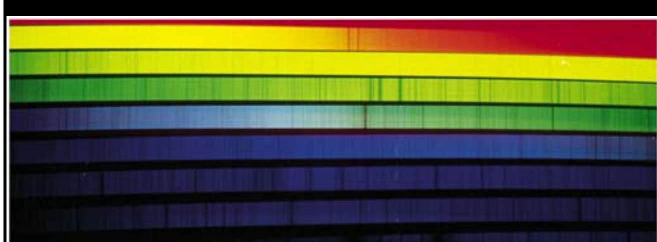
Clues: Continuous & Discrete spectra of Elements



Visible Spectrum of Sun Through a Prism



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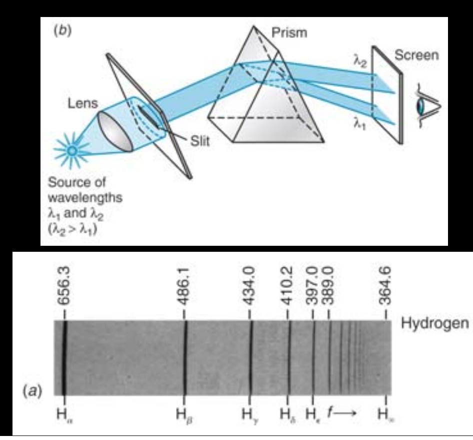
Emission & Absorption Line Spectra of Elements



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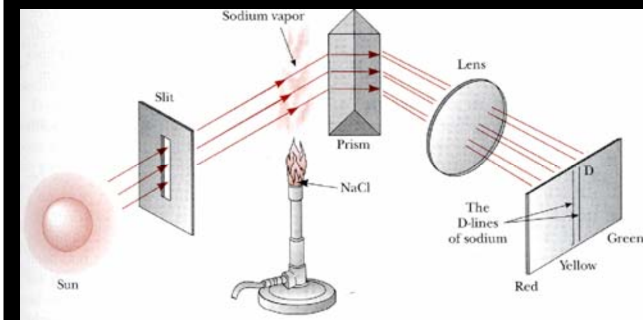
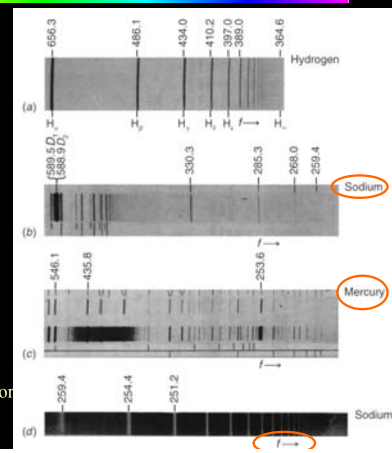
Kirchhoff' Experiment : "D" Lines in Na



D lines **darken** noticeably when Sodium vapor introduced
Between slit and prism

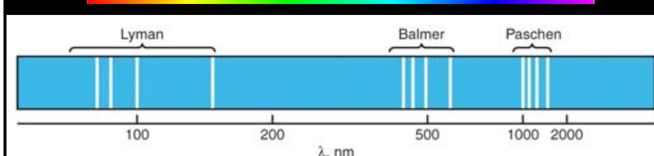
Emission & Absorption Line Spectrum of Elements

Emission line appear dark because of photographic exposure



Absorption spectrum of Na
While light passed thru Na vapor is absorbed at specific λ

Spectral Observations : series of lines with a pattern



- Empirical observation (by trial & error)
- All these series can be summarized in a simple formula

$$\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right), n_f > n_i, n_i = 1, 2, 3, 4..$$

Fitting to spectral line series data

$R = 1.09737 \times 10^7 m^{-1}$

How does one explain this ?

The Rapidly Vanishing Atom: A Classical Disaster !

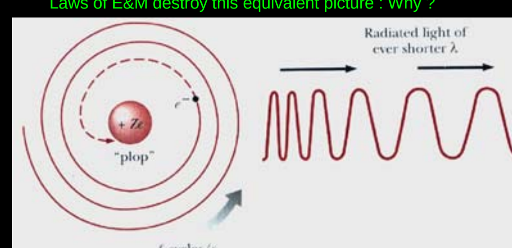
Not too hard to draw analogy with dynamics under another Central Force

Think of the Gravitational Force between two objects and their circular orbits.

Perhaps the electron rotates around the Nucleus and is bound by their electrical charge

$$F = G\frac{M_1 M_2}{r^2} \Rightarrow k\frac{Q_1 Q_2}{r^2}$$

Laws of E&M destroy this equivalent picture : Why ?



Classical Trajectory of The Orbiting Electron

Classical model of Hydrogenic Atom (Z protons) is mechanically stable but is electrically unstable !

Mechanically balanced : $F = \frac{kZe^2}{r^2} = \frac{mv^2}{r}$ (Coulomb force = Centripetal force)

But electron is always accelerating towards center of circle. Laws of classical electrodynamics predict that accelerating charge will radiate light of frequency f = freq. of periodic motion

$$f = \frac{v}{2\pi r} = \left(\frac{kZe^2}{rm}\right)^{\frac{1}{2}} \frac{1}{2\pi r} = \left(\frac{kZe^2}{4\pi^2 m}\right)^{\frac{1}{2}} \frac{1}{r^{\frac{3}{2}}} \sim \frac{1}{r^{\frac{3}{2}}}$$

And Total energy $E = KE+U = \frac{mv^2}{2} + \left(-\frac{kZe^2}{r}\right)$, but since $\boxed{\frac{kZe^2}{2r} = \frac{mv^2}{2}}$

$$\Rightarrow E = \frac{kZe^2}{2r} - \frac{kZe^2}{r} = \frac{kZe^2}{2r} \sim \boxed{-\frac{1}{r}}$$

Thus Classical physics predicts that as energy is lost to radiation, electron's orbit will become smaller and smaller while frequency of radiation will become larger and larger!

The electron will reach the Nucleus in $\sim 1\mu s$!!

In reality, this does not occur. Unless excited by external means, atoms do not radiate AT ALL!

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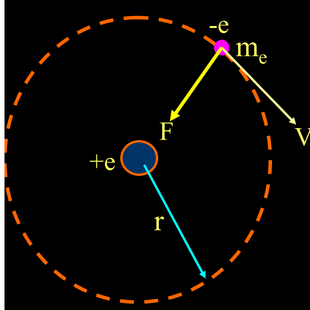
Bohr's Bold Model of Atom: Semi Quantum/Classical



$$U(r) = -k\frac{e^2}{r}$$

$$KE = \frac{1}{2}m_e v^2$$

1. Electron in circular orbit around proton with vel=v
2. Only stationary orbits allowed . Electron does not radiate when in these stable (stationary) orbits
3. Orbits quantized:
   - $M_e v\, r = n\, h/2\pi$ (n=1,2,3…)
4. Radiation emitted when electron "jumps" from a stable orbit of higher energy → stable orbit of lower energy $E_f - E_i = hf = hc/\lambda$
5. Energy change quantized
   - f = frequency of radiation

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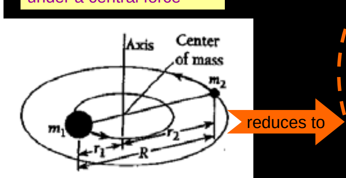
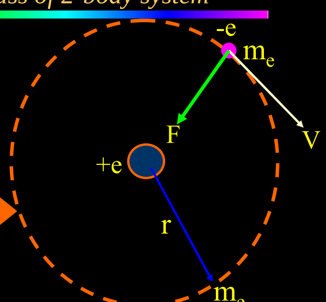
Reduced Mass of 2-body system

General two body motion under a central force





- Both Nucleus & e^- revolve around their common center of mass (CM)
- Such a system is equivalent to single particle of "reduced mass" μ that revolves around position of Nucleus at a distance of (e^--N) separation
  - $\mu = (m_e M)/(m_e + M)$, when M>>m, μ=m (Hydrogen atom)
  - Not so when calculating Muon ($m_\mu = 207\, m_e$) or equal mass charges rotating around each other (similar to what you saw in gravitation)

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Allowed Energy Levels & Orbit Radii in Bohr Model

$E = KE + U = \frac{1}{2}m_e v^2 - k\frac{e^2}{r}$

Force Equality for Stable Orbit

⇒ Coulomb attraction = CP Force

$$\boxed{k\frac{e^2}{r^2} = \frac{m_e v^2}{r}}$$

$$\Rightarrow KE = \frac{m_e v^2}{2} = k\frac{e^2}{2r}$$

Total Energy $\boxed{E = KE+U = -k\frac{e^2}{2r}}$

Negative E ⇒ Bound system

This much energy must be added to the system to break up the bound atom

Radius of Electron Orbit :

$mvr = n\hbar$

$\Rightarrow v = \frac{n\hbar}{mr}$,

substitute in $KE = \frac{1}{2}m_e v^2 = \frac{ke^2}{2r}$

$\Rightarrow r_n = \frac{n^2\hbar^2}{mke^2}$, $n = 1, 2, \ldots\infty$

$n = 1 \Rightarrow$ Bohr Radius a_0

$a_0 = \frac{1^2\hbar^2}{mke^2} = 0.529 \times 10^{-10} m$

In general $r_n = n^2 a_0$; $n = 1, 2, \ldots\infty$

Quantized orbits of rotation

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Energy Level Diagram and Atomic Transitions

$E_n = K + U = \frac{-ke^2}{2r}$

since $r_n = a_0 n^2$, n = quantum number

$E_n = \frac{-ke^2}{2a_0 n^2} = -\frac{13.6}{n^2} eV$, $n = 1, 2, 3..\infty$

Interstate transition: $n_i \to n_f$

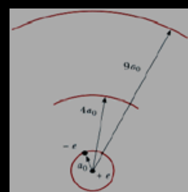
$\Delta E = hf = E_i - E_f$

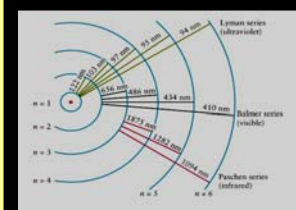
$= \frac{-ke^2}{2a_0}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$

$f = \frac{ke^2}{2ha_0}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

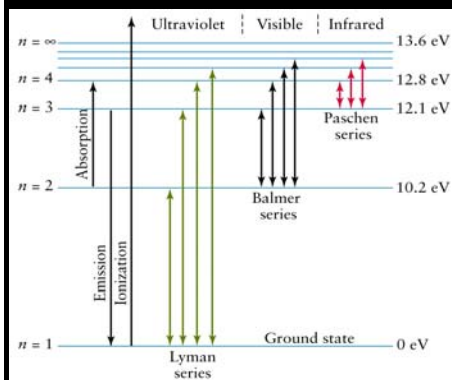
$\frac{1}{\lambda} = \frac{f}{c} = \frac{ke^2}{2hca_0}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$

$= R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$





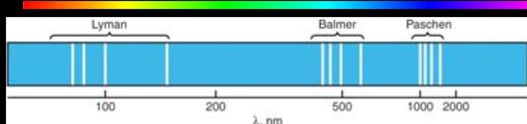
Hydrogen Spectrum: as explained by Bohr



$$E_n = -\left(\frac{ke^2}{2a_0}\right)\frac{Z^2}{n^2}$$

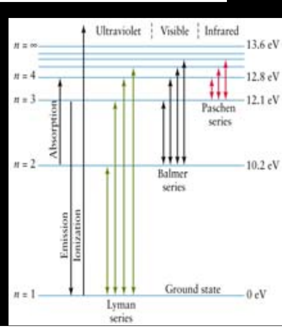
Bohr's "R" same as Rydberg Constant **R** derived emperically from spectral series

A Look Back at the Spectral Lines With Bohr's Optic

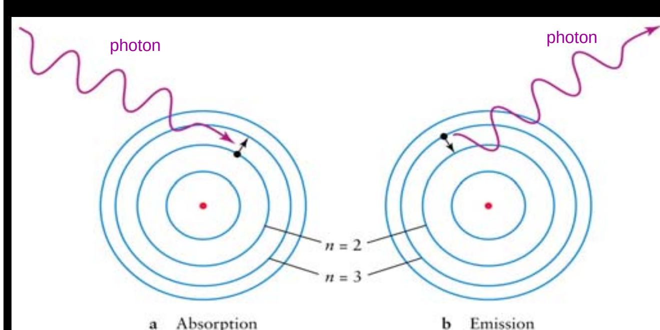


$$E_n = -\left(\frac{ke^2}{2a_0}\right)\frac{Z^2}{n^2}$$

Rydberg Constant



Bohr's Atom: Emission & Absorption Spectra



Some Notes About Bohr Like Atoms

- Ground state of Hydrogen atom (n=1) E_0= -13.6 eV
- Method for calculating energy levels etc applies to all Hydrogen-like atoms → -1e around +Ze
  - Examples : He^+, Li^{++}
- Energy levels would be different if replace electron with Muons
  - Reduced Mass
  - Necessity of Reduced Mass calculation enhanced for "positronium" like systems
- Bohr's method can be applied in general to all systems under a central force (e.g. gravitational instead of Coulombic)

$$\text{If change } U(r) = k\frac{Q_1Q_2}{r} \to G\frac{M_1M_2}{r}$$

Changes every thing: E, r , f etc

"Importance of constants in your life"

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Bohr's Correspondence Principle

- It now appears that there are two different worlds with different laws of physics governing them
  - The macroscopic world
  - The microscopic world
- How does one transcend from one world to the other ?
  - Bohr's correspondence Principle
    - predictions of quantum theory must correspond to predictions of the classical physics in the regime of sizes where classical physics is known to hold.

when n→ ∞ [Quantum Physics] = [Classical Physics]

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Correspondence Principle for Bohr Atom

- When n >> 1, quantization should have little effect, classical and quantum calculations should give same result: Check this →

Compare frequency of transition between level $n_i = n$ and $n_f = n-1$

$$\text{In Bohr Model : } f = \frac{c}{\lambda} = \frac{Z^2mk^2e^4}{4\pi\hbar^3}\left(\frac{1}{(n-1)^2} - \frac{1}{n^2}\right)$$

$$= \frac{Z^2mk^2e^4}{4\pi\hbar^3}\frac{2n-1}{n^2(n-1)^2} \approx \boxed{\frac{Z^2mk^2e^4}{4\pi\hbar^3}\frac{1}{n^3}}$$ (since when n>>1, n-1 ≈ n)

$$\text{And Classically: } f_{rev} = \frac{v}{2\pi r}; \text{ using } \boxed{v = \frac{n\hbar}{mr}} \text{ and } \boxed{r = \frac{n^2\hbar^2}{mkZe^2}}$$

$$\Rightarrow f_{rev} = \frac{n\hbar/mr}{2\pi r} = \frac{n\hbar}{2\pi mr^2} = \frac{n\hbar}{2\pi m(n^2\hbar^2/mkZe^2)^2} = \boxed{\frac{mk^2Z^2e^4}{2\pi\hbar^3n^3}}$$

$\Rightarrow$ *Same*!

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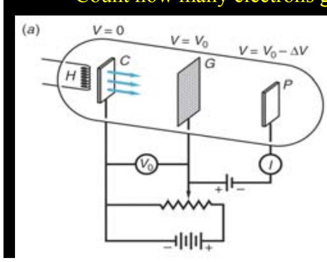
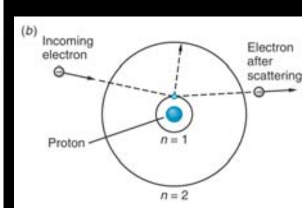
Atomic Excitation by Electrons: Franck-Hertz Expt

Other ways of Energy exchange are also quantized ! Example:

- Transfer energy to atom by colliding electrons on it
  - Elastic and inelastic collisions with a heavy atom (Hg)
- Accelerate electrons, collide with Hg atoms, measure energy transfer in inelastic collision (by applying retarding voltage)
- Count how many electrons get thru and arrive at plate P





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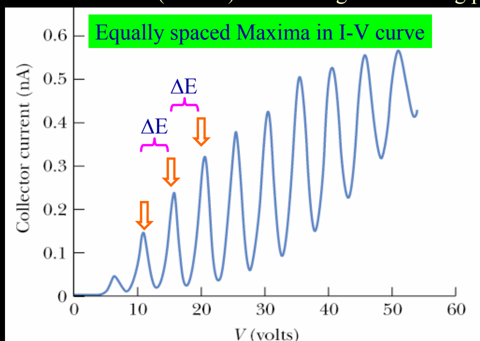
Atomic Excitation by Electrons: Franck-Hertz Expt

Plot # of electrons/time (current) overcoming the retarding potential (V)



Atoms accept only discrete amount of Energy, no matter the fashion in which energy is transfered

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Bohr's Explanation of Hydrogen like atoms

- Bohr's Semiclassical theory explained some spectroscopic data → Nobel Prize : 1922
- The "hotch-potch" of clasical & quantum attributes left many (Einstein) unconvinced
  - "appeared to me to be a miracle – and appears to me to be a miracle today ...... One ought to be ashamed of the successes of the theory"
- Problems with Bohr's theory:
  - Failed to predict INTENSITY of spectral lines
  - Limited success in predicting spectra of multi-electron atoms (He)
  - Failed to provide "time evolution " of system from some initial state
  - Overemphasized Particle nature of matter-could not explain the wave-particle duality of light
  - No general scheme applicable to non-periodic motion in subatomic systems
- "Condemned" as a one trick pony ! Without fundamental insight …raised the question : Why was Bohr successful?

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Prince Louise de Broglie & Matter Waves

- Key to Bohr atom was Angular momentum quantization
- Why this Quantization: $mvr = |L| = nh/2\pi$?
- Invoking symmetry in nature, Prince Louise de Broglie conjectured:

Because photons have wave and particle like nature → particles may have wave like properties !!

Electrons have accompanying "pilot" wave (not EM) which guide particles thru spacetime.

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A PhD Thesis Fit For a Prince !

- Matter Wave !
  - "Pilot wave" of $\lambda = h/p = h / (\gamma m v)$
  - Frequency of pilot wave $f = E/h$
- Consequence:
  - If matter has wave like properties then there would be interference (destructive & constructive) of some kind!
    - Analogy of standing waves on a plucked string to explain the quantization condition of Bohr orbits

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Matter Waves : How big, how small ?

1.Wavelength of baseball, m=140g, v=27m/s

$$\lambda=\frac{h}{p}=\frac{h}{mv}=\frac{6.63\times10^{-34}\,J.s}{(.14kg)(27m/s)}=1.75\times10^{-34}\,m$$

$\Rightarrow$ $\boxed{\lambda_{baseball} <<< \text{ size of nucleus}}$

$\Rightarrow$ Baseball "looks" like a particle

2. Wavelength of electron K=120eV (assume NR)

$$K=\frac{p^2}{2m}\Rightarrow p=\sqrt{2mK}$$

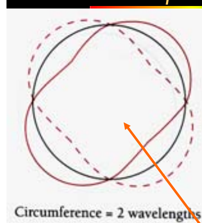
$$=\sqrt{2(9.11\times10^{-31})(120eV)(1.6\times10^{-19})}$$

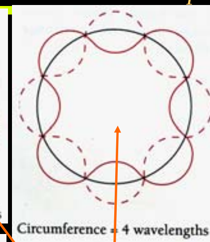
$$=5.91\times\ 10^{-24}\,Kg.m/s$$

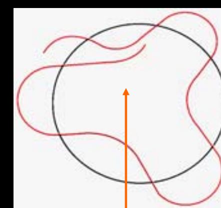
$$\lambda_e=\frac{h}{p}=\frac{6.63\times10^{-34}\,J.s}{5.91\times10^{-24}\,kg.m/s}=1.12\times10^{-10}\,m$$

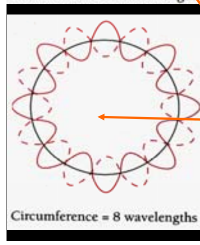
$\Rightarrow$ $\boxed{\lambda_e \simeq \text{ Size of atom}}$!!

Models of Vibrations on a Loop: Model of e in atom







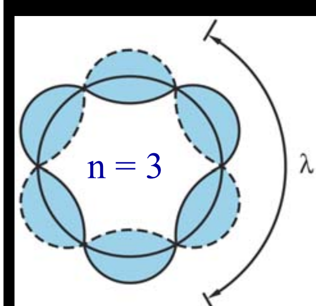


Modes of vibration when a integral # of λ fit into loop

(Standing waves) vibrations continue Indefinitely

Fractional # of waves in a loop can not persist due to destructive interference

De Broglie's Explanation of Bohr's Quantization



Standing waves in H atom:

Constructive interference when

$n\lambda = 2\pi r$

since $\lambda=\frac{h}{p}=\frac{h}{mv}$ ......(NR)

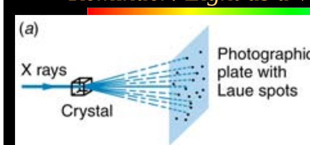
$\Rightarrow \frac{nh}{mv}=2\pi r$

$\Rightarrow \boxed{n\hbar = mvr}$

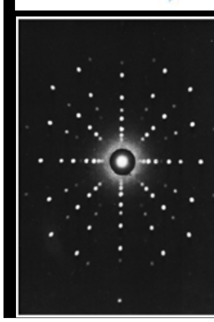
Angular momentum Quantization condition!

This is too intense ! Must verify such "loony tunes" with experiment

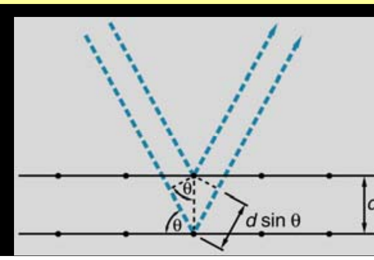
Reminder: Light as a Wave : Bragg Scattering Expt

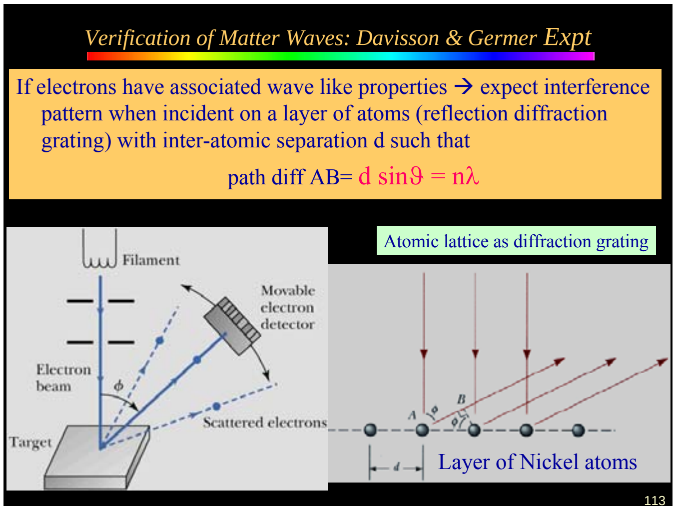


X-ray scatter off a crystal sample
X-rays constructively interfere from certain planes producing bright spots



Interference → Path diff=2dsinϑ = nλ




Verification of Matter Waves: Davisson & Germer Expt
If electrons have associated wave like properties → expect interference pattern when incident on a layer of atoms (reflection diffraction grating) with inter-atomic separation d such that
path diff AB= d sinϑ = nλ
Filament
Movable electron detector
Electron beam
Target
Scattered electrons
Atomic lattice as diffraction grating
Layer of Nickel atoms
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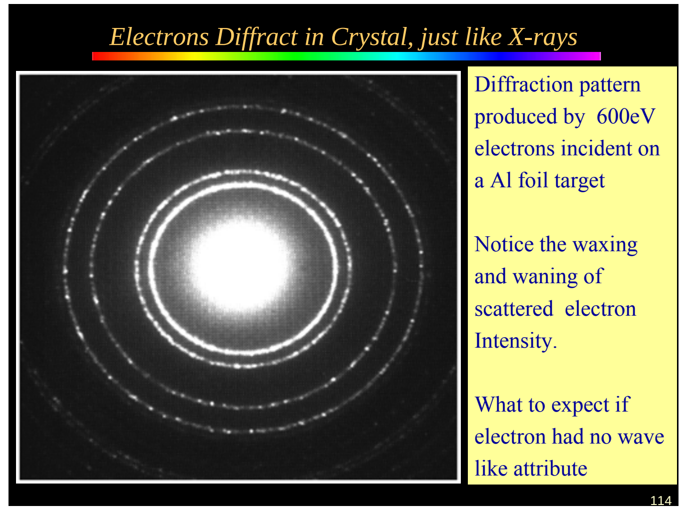
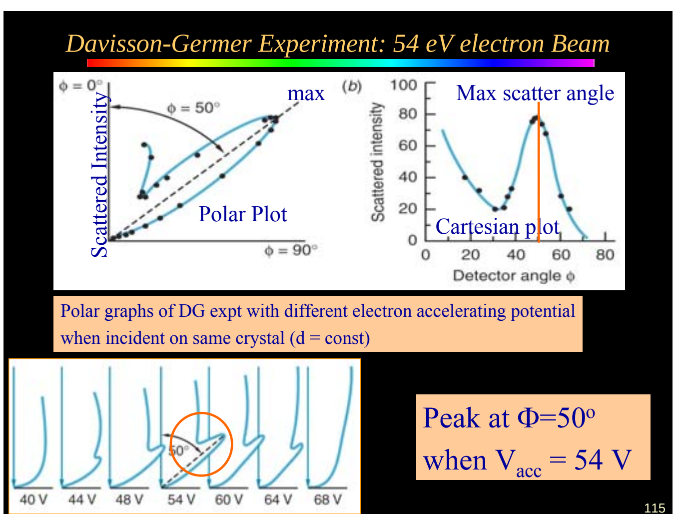
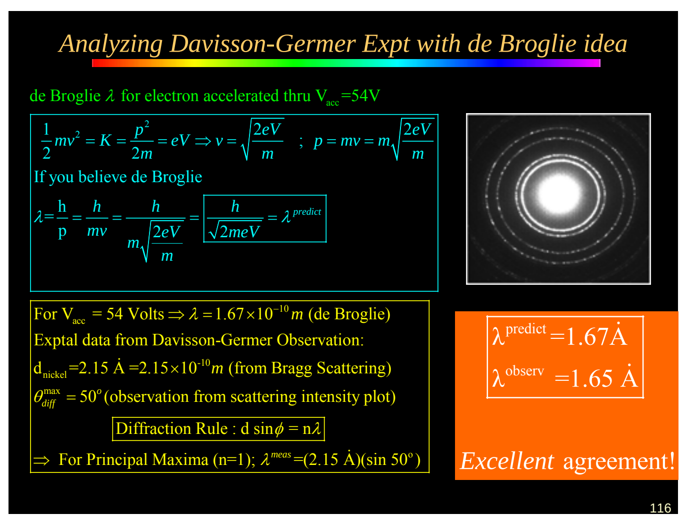

Electrons Diffract in Crystal, just like X-rays
Diffraction pattern produced by 600eV electrons incident on a Al foil target
Notice the waxing and waning of scattered electron Intensity.
What to expect if electron had no wave like attribute
114


Davisson-Germer Experiment: 54 eV electron Beam
φ = 0°
φ = 50°
max
Scattered Intensity
Polar Plot
φ = 90°
Max scatter angle
Scattered intensity
Cartesian plot
Detector angle φ
Polar graphs of DG expt with different electron accelerating potential when incident on same crystal (d = const)
40 V
44 V
48 V
54 V
60 V
64 V
68 V
Peak at Φ=50° when V_{acc} = 54 V
115


Analyzing Davisson-Germer Expt with de Broglie idea
de Broglie λ for electron accelerated thru V_{acc}=54V
$\frac{1}{2}mv^2 = K = \frac{p^2}{2m} = eV \Rightarrow v = \sqrt{\frac{2eV}{m}}$; $p = mv = m\sqrt{\frac{2eV}{m}}$
If you believe de Broglie
$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{m\sqrt{\frac{2eV}{m}}} = \frac{h}{\sqrt{2meV}} = \lambda^{predict}$
For V_{acc} = 54 Volts ⇒ $\lambda = 1.67\times10^{-10}\,m$ (de Broglie)
Exptal data from Davisson-Germer Observation:
d_{nickel}=2.15 Å =$2.15\times10^{-10}\,m$ (from Bragg Scattering)
θ^{max}_{diff} = 50° (observation from scattering intensity plot)
Diffraction Rule : d sinφ = nλ
⇒ For Principal Maxima (n=1); λ^{meas}=(2.15 Å)(sin 50°)
$\lambda^{predict}$=1.67Å
λ^{observ} =1.65 Å
Excellent agreement!
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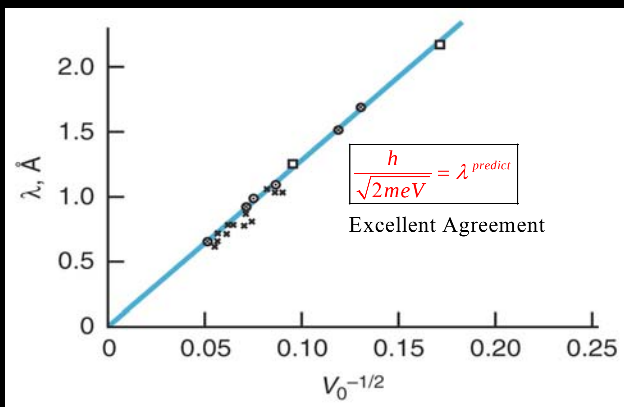
Davisson Germer Experiment: Matter Waves !



$$\frac{h}{\sqrt{2meV}} = \lambda^{predict}$$

Excellent Agreement

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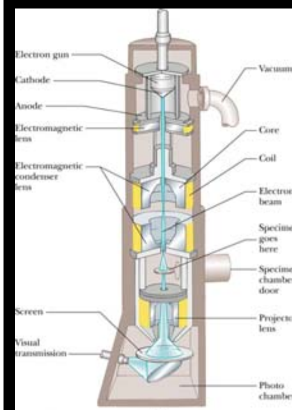
Practical Application : Electron Microscope



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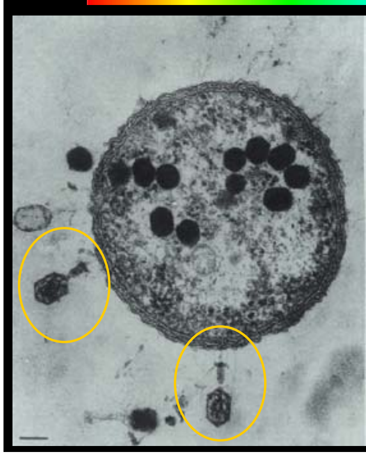
Electron Microscope : Excellent Resolving Power



Electron Micrograph showing Bacteriophage viruses in E. Coli bacterium

The bacterium is ≅ 1μ size

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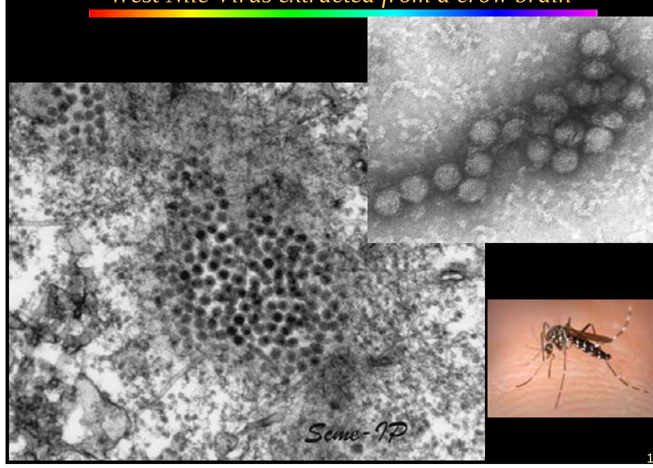
West Nile Virus extracted from a crow brain



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Just What is Waving in Matter Waves ?

For waves in an ocean, it's the water that "waves"
For sound waves, it's the molecules in medium
For light it's the **E** & **B** vectors that oscillate

Just What's "**waving**" in matter waves ?

- **It's the PROBABLILITY OF FINDING THE PARTICLE that waves !**
- **Particle can be represented by a wave packet**
  - At a certain location (x)
  - At a certain time (t)
  - **Made by superposition of many sinusoidal waves of different amplitudes, wavelengths λ and frequency f**
  - **It's a "pulse" of probability in spacetime**

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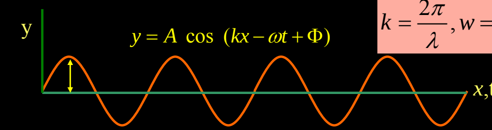
What Wave Does Not Describe a Particle



$k = \frac{2\pi}{\lambda}, w = 2\pi f$

- What wave form can be associated with particle's pilot wave?
- A traveling sinusoidal wave? $y = A\ \cos\ (kx - \omega t + \Phi)$
- Since de Broglie "pilot wave" represents particle, it must travel with same speed as particle ……(like me and my shadow)

Phase velocity (v_p) of sinusoidal wave: $v_p = \lambda f$

In Matter:

(a) $\lambda = \frac{h}{p} = \frac{h}{\gamma m v}$

(b) $f = \frac{E}{h} = \frac{\gamma m c^2}{h}$

$\Rightarrow v_p = \lambda f = \frac{E}{p} = \frac{\gamma m c^2}{\gamma m v} = \frac{c^2}{v} > c!$

Conflicts with Relativity → Unphysical

Single sinusoidal wave of infinite extent does not represent particle localized in space

Need "wave packets" localized Spatially (x) and Temporally (t)

122

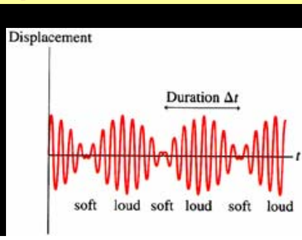
How To Make Wave Packets : Just Beat it !

Superposition of two sound waves of slightly different frequencies f_1 and f_2, $f_1 \cong f_2$

Pattern of beats is a series of wave packets

Beat frequency $f_{beat} = f_2 - f_1 = \Delta f$

Δf = range of frequencies that are superimposed to form the wave packet



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Addition of 2 Waves with slightly different λ and slightly different ω

Resulting wave's "displacement" $y = y_1 + y_2$:

$y = A\left[\cos(k_1 x - w_1 t) + \cos(k_2 x - w_2 t)\right]$

Trignometry : $\cos A + \cos B = 2\cos(\frac{A+B}{2})\cos(\frac{A-B}{2})$

$\therefore\ y = 2A\left[\left(\cos(\frac{k_2 - k_1}{2}x - \frac{w_2 - w_1}{2}t)\right)\left(\cos(\frac{k_2 + k_1}{2}x - \frac{w_2 + w_1}{2}t)\right)\right]$

since $k_2 \cong k_1 \cong k_{ave}$, $w_2 \cong w_1 \cong w_{ave}$, $\Delta k \ll k, \Delta w \ll w$

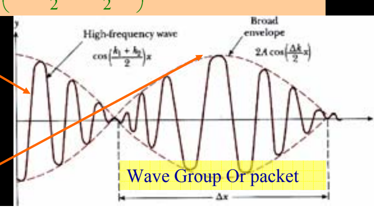
$\therefore\ y = 2A\left[\left(\cos(\frac{\Delta k}{2}x - \frac{\Delta w}{2}t)\right)\cos(kx - wt)\right] \equiv\ y = A'\ \cos(kx - wt)$,

A' oscillates in x,t ; $A' = 2A\left(\cos(\frac{\Delta k}{2}x - \frac{\Delta w}{2}t)\right)$ = modulated amplitude

Phase Vel $V_p = \frac{w_{ave}}{k_{ave}}$

Group Vel $V_g = \frac{\Delta w}{\Delta k}$

V_g : Vel of envelope$= \frac{dw}{dk}$



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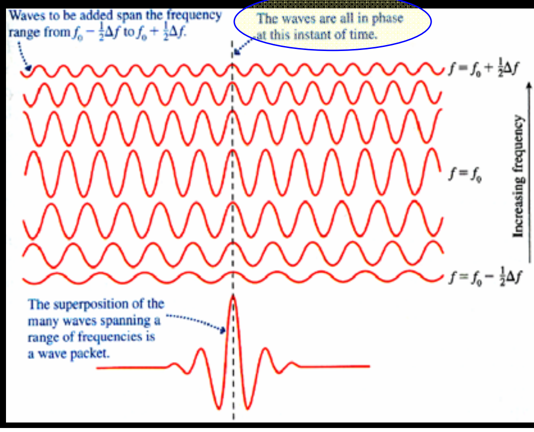
Non-repeating wave packet can be created thru superposition Of many waves of similar (but different) frequencies and wavelengths



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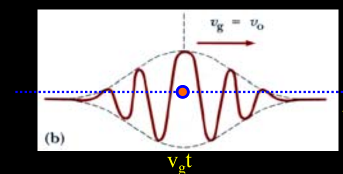
Wave Packet : Localization

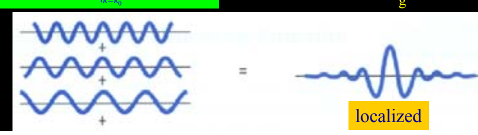
Finite # of diff. Monochromatic waves always produce INFINTE sequence of repeating wave groups → can't describe (localized) particle
To make localized wave packet, add " infinite" # of waves with Well chosen Amplitude A, Wave number k and ang. f requency ω

$\psi(x,t) = \int_{-\infty}^{\infty} A(k)\, e^{i(kx-wt)} dk$

$A(k)$ = Amplitude distribution Fn
$\Rightarrow$ diff waves of diff k have different amplitudes A(k)
w = w(k), depends on type of wave, media

Group Velocity $V_g = \left.\frac{dw}{dk}\right|_{k=k_0}$





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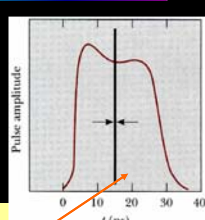
Group Velocity, Phase Velocity and Dispersion

In a Wave Packet: $w = w(k)$

Group Velocity $V_g = \left.\frac{dw}{dk}\right|_{k=k_0}$

Since $V_p = \frac{w}{k}$ (def) $\Rightarrow w = kV_p$

$\therefore V_g = \left.\frac{dw}{dk}\right| = V_p\big|_{k=k_0} + k\left.\frac{dV_p}{dk}\right|_{k=k_0}$



usually $V_p = V_p(\lambda)$
Material in which V_p varies with λ are said to be Dispersive
Individual harmonic waves making a wave pulse travel at different V_p thus changing shape of pulse and become spread out
In non-dispersive media, $V_g = V_p$; Example: EM waves in vaccum
Wave packet maintains its shape as it moves.
In dispersive media $V_g \neq V_p$, depends on $\frac{dV_p}{dk}$; shape changes with time
Example: Water wave, EM waves in a medium

1 ns laser pulse disperse by x30 after traveling 1km in optical fiber

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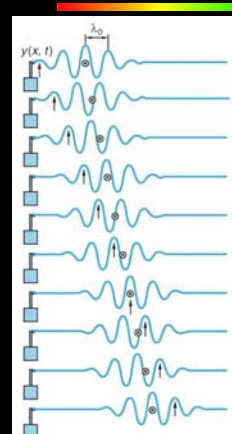
Example: Water Wave packet With $V_g = V_p/2$



Wave packet for which the group velocity=1/2 phase velocity

The ↑, representing a point of constant phase for the dominant λ, travels with V_p

The ⊕ at center of group travels with group velocity (V_g)

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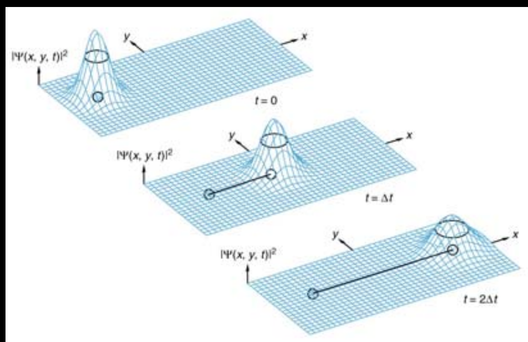
A Dispersive Wave Packet Moving Along X Axis



The O indicates position of the classical particle. The Wave packet spreads out in x & y directions since V_p of constituent waves depends on wavelength λ of the wave

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Group Velocity v_g of Matter Wave Packets

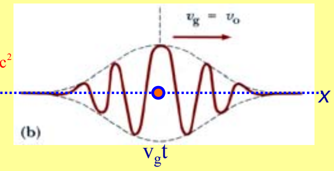
Consider An Electron:

mass = m velocity = v, momentum = p

Energy $E = hf = \gamma mc^2$; $\omega = 2\pi f = \frac{2\pi}{h}\gamma mc^2$

Wavelength $\lambda = \frac{h}{p}$; $k = \frac{2\pi}{\lambda} \Rightarrow k = \frac{2\pi}{h}\gamma mv$

Group Velocity : $V_g = \frac{dw}{dk} = \frac{dw/dv}{dk/dv}$



$$\frac{dw}{dv} = \frac{d}{dv}\left[\frac{\frac{2\pi}{h}mc^2}{[1-(\frac{v}{c})^2]^{1/2}}\right] = \frac{2\pi mv}{h[1-(\frac{v}{c})^2]^{3/2}} \quad \& \quad \frac{dk}{dv} = \frac{d}{dv}\left[\frac{2\pi}{h[1-(\frac{v}{c})^2]^{1/2}}mv\right] = \frac{2\pi m}{h[1-(\frac{v}{c})^2]^{3/2}}$$

$V_g = \frac{dw}{dk} = \frac{dw/dv}{dk/dv} = v \Rightarrow$ Group velocity of electron Wave packet "pilot wave"

is same as electron's physical velocity

But velocity of individual waves making up the wave packet $V_p = \frac{w}{k} = \frac{c^2}{v} > c!$ (not physical)

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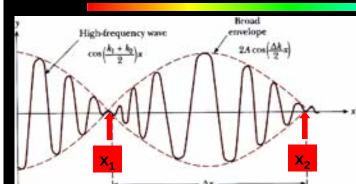
Wave Packets & Uncertainty Principles



$$y = 2A\left[\left(\cos(\frac{\Delta k}{2}x - \frac{\Delta w}{2}t)\right)\cos(kx - wt)\right]$$

What can we learn from this simple model ?

- Distance ΔX between adjacent minima = $(X_2)_{node} - (X_1)_{node}$
- Define X_1=0 then phase diff from $X_1 \rightarrow X_2 = \pi$ (similarly for $t_1 \rightarrow t_2$)

Node at y = 0 = 2A cos $(\frac{\Delta w}{2}t - \frac{\Delta k}{2}x)$, Examine x or t behavior

$\Rightarrow$ in x: $\boxed{\Delta k.\Delta x = \pi}$ $\Rightarrow$ Need to combine many waves of diff. k to make small Δx pulse

$\Delta x = \frac{\pi}{\Delta k}$, for small $\Delta x \rightarrow 0 \Rightarrow \Delta k \rightarrow \infty$ & Vice Verca

and In t : $\boxed{\Delta w.\Delta t = \pi}$ $\Rightarrow$ Need to combine many waves of diff ω to make small Δt pulse

$\Delta t = \frac{\pi}{\Delta \omega}$, for small $\Delta t \rightarrow 0 \Rightarrow \Delta\omega \rightarrow \infty$ & Vice Verca

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Signal Transmission and Bandwidth Theory

- Short duration pulses are used to transmit digital info
  - Over phone line as brief tone pulses
  - Over satellite link as brief radio pulses
  - Over optical fiber as brief laser light pulses
- Ragardless of type of wave or medium, any wave pulse must obey the fundamental relation
  - $\Delta\omega\Delta t \cong \pi$
- Range of frequencies that can be transmitted are called bandwidth of the medium
- Shortest possible pulse that can be transmitted thru a medium is

$\Delta t_{min} \cong \pi/\Delta\omega$

- Higher bandwidths transmits shorter pulses & allows high data rate

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Wave Packets & The Uncertainty Principles of Subatomic Physics

in space x: $\boxed{\Delta k.\Delta x = \pi}$ $\Rightarrow$ since $k = \frac{2\pi}{\lambda}$, $p = \frac{h}{\lambda}$

$\Rightarrow$ $\boxed{\Delta p.\Delta x = h/2}$

usually one writes $\boxed{\Delta p.\Delta x \geq \hbar/2}$ approximate relation

In time t : $\boxed{\Delta w.\Delta t = \pi}$ $\Rightarrow$ since $\omega = 2\pi f$, $E = hf$

$\Rightarrow$ $\boxed{\Delta E.\Delta t = h/2}$

usually one writes $\boxed{\Delta E.\Delta t \geq \hbar/2}$ approximate relation

What do these inequalities mean physically?

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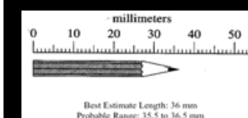
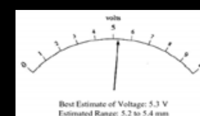
Know the Error of Thy Ways: Measurement Error → Δ

- Measurements are made by observing something : length, time, momentum, energy
- All measurements have some (limited) precision….no matter the instrument used
- Examples:
  - How long is a desk ? L = (5 ± 0.1) m = L ± ΔL (depends on ruler used)
  - How long was this lecture ? T = (50 ± 1)minutes = T ± ΔT (depends on the accuracy of your watch)
  - How much does Prof. Sharma weigh ? M = (1000 ± 700) kg = m ± Δm
    - Is this a correct measure of my weight ?
      - Correct (because of large error reported) but imprecise
      - My correct weight is covered by the (large) error in observation



Length Measure



Voltage (or time) Measure

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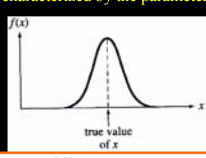
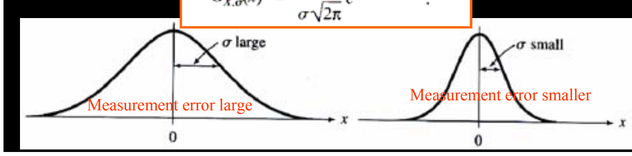
Measurement Error : x ± Δx

- Measurement errors are unavoidable since the measurement procedure is an experimental one
- True value of an measurable quantity is an abstract concept
- In a set of repeated measurements with random errors, the distribution of measurements resembles a Gaussian distribution characterized by the parameter σ or Δ characterizing the width of the distribution



The Gauss, or Normal, Distribution

$$G_{X,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-X)^2/2\sigma^2}.$$



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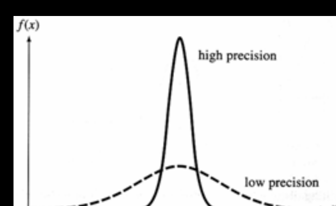
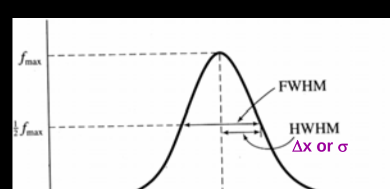
Measurement Error : x ± Δx





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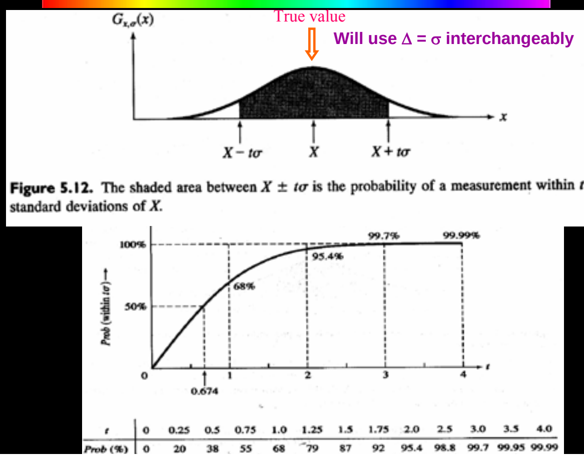
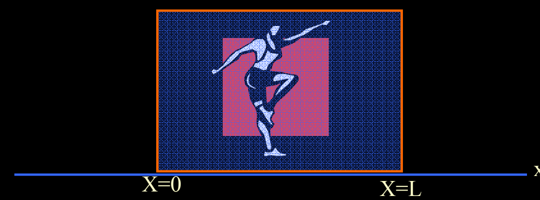
Interpreting Measurements with random Error : Δ



Where in the World is Carmen San Diego?

Carmen San Diego hidden inside a big box of length L

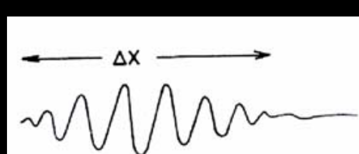
Suppose you can't see thru the (blue) box, what is you best estimate of her location inside box (she could be anywhere inside the box)



Your best unbiased measure would be $x = L/2 \pm L/2$

There is no perfect measurement, there are always measurement error

Wave Packets & Matter Waves



- What is the Wave Length of this wave packet?
  - made of waves with $\lambda-\Delta\lambda < \lambda < \lambda+\Delta\lambda$
  - De Broglie wavelength $\lambda = h/p$
    - → Momentum Uncertainty: $p-\Delta p < p < p+\Delta p$
- Similarly for frequency ω or f
  - made of waves with $\omega-\Delta\omega < \omega < \omega+\Delta\omega$

  Planck's condition $E = hf = h\omega/2$

  → Energy Uncertainty: $E-\Delta E < E < E + \Delta E$

Back to Heisenberg's Uncertainty Principle

- $\Delta x . \Delta p \geq h/4\pi \Rightarrow$ If the measurement of the position of a particle is made with a precision Δx and a SIMULTANEOUS measurement of its momentum p_x in the X direction , then the product of the two uncertainties (measurement errors) can never be smaller than $\cong h/4\pi$ irrespective of how precise the measurement tools

- $\Delta E . \Delta t \geq h/4\pi \Rightarrow$ If the measurement of the energy E of a particle is made with a precision ΔE and it took time Δt to make that measurement, then the product of the two uncertainties (measurement errors) can never be smaller than $\cong h/4\pi$ irrespective of how precise the measurement tools

These rules arise from the way we constructed the wave packets describing Matter "pilot" waves

Perhaps these rules are bogus, can we verify this with some physical picture ??

Are You Experienced ?

- What you experience is what you observe
- What you observe is what you measure
- No measurement is perfect, they all have measurement error: question is of the degree
  - Small or large Δ
- Uncertainty Principle and Breaking of Conservation Rules
  - Energy Conservation
  - Momentum Conservation

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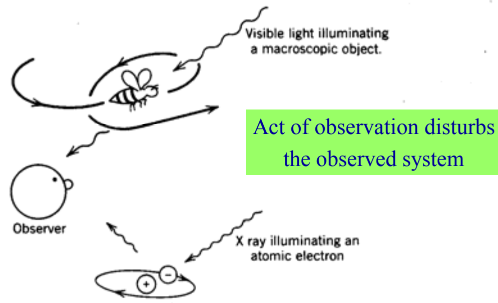
The Act of Observation (Compton Scattering)

Observations of particle motion by means of scattered illumination. When the incident wavelength is reduced to accommodate the size of the particle, the momentum transferred by the photon becomes large enough to disturb the observed motion.



Act of observation disturbs the observed system

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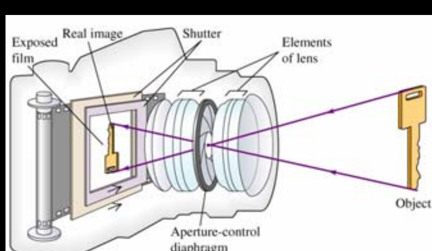
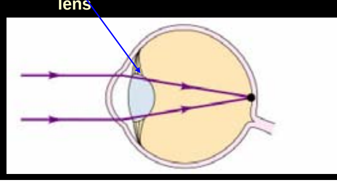
Act of Observation Tells All



lens



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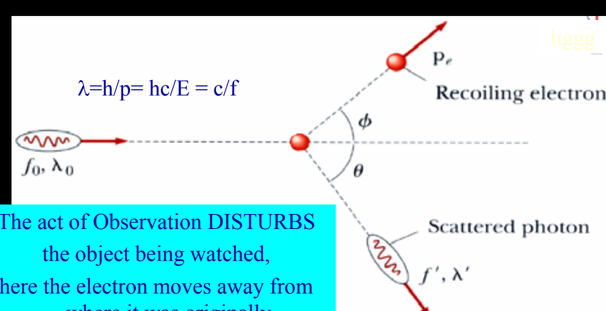
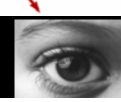
Compton Scattering: Shining light to observe electron

Photon scattering off an electron, Seeing→ the photon enters my eye



The act of Observation DISTURBS the object being watched, here the electron moves away from where it was originally



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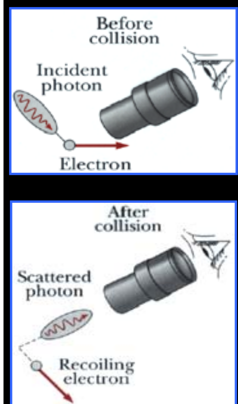
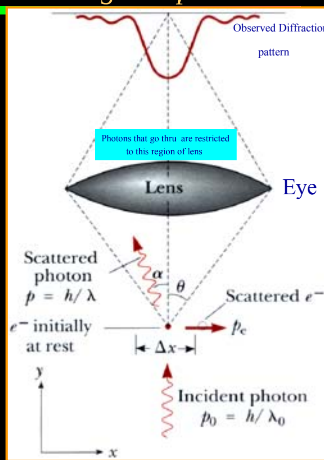
Act of Watching: A Thought Experiment





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Diffraction By a Circular Aperture (Lens)

See Resnick, Halliday Walker 6th Ed (on S.Reserve), Ch 37, pages 898-900

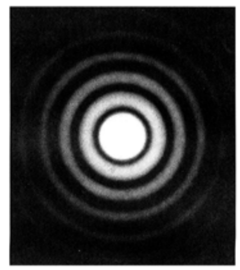

Fig. 37-9 The diffraction pattern of a circular aperture. Note the central maximum and the circular secondary maxima. The figure has been overexposed to bring out these secondary maxima, which are much less intense than the central maximum.

Diffracted image of a point source of light thru a lens (circular aperture of size d)

First minimum of diffraction pattern is located by

$$\sin\theta = 1.22\frac{\lambda}{d}$$

See previous picture for definitions of ϑ, λ, d

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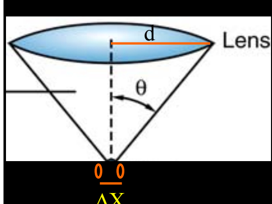
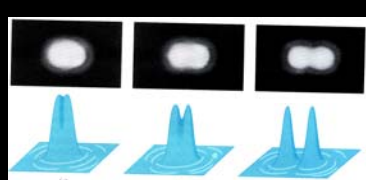
Resolving Power of Light Thru a Lens

Image of 2 separate point sources formed by a converging lens of diameter d, ability to resolve them depends on λ & d because of the Inherent diffraction in image formation





Not resolved Barely resolved Resolved

Resolving power $\Delta x \simeq \frac{\lambda}{2\sin\theta}$

θ depends on lens radius d

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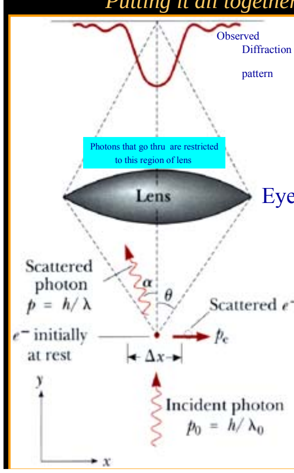
Putting it all together: Act of Observing an Electron



- Incident light (p,λ) scatters off electron
- To be collected by lens → γ must scatter thru angle α
  - $-\vartheta \le \alpha \le \vartheta$
- Due to Compton scatter, electron picks up momentum
  - P_X , P_Y

$$-\frac{h}{\lambda}\sin\theta \le P_x \le \frac{h}{\lambda}\sin\theta$$

electron momentum uncertainty is

$$\Delta p \cong \frac{\sim 2h}{\lambda}\sin\theta$$

- After passing thru lens, photon diffracts, lands somewhere on screen, image (of electron) is fuzzy
- How fuzzy ? Optics says shortest distance between two resolvable points is :

$$\Delta x = \frac{\lambda}{2\sin\theta}$$

- Larger the lens radius, larger the $\vartheta \Rightarrow$ better resolution

$$\Rightarrow \Delta p.\Delta x \simeq \left(\frac{2h\sin\theta}{\lambda}\right)\left(\frac{\lambda}{2\sin\theta}\right) = h$$

$$\Rightarrow \Delta p.\Delta x \ge \hbar/2$$

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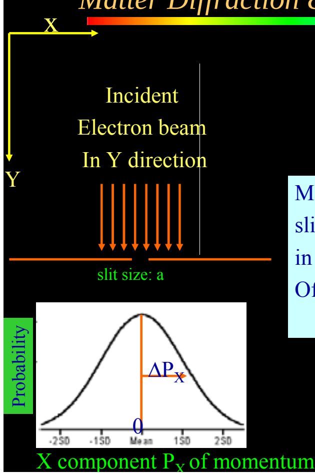
Aftermath of Uncertainty Principle

- Deterministic (Newtonian) physics topples over
  - Newton's laws told you all you needed to know about trajectory of a particle
    - Apply a force, watch the particle go !
      - Know every thing ! X, v, p , F, a
      - Can predict exact trajectory of particle if you had perfect device
- No so in the subatomic world !
  - Of small momenta, forces, energies
  - Can't predict anything exactly
    - Can only predict probabilities
      - There is so much chance that the particle landed here or there
      - Cant be sure !....cognizant of the errors of thy observations

All Measurements Have Associated Errors

- If your measuring apparatus has an intrinsic inaccuracy (error) of amount Δp
- Then results of measurement of momentum p of an object at rest can easily yield a range of values accommodated by the measurement imprecision :
  - $-\Delta p \leq p \leq \Delta p$: you will measure any of these values for the momentum of the particle
- Similarly for all measurable quantities like x, t, Energy !

Matter Diffraction & Uncertainty Principle

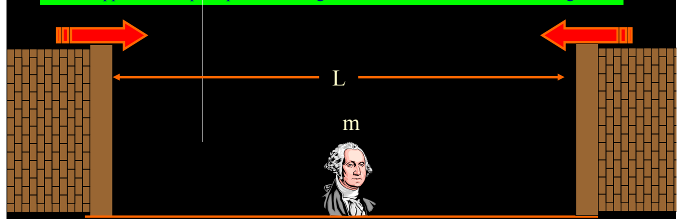


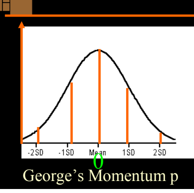
Momentum measurement beyond slit show particle not moving exactly in Y direction, develops a X component Of motion $-\Delta p_x \leq p_x \leq \Delta p_x$ with

$\Delta p_X = h/(2\pi a)$

Particle at Rest Between Two Walls

Object of mass M at rest between two walls originally at infinity
What happens to our perception of George's momentum as the walls are brought in ?



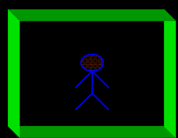


On average, measure <p> = 0
but there are quite large fluctuations!
Width of Distribution $= \Delta P$

$\Delta P = \sqrt{(P^2)_{ave} - (P_{ave})^2}$; $\Delta P \sim \frac{\hbar}{L}$

Implications of Uncertainty Principles

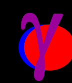
A bound "particle" is one that is confined in some finite region of space.



One of the cornerstones of Quantum mechanics is that bound particles can not be stationary – <u>even at Zero absolute temperature !</u>

There is a non-zero limit on the kinetic energy of a bound particle

Matter-Antimatter Collisions and Uncertainty Principle



Look at Rules of Energy and Momentum Conservation : Are they ?

$E_{before} = mc^2 + mc^2$ and $E_{after} = 2mc^2$

$P_{before} = 0$ but since photon produced in the annihilation → $P_{after} = 2mc$!

Such violation are allowed but must be consumed instantaneously !
Hence the name "virtual" particles

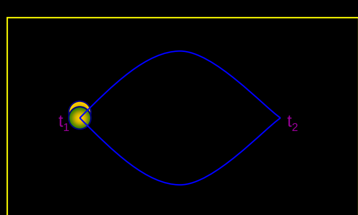
Fluctuations In The Vacuum : Breaking Energy Conservation Rules

Vacuum, at any energy, is bubbling with particle creation and annihilation

$\Delta E . \Delta t \approx h/2\pi$ implies that you can (in principle) pull out an **<u>elephant + anti-elephant</u>** from NOTHING (Vaccum) but for a very very short time Δt !!

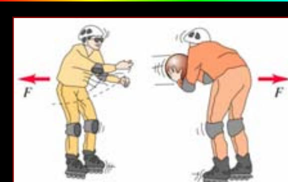
How Much Time : $\Delta t = \dfrac{\hbar}{2Mc^2}$

How cool is that !



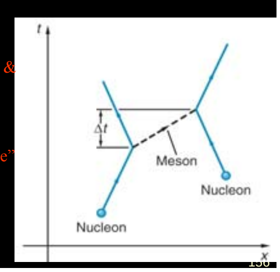
K rz#idu#fdq#wkh#yluwxdo#sduwlfohv#sursdjdwh#B#G hshqgv#rq#wkhlu#p dvv

Strong Force Within Nucleus → Exchange Force and Virtual Particles



Repulsive force

- Strong Nuclear force can be modeled as exchange of virtual particles called $\pi^{\pm}$ mesons by nucleons (protons & neutrons)
- $\pi^{\pm}$ mesons are emitted by proton and reabsorbed by a neutron
- The short range of the Nuclear force is due to the "large" mass of the exchanged meson
- $M_{\pi} = 140\ MeV/c^2$



Range of Nuclear Exchange Force

How long can the emitted virtual particle last?

$\Delta E \times \Delta t \geq \hbar$

The virtual particle has rest mass + kinetic energy

$\Rightarrow$ Its energy $\boxed{\Delta E \geq Mc^2}$

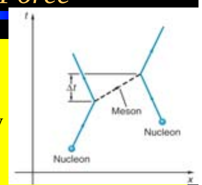
$\Rightarrow$ Particle can not live for more than $\boxed{\Delta t \leq \hbar / Mc^2}$

Range R of the meson (and thus the exchange force)

R= $c\Delta t = c\hbar / Mc^2 = \hbar / Mc$

For M=140 MeV/c^2 $\Rightarrow R \simeq \dfrac{1.06\times10^{-34}\,J.s}{(140 MeV/c^2)\times c^2\times(1.60\times10^{-13}\,J/MeV)}$

$\boxed{R \simeq 1.4\times10^{-15}\,m = 1.4\,fm}$



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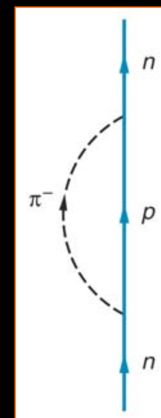
Subatomic Cinderella Act

- Neutron emits a charged pion for a time Δt and becomes a (charged) proton
- After time Δt , the proton reabsorbs charged pion particle (π^-) to become neutron again
- But in the time Δt that the positive proton and π^- particle exist, they can interact with other charged particles
- After time Δt strikes , the Cinderella act is over !



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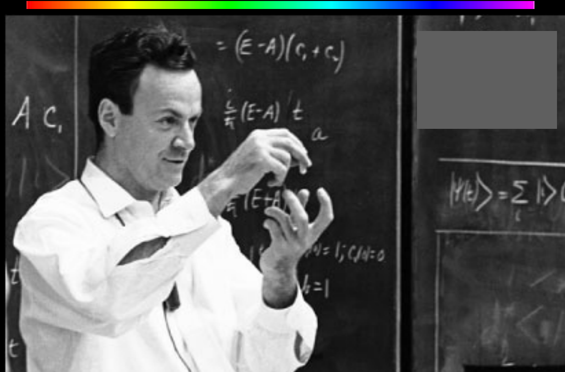
Quantum Behavior : Richard Feynman



See Chapters 1 & 2 of Feynman Lectures in Physics Vol III

Or Six Easy Pieces by Richard Feynman : Addison Wesley Publishers

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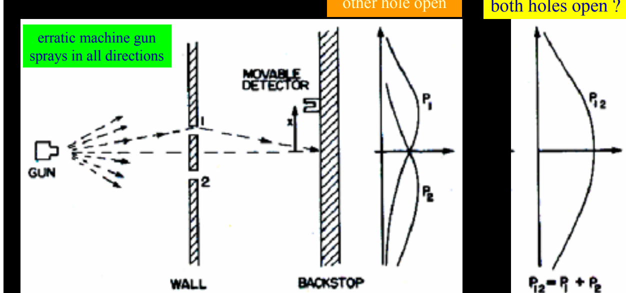
An Experiment with Indestructible Bullets

Prob.when one or other hole open

Probability P_{12} when both holes open ?



made of armor plate

sandbox

$P_{12} = P_1 + P_2$

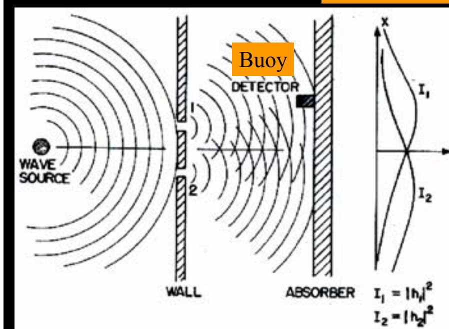
160

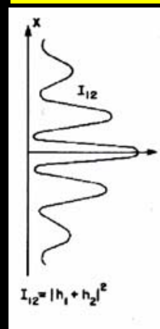
An Experiment With Water Waves

Measure Intensity of Water Waves
(by measuring detector displacement)

when one or other hole open

Intensity I_{12} when Both holes open





$$I_{12} = |h_1 + h_2|^2 = I_1 + I_2 + 2\sqrt{I_1 I_2}\cos\delta$$

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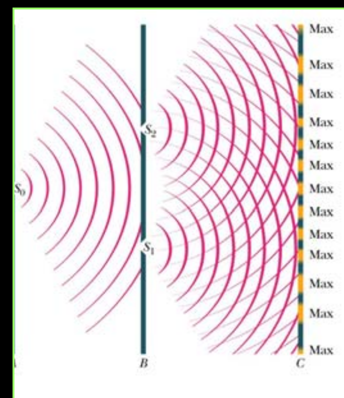
Wave Phenomena → Interference and Diffraction



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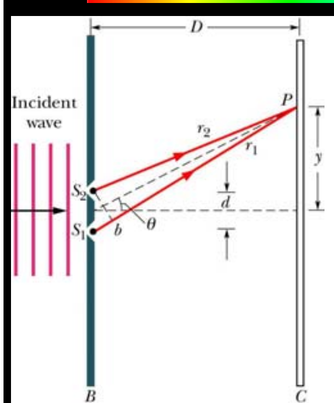
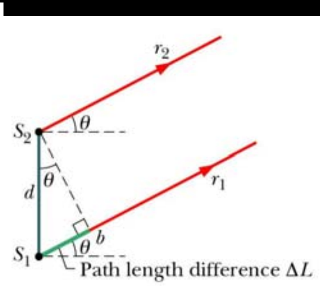
Interference Phenomenon in Waves





$$n\lambda = d\sin\theta$$

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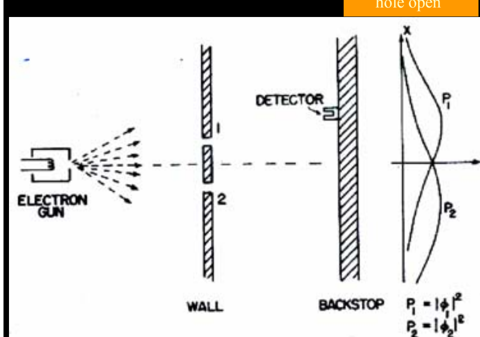
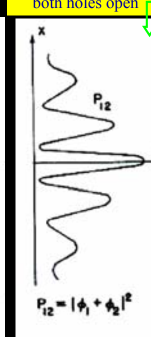
An Experiment With (indestructible) Electrons

when one or other hole open

Probability P_{12} when both holes open





$P_{12} \neq P_1 + P_2$

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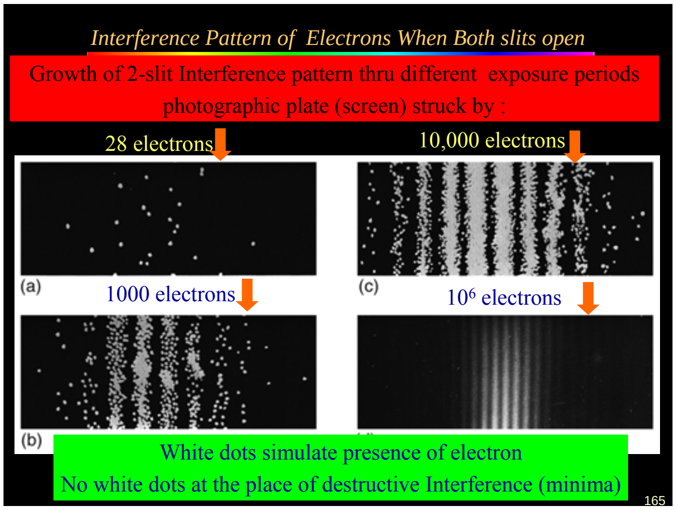
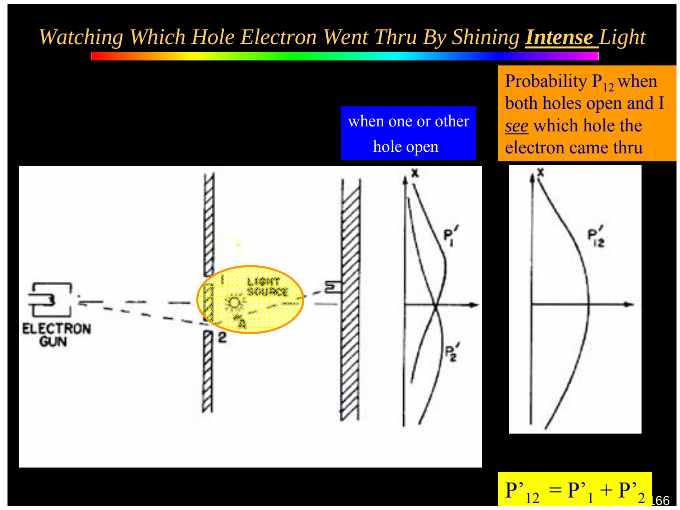
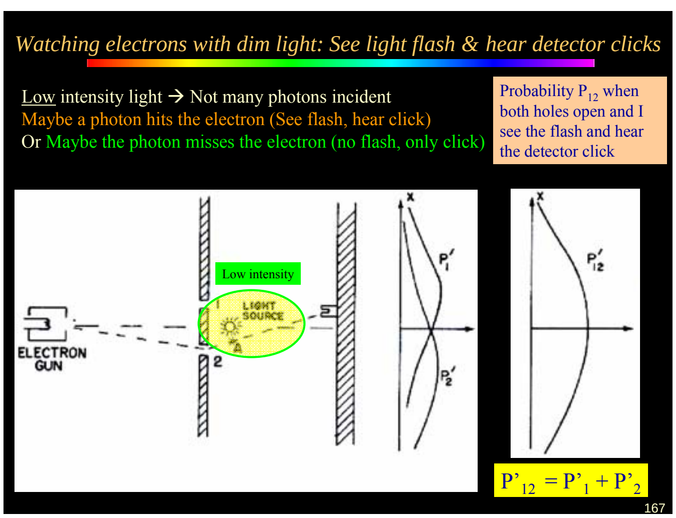
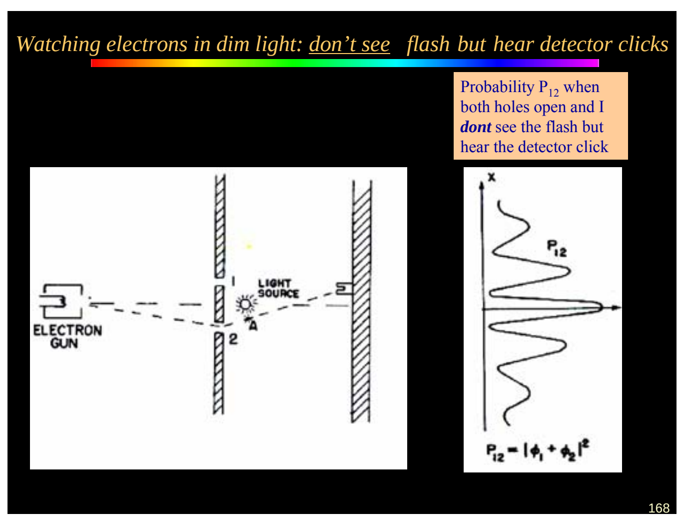
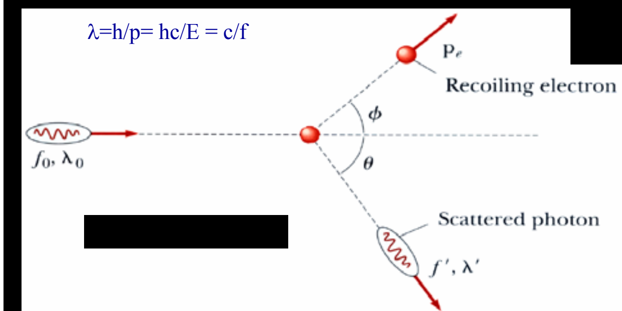

Interference Pattern of Electrons When Both slits open
Growth of 2-slit Interference pattern thru different exposure periods
photographic plate (screen) struck by :
28 electrons
10,000 electrons
(a)
1000 electrons
(c)
10⁶ electrons
(b)
White dots simulate presence of electron
No white dots at the place of destructive Interference (minima)
165


Watching Which Hole Electron Went Thru By Shining Intense Light
when one or other hole open
Probability P_{12} when both holes open and I see which hole the electron came thru
ELECTRON GUN
LIGHT SOURCE
1
2
A
x
P_1'
P_2'
P_{12}'
$P'_{12} = P'_1 + P'_2$
166

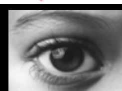

Watching electrons with dim light: See light flash & hear detector clicks
Low intensity light → Not many photons incident
Maybe a photon hits the electron (See flash, hear click)
Or Maybe the photon misses the electron (no flash, only click)
Probability P_{12} when both holes open and I see the flash and hear the detector click
Low intensity
ELECTRON GUN
LIGHT SOURCE
1
2
A
x
P_1'
P_2'
P_{12}'
$P'_{12} = P'_1 + P'_2$
167


Watching electrons in dim light: don't see flash but hear detector clicks
Probability P_{12} when both holes open and I dont see the flash but hear the detector click
ELECTRON GUN
LIGHT SOURCE
1
2
A
x
P_{12}
$P_{12} = |\phi_1 + \phi_2|^2$
168

Compton Scattering: Shining light to observe electron



The act of Observation DISTURBS the object being watched, here the electron moves away from where it was originally



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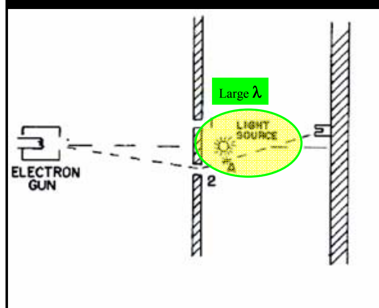
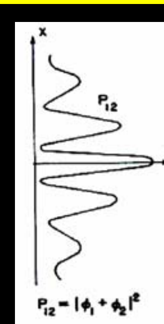
Watching Electrons With Light of λ >> slit size but High Intensity

Probability P_{12} when both holes open but can't tell, from the location of flash, which hole the electron came thru





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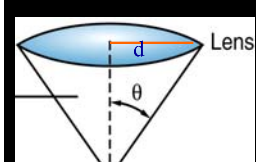
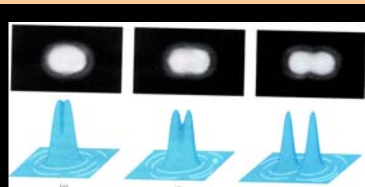
Why Fuzzy Flash? → Resolving Power of Light

Image of 2 separate point sources formed by a converging lens of diameter d, ability to resolve them depends on λ & d because of the Inherent diffraction in image formation



0_0

ΔX



Not resolved barely resolved resolved

$$\text{Resolving power } \Delta x \simeq \frac{\lambda}{2\sin\theta}$$

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Summary of Experiments So Far

1. Probability of an event is given by the square of amplitude of a complex # Ψ: Probability Amplitude
2. When an event occurs in several alternate ways, probability amplitude for the event is sum of probability amplitudes for each way considered seperately. There is interference:
   - $\Psi = \Psi_1 + \Psi_2$

     $P_{12} = |\Psi_1 + \Psi_2|^2$
3. If an experiment is done which is capable of determining whether one or other alternative is actually taken, probability for event is just sum of each alternative
   - Interference pattern is LOST !

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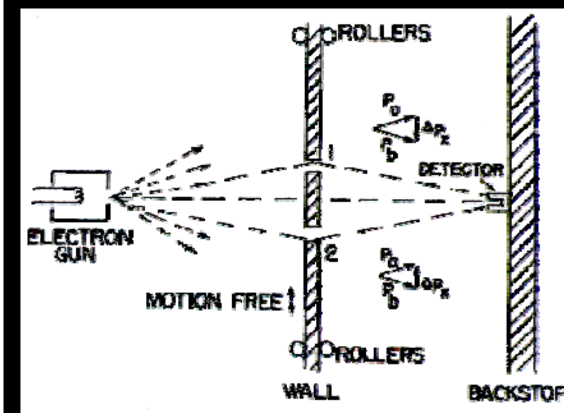
Is There No Way to Beat Uncertainty Principle?

- How about NOT watching the electrons!
- Let's be a bit crafty !!
- Since this is a Thought experiment→ ideal conditions
  - Mount the wall on rollers, put a lot of grease → frictionless
  - Wall will move when electron hits it
  - Watch recoil of the wall containing the slits when the electron hits it
  - By watching whether wall moved up or down I can tell
    -
    -
- Will my ingenious plot succeed?

Measuring The Recoil of The Wall → Not Watching Electron !



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Losing Out To Uncertainty Principle

- To measure the RECOIL of the wall ⇒
  - must know the initial momentum of the wall before electron hit it
  - Final momentum after electron hits the wall
  - Calculate vector sum → recoil
- Uncertainty principle :
  - To do this ⇒ $\Delta P = 0$ → $\Delta X = \infty$ [can not know the position of wall exactly]
  - If don't know the wall location, then down know where the holes are
  - Holes will be in different place for every electron that goes thru
  - → The center of interference pattern will have different (random) location for each electron
  - Such random shift is just enough to Smear out the pattern so that no interference is observed !

Summary

- Probability of an event in an ideal experiment is given by the square of the absolute value of a complex number Ψ which is call probability amplitude
  - P = probability
  - Ψ= probability amplitude, $P=|\Psi|^2$
- When an even can occur in several alternative ways, the probability amplitude for the event is the sum of the probability amplitudes for each way considered separately. There is interference:
  - $\Psi= \Psi_1+ \Psi_2$
  - $P=|\Psi_1+ \Psi_2|^2$
- If an experiment is performed which is capable of determining whether one or other alternative is actually taken, the probability of the event is the sum of probabilities for each alternative. The interference is lost: $P = P_1 + P_2$

The Lesson Learnt

- In trying to determine which slit the particle went through, we are examining particle-like behavior
- In examining the interference pattern of electron, we are using wave like behavior of electron

Bohr's Principle of Complementarity:

It is not possible to simultaneously determine physical observables in terms of both particles and waves

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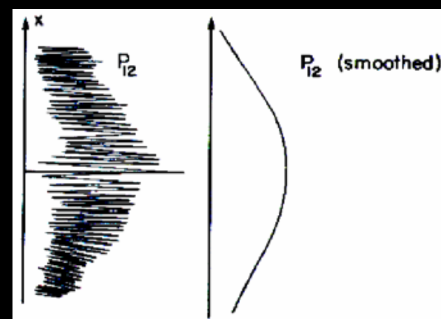
The Bullet Vs The Electron: Each Behaves the Same Way



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Quantum Mechanics of Subatomic Particles

- Act of Observation destroys the system (No watching!)
- If can't watch then all conversations can only be in terms of Probability P
- Every particle under the influence of a force is described by a Complex wave function $\Psi(x,y,z,t)$
- Ψ is the ultimate DNA of particle: contains all info about the particle under the force (in a potential e.g Hydrogen)
- Probability of per unit volume of finding the particle at some point (x,y,z) and time t is given by
  - $P(x,y,z,t) = \Psi(x,y,z,t) \,.\, \Psi^*(x,y,z,t) = |\Psi(x,y,z,t)|^2$
- When there are more than one path to reach a final location then the probability of the event is
  - $\Psi = \Psi_1 + \Psi_2$
  - $P = |\Psi^* \Psi| = |\Psi_1|^2 + |\Psi_2|^2 + 2\,|\Psi_1|\,|\Psi_2| \cos\phi$

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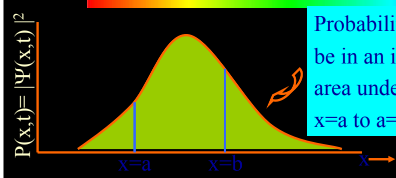
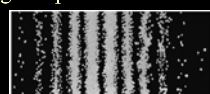
Wave Function of "Stuff" & Probability Density



Probability of a particle to be in an interval a ≤ x ≤b is area under the curve from x=a to a=b

- Although not possible to specify with certainty the location of particle, its possible to assign probability P(x)dx of finding particle between x and x+dx
- P(x) dx = | Ψ(x,t)|² dx
- E.g intensity distribution in light diffraction pattern is a measure of the probability that a photon will strike a given point within the pattern



Ψ: The Wave function Of A Particle

- The particle must be some where

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2 \, dx = 1$$

- Any Ψ satisfying this condition is NORMALIZED
- Prob of finding particle in finite interval

$$P(a \le x \le b) = \int_a^b \psi^*(x,t)\ \psi(x,t)dx$$

- Fundamental aim of Quantum Mechanics
  - Given the wavefunction at some instant (say t=0) find Ψ at some subsequent time t
  - Ψ(x,t=0) → Ψ(x,t) …evolution
  - Think of a probabilistic view of particle's "newtonian trajectory"
    - We are replacing Newton's 2nd law for subatomic systems

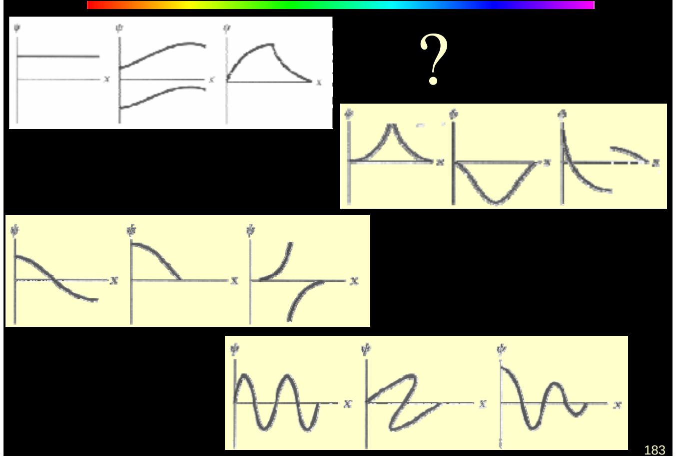
The Wave Function is a mathematical function that describes a physical object → Wave function must have some rigorous properties :

- Ψ must be finite
- Ψ must be continuous fn of x,t
- Ψ must be single-valued
- Ψ must be smooth fn →

$\frac{d\psi}{dx}$ must be continuous

WHY ?

Bad Wave Functions Of Physical Systems : You Decide Why



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A Simple Wave Function : Free Particle

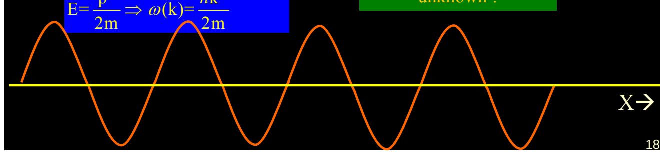
- Imagine a free particle of mass m , momentum p and K=p²/2m
- Under no force , no attractive or repulsive potential to influence it
- Particle is where it wants : can be any where [- ∞ ≤ x ≤ + ∞]
  - Has No relationship, no mortgage , no quiz, no final exam….its essentially a **bum** !
  - how to describe a **quantum mechanical bum** ?
    - Ψ(x,t)= $Ae^{i(kx-\omega t)}$ =A(Cos(kx-ωt)+ i sin (kx-ωt))

$k = \frac{p}{\hbar}$; $\omega = \frac{E}{\hbar}$

For non-relativistic particles

$E = \frac{p^2}{2m} \Rightarrow \omega(k) = \frac{\hbar k^2}{2m}$

Has definite momentum and energy but location unknown !



Wave Function of Different Kind of Free Particle : Wave Packet

Sum of Plane Waves:

$$\Psi(x,0) = \int_{-\infty}^{+\infty} a(k) e^{ikx} dk$$

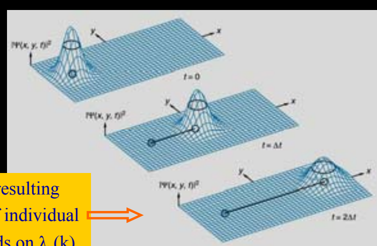
$$\Psi(x,t) = \int_{-\infty}^{+\infty} a(k) e^{i(kx-\omega t)} dk$$

Wave Packet initially localized in ΔX, Δt undergoes dispersion

Combine many free waves to create a localized wave packet (group)

The more you know now,
The less you will know later
Why ?

Spreading is due to DISPERSION resulting from the fact that phase velocity of individual waves making up the packet depends on λ (k)



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Normalization Condition: Particle Must be Somewhere

Example: $\psi(x,0) = Ce^{-\left|\frac{x}{x_0}\right|}$, C & x_0 are constants

This is a symmetric wavefunction with diminishing amplitude

The Amplitude is maximum at x =0 ⇒ Probability is max too

Normalization Condition: How to figure out C ?

A real particle must be somewhere: Probability of finding particle is finite

$$P(-\infty \le x \le +\infty) = \int_{-\infty}^{+\infty} |\psi(x,0)|^2 dx = \int_{-\infty}^{+\infty} C^2 e^{-2\left|\frac{x}{x_0}\right|} dx = 1$$

$$\Rightarrow 1 = 2C^2 \int_0^{\infty} e^{-2\left|\frac{x}{x_0}\right|} dx = 2C^2\left[\frac{x_0}{2}\right] = C^2 x_0$$

$$\Rightarrow \psi(x,0) = \frac{1}{\sqrt{x_0}} e^{-\left|\frac{x}{x_0}\right|}$$

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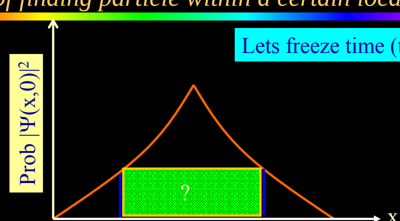
Probability of finding particle within a certain location x ± Δx

Lets freeze time (t=0)



$$P(-x_0 \le x \le +x_0) = \int_{-x_0}^{+x_0} |\psi(x,0)|^2 dx = \int_{-x_0}^{+x_0} C^2 e^{-2\left|\frac{x}{x_0}\right|} dx$$

$$= 2C^2\left[\frac{x_0}{2}\right]\left[1-e^{-2}\right] = \left[1-e^{-2}\right] = 0.865 \Rightarrow 87\%$$

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Where Do Wave Functions Come From ?

- Are solutions of the time dependent Schrödinger Differential Equation (inspired by Wave Equation seen in 2C)

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

- Given a potential U(x) → particle under certain force
  - $F(x) = -\dfrac{\partial U(x)}{\partial x}$

Schrodinger had an interesting life

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Introducing the Schrodinger Equation

Consider for simplicity just a *one*-dimensional system

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

- U(x) = characteristic Potential of the system
- Different potential for different types of forces
- Hence different solutions for the S eqn.
- → characteristic wavefunctions for a particular U(x)

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Schrodinger Equation in 1, 2, 3 dimensional systems

1-dimension

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

2-dimension

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

3-dimension

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

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Schrodinger Wave Equation in Quantum Mechanics

Wavefunction ψ which is a sol. of the Sch. Equation embodies all modern physics experienced/learnt so far:

$E=hf$, $p=\frac{h}{\lambda}$, $\Delta x.\Delta p \sim \hbar$, $\Delta E.\Delta t \sim \hbar$, quantization etc

Schrodinger Equation is a Dynamical Equation much like Newton's Equation $\vec{F}= m\,\vec{a}$

$\psi(x,0) \rightarrow \vec{\text{Force}}\,(\text{potential}) \rightarrow \psi(x,t)$

Evolves the System as a function of space-time

The Schrodinger Eq. propogates the system forward & backward in time:

$$\psi(x,\delta t) = \psi(x,0) \pm \left[\frac{d\psi}{dt}\right]_{t=0} \delta t$$

Where does it come from ?? ..."First Principles"

......no real "derivation" exists............

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Time Independent S. Equation

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

Sometimes (depending on the character of the Potential U(x,t))

The Wave function is factorizable: can be broken up

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

Example: Plane Wave $\Psi(x,t)=e^{i(kx-\omega t)}=e^{i(kx)}e^{-i(\omega t)}$

In such cases, use seperation of variables to get :

$$\frac{-\hbar^2}{2m}\phi(t).\frac{\partial^2\psi(x)}{\partial^2 x}+U(x)\psi(x)\phi(t)=i\hbar\psi(x)\frac{\partial\phi(t)}{\partial t}$$

Divide throughout by $\Psi(x,t)=\psi(x)\phi(t)$

$$\Rightarrow \frac{-\hbar^2}{2m}\frac{1}{\psi(x)}.\frac{\partial^2\psi(x)}{\partial^2 x}+U(x)=i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

LHS is a function of x; RHS is fn of t

x and t are independent variables, hence :

$\Rightarrow$ RHS = LHS = Constant = E

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Factorization Condition For Wave Function Leads to:

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

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

What is the Constant E ? How to Interpret it ?

Back to a Free particle :

$\Psi(x,t)= Ae^{ikx}e^{-i\omega t}$, $\psi(x)= Ae^{ikx}$

$U(x,t) = 0$

Plug it into the Time Independent Schrodinger Equation (TISE) $\Rightarrow$

$$\frac{-\hbar^2}{2m}\frac{d^2(Ae^{(ikx)})}{dx^2}+0=E\ Ae^{(ikx)}\ \Rightarrow E=\frac{\hbar^2k^2}{2m}=\frac{p^2}{2m}=\text{(NR Energy)}$$

Stationary states of the free particle: $\Psi(x,t)=\psi(x)e^{-i\omega t}$

$\Rightarrow |\Psi(x,t)|^2=|\psi(x)|^2$

Probability is static in time t, character of wave function depends on $\psi(x)$

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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

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

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

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

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

Schrodinger Eqn: Stationary State Form

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

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

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

$\therefore \ln\phi(t)-\ln\phi(0)=-\frac{iE}{\hbar}t$, 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 $\Psi(x,t)=\psi(x)e^{-\frac{iE}{\hbar}t}$ where E = energy of system

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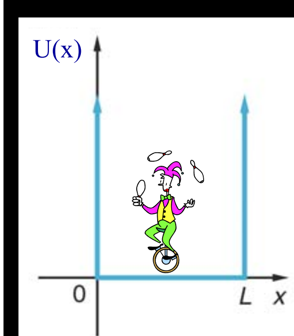
A More Interesting Potential : Particle In a Box



Write the Form of Potential: Infinite Wall

$U(x,t) = \infty;\ x \le 0,\ x \ge L$

$U(x,t) = 0\ ;\ 0 < X < L$

- Classical Picture:
  - Particle dances back and forth
  - Constant speed, const KE
  - Average <P> = 0
  - No restriction on energy value
    - E=K+U = K+0
  - Particle can not exist outside box
    - Can't get out because needs to borrow infinite energy to overcome potential of wall

What happens when the joker is subatomic in size ??

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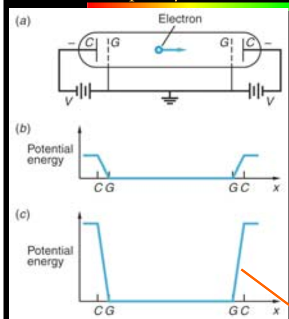
Example of a Particle Inside a Box With Infinite Potential



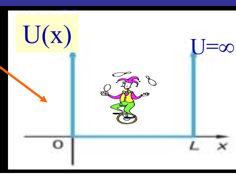
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

However in the regions between each C & G is a repelling electric field whose strength depends on the magnitude of V

(b) If V is small, then electron's potential energy vs x has low sloping "walls"

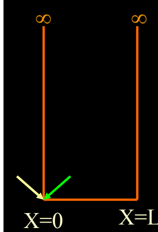
(c) If V is large, the "walls"become very high & steep becoming infinitely high for $V \to \infty$

(d) The straight infinite walls are an approximation of such a situation



Ψ(x) for Particle Inside 1D Box with Infinite Potential Walls

Why can't the particle exist Outside the box ?
→ E Conservation



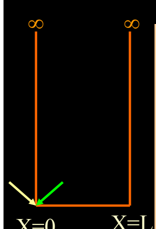
Inside the box, no force $\Rightarrow$ U=0 or constant (same thing)

$$\Rightarrow \boxed{\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + 0\ \psi(x) = E\ \psi(x)}$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)\ ;\ k^2 = \frac{2mE}{\hbar^2}$$

$$or\ \boxed{\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0} \Leftarrow$$ figure out what $\psi(x)$ solves this diff eq.

Ψ(x) for Particle Inside 1D Box with Infinite Potential Walls



Need to figure out values of A, B : How to do that ?

Apply BOUNDARY Conditions on the Wavefunction

Since $\psi(x)$ *must be continuous* everywhere

$\Rightarrow$ match the wavefunction just outside box with the wavefunction value just inside the box

$\Rightarrow$ $\boxed{\text{At } x = 0 \Rightarrow \psi(x=0) = 0}$ & $\boxed{\text{At } x = L \Rightarrow \psi(x=L) = 0}$

$\therefore\ \psi(x=0) = B = 0$ (Continuity condition at x =0)

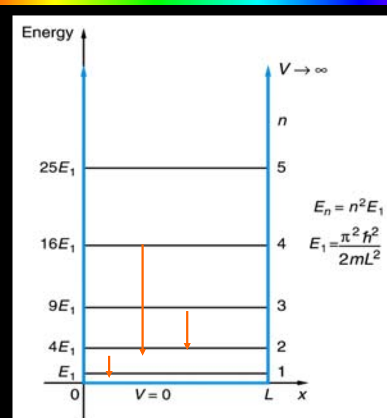
& $\boxed{\psi(x=L) = 0}$ $\Rightarrow$ A Sin kL = 0 (Continuity condition at x =L)

$$\Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}, n = 1, 2, 3, ...\infty$$

So what does this say about Energy E ? : $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$

Quantized (not Continuous)!

Quantized Energy levels of Particle in a Box



What About the Wave Function Normalization ?

The particle's Energy and Wavefunction are determined by a number n

We will call n $\rightarrow$ Quantum Number , just like in Bohr's Hydrogen atom

What about the wave functions corresponding to each of these energy states?

$$\psi_n = A\sin(kx) = A\sin(\frac{n\pi x}{L}) \quad \text{for} \quad 0<x<L$$
$$= 0 \quad \text{for } x \geq 0,\ x \geq L$$

Normalized Condition :

$$1 = \int_0^L \psi_n^* \psi_n dx = A^2 \int_0^L Sin^2(\frac{n\pi x}{L}) \qquad \text{Use } 2Sin^2\theta = 1 - 2Cos2\theta$$

$$1 = \frac{A^2}{2}\int_0^L \left(1 - \cos(\frac{2n\pi x}{L})\right) \quad \text{and since } \int \cos\theta = \sin\theta$$

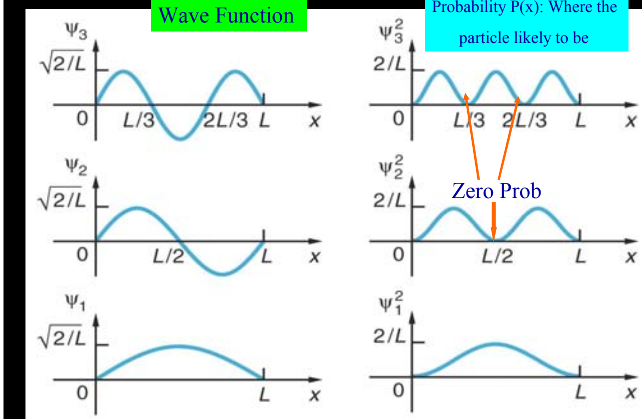
$$1 = \frac{A^2}{2}L \quad \Rightarrow A = \sqrt{\frac{2}{L}}$$

So $\psi_n = \sqrt{\frac{2}{L}}\sin(kx) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$ ...What does this look like?

Wave Functions : Shapes Depend on Quantum # n

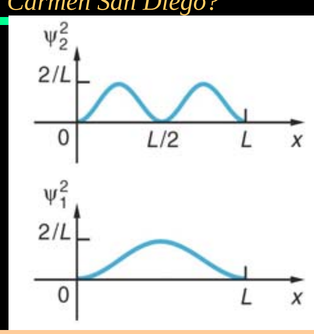
Wave Function

Probability P(x): Where the particle likely to be



Where in The World is Carmen San Diego?

- We can only guess the probability of finding the particle somewhere in x
  - For n=1 (ground state) particle most likely at x = L/2
  - For n=2 (first excited state) particle most likely at L/4, 3L/4
    - Prob. Vanishes at x = L/2 & L
      - How does the particle get from just before x=L/2 to just after?
        - QUIT thinking this way, particles don't have trajectories
        - Just probabilities of bei[ng] somewhere



Classically, where is the particle most Likely to be : Equal prob of being anywhere inside the Box

NOT SO says Quantum Mechanics!

Remember Sesame Street?

This particle in the box is brought to you by the letter

n

Its the Big Boss Quantum Number

The QM Prob. of Finding Particle in Some Region in Space

Consider n =1 state of the particle

Ask : What is P $(\frac{L}{4} \le x \le \frac{3L}{4})$?

$$P = \int_{\frac{L}{4}}^{\frac{3L}{4}} |\psi_1|^2 \, dx = \frac{2}{L} \int_{\frac{L}{4}}^{\frac{3L}{4}} \sin^2 \frac{\pi x}{L} dx = \left(\frac{2}{L}\right) \cdot \frac{1}{2} \int_{\frac{L}{4}}^{\frac{3L}{4}} (1 - \cos \frac{2\pi x}{L}) dx$$

$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi} \sin \frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin \frac{2\pi}{L} \cdot \frac{3L}{4} - \sin \frac{2\pi}{L} \cdot \frac{L}{4}\right)$$

$$P = \frac{1}{2} - \frac{1}{2\pi}(-1-1) = 0.818 \Rightarrow \quad 81.8\%$$

Classically $\Rightarrow$ 50% (equal prob over half the box size)

$\Rightarrow$ Substantial difference between Classical & Quantum predictions

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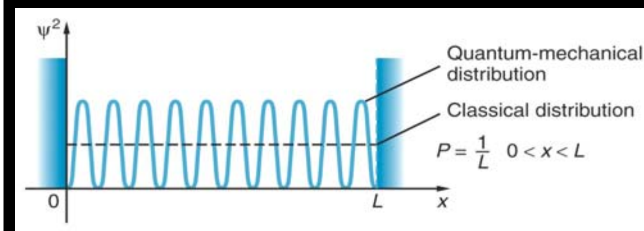
When The Classical & Quantum Pictures Merge: $n \to \infty$



But one issue is irreconcilable:

Quantum Mechanically the particle can not have E = 0

This is a direct consequence of the Uncertainty Principle

The particle moves around with KE inversely proportional to the length Of the (1D) Box

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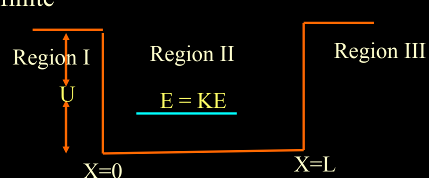
Finite Potential Barrier

- There are no Infinite Potentials in the real world
  - Imagine the cost of as battery with infinite potential diff
    - Will cost infinite $ sum + not available at Radio Shack
- Imagine a realistic potential : Large U compared to KE but not infinite



Classical Picture : A bound particle (no escape) in 0<x<L

Quantum Mechanical Picture : Use ΔE.Δt ≤ h/2π

Particle can leak out of the Box of finite potential P(|x|>L) ≠0

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Finite Potential Well

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

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

$$= \alpha^2 \psi(x); \ \alpha = \sqrt{\frac{2m(U-E)}{\hbar^2}}$$

$\Rightarrow$General Solutions : $\psi(x) = Ae^{+\alpha x} + Be^{-\alpha x}$

Require finiteness of $\psi(x)$

$\Rightarrow \psi(x) = Ae^{+\alpha x}$ .....x<0 (region I)

$\psi(x) = Ae^{-\alpha x}$ .....x>L (region III)

Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

But note that wave fn at $\psi(x)$ at (x =0, L) $\neq 0$!! (why?)

Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

These lead to rather different wave functions

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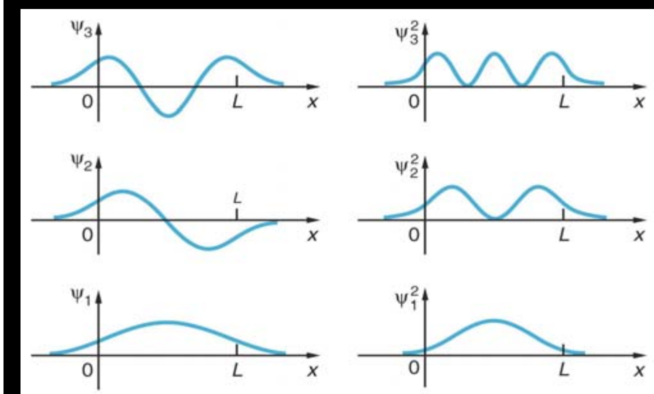
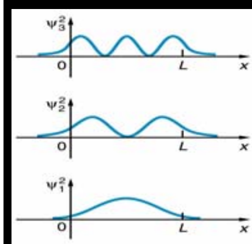
Finite Potential Well: Particle can Burrow Outside Box!



Finite Potential Well: Particle can Burrow Outside Box



Particle can be outside the box but only for a time $\Delta t \approx h/\Delta E$

ΔE = Energy particle needs to borrow to Get outside ΔE = U-E + KE

The Cinderella act (of violating E conservation cant last very long

Particle must hurry back (cant be caught with its hand inside the cookie-jar)

Penetration Length $\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U-E)}}$

If U>>E $\Rightarrow$ Tiny penetration

If U $\rightarrow \infty \Rightarrow \delta \rightarrow 0$

Finite Potential Well: Particle can Burrow Outside Box

Penetration Length $\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U-E)}}$

If U>>E $\Rightarrow$ Tiny penetration

If U $\rightarrow \infty \Rightarrow \delta \rightarrow 0$

$$E_n = \frac{n^2\pi^2\hbar^2}{2m(L+2\delta)^2}, n = 1, 2, 3, 4...$$

When E=U then solutions blow up

$\Rightarrow$ Limits to number of bound states($E_n < U$)

When E>U, particle is not bound and can get either reflected or transmitted across the potential "barrier"

Measurement Expectation: Statistics Lesson

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

$$<x> = \frac{n_1x_1 + n_2x_2 + n_3x_3 + ...n_ix_i}{n_1 + n_2 + n_3 + ...n_i} = \frac{\sum_{i=1}^{n} n_i x_i}{N} = \frac{\int_{-\infty}^{\infty} xP(x)dx}{\int_{-\infty}^{\infty} P(x)dx}$$

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 Distr:

Scatter around average

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

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

σ = small $\rightarrow$ Sharp distr.

Uncertainty $\Delta X = \sigma$

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

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

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

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

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

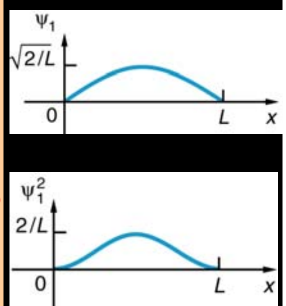
$\Rightarrow <x>=\frac{2L}{2\pi^2}\left[\int_0^{\pi}\theta d\theta - \int_0^{\pi}\theta\cos 2\theta d\theta\right]$ use $\int udv=uv-\int vdu$

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

Similarly $<x^2>=\int_0^L x^2\sin^2(\frac{\pi}{L}x)dx=\frac{L^2}{3}-\frac{L^2}{2\pi^2}$

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

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



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

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

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

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

gives the value of average mometum in the following way:

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

Similerly :

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

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

Similerly

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

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

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

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

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

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

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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!

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

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

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

Since $\int \text{sinax cosax dx} = \frac{1}{2a}\sin^2 ax$ ...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

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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 ≠ 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

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

Be careful when being "lazy"

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

Does similar logic apply??

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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.

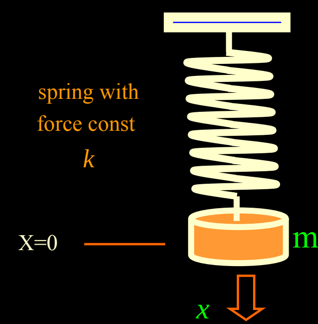
These are called "stationary" states because Prob is independent of time

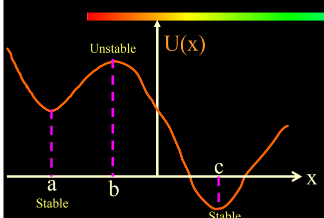
Examples : Particle in a box (why?)

: Quantum Oscillator (why?)

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

Simple Harmonic Oscillator:Quantum and Classical





Particle of mass m within a potential U(x)

$\vec{F}(x) = -\frac{dU(x)}{dx}$

$\vec{F}(x=a) = -\left.\frac{dU(x)}{dx}\right|_{x=a} = 0,$

$\vec{F}(x=b) = 0$, $\vec{F}(x=c) = 0$ ...But...

look at the Curvature:

$\frac{\partial^2 U}{\partial x^2} > 0$ (stable), $\frac{\partial^2 U}{\partial x^2} < 0$ (unstable)

Stable Equilibrium: General Form :

$U(x) = U(a) + \frac{1}{2}k(x-a)^2$

Rescale $\Rightarrow U(x) = \frac{1}{2}k(x-a)^2$

Motion of a Classical Oscillator (ideal)

Ball originally displaced from its equilibibirium position, motion confined between x=0 & x=A

$U(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2 ; \omega = \sqrt{\frac{k}{m}} = Ang.\ Freq$

$E = \frac{1}{2}kA^2 \Rightarrow$ Changing A changes E

E can take any value & if $A \rightarrow 0$, $E \rightarrow 0$

Max. KE at x = 0, KE= 0 at $x = \pm A$

Quantum Picture: Harmonic Oscillator

Find the Ground state Wave Function $\psi(x)$

Find the Ground state Energy E when $U(x) = \frac{1}{2}m\omega^2x^2$

Time Dependent Schrodinger Eqn: $\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x} + \frac{1}{2}m\omega^2x^2\psi(x) = E\ \psi(x)$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2}(E - \frac{1}{2}m\omega^2x^2)\psi(x) = 0$$ What $\psi(x)$ solves this?

Two guesses about the simplest Wavefunction:

1. $\psi(x)$ should be symmetric about x 2. $\psi(x) \rightarrow 0$ as $x \rightarrow \infty$

\+ $\psi(x)$ should be continuous & $\frac{d\psi(x)}{dx}$ = continuous

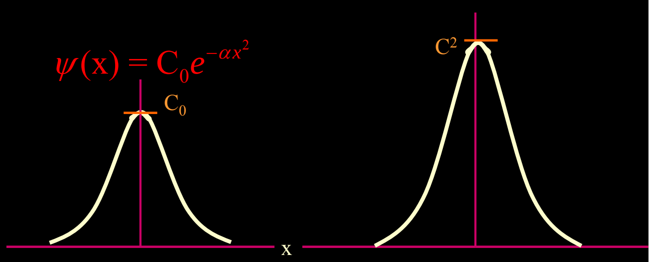
My guess: $\psi(x) = C_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

$P(x) = C^2_0 e^{-2\alpha x^2}$

$\psi(x) = C_0 e^{-\alpha x^2}$



How to Get C_0 & α ?? …Try plugging in the wave-function into the time-independent Schr. Eqn.

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Time Independent Sch. Eqn & The Harmonic Oscillator

Master Equation is : $\frac{\partial^2\psi(x)}{\partial x^2} = \frac{2m}{\hbar^2}[\frac{1}{2}m\omega^2x^2 - E]\psi(x)$

Since $\psi(x) = C_0 e^{-\alpha x^2}$, $\frac{d\psi(x)}{dx} = C_0(-2\alpha x)e^{-\alpha x^2}$,

$\frac{d^2\psi(x)}{dx^2} = C_0\frac{d(-2\alpha x)}{dx}e^{-\alpha x^2} + C_0(-2\alpha x)^2e^{-\alpha x^2} = C_0[4\alpha^2x^2 - 2\alpha]e^{-\alpha x^2}$

$\Rightarrow C_0[\boxed{4\alpha^2x^2} - \boxed{2\alpha}]e^{-\alpha x^2} = \frac{2m}{\hbar^2}[\boxed{\frac{1}{2}m\omega^2x^2} - E]C_0e^{-\alpha x^2}$

Match the coeff of x^2 and the Constant terms on LHS & RHS

$\Rightarrow 4\alpha^2 = \frac{2m}{\hbar^2}\frac{1}{2}m\omega^2$ or $\alpha = \frac{m\omega}{2\hbar}$

& the other match gives $2\alpha = \frac{2m}{\hbar^2}E$, substituing $\alpha \Rightarrow$

$\boxed{E = \frac{1}{2}\hbar\omega = hf}$!!!!......(Planck's Oscillators)

What about C_0? We learn about that from the Normalization cond.

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SHO: Normalization Condition

$\int_{-\infty}^{+\infty} |\psi_0(x)|^2\, dx = 1 = \int_{-\infty}^{+\infty} C_0^2 e^{\frac{-m\omega x^2}{\hbar}}\, dx$

Since $\int_{-\infty}^{+\infty} e^{-ax^2}\, dx = \sqrt{\frac{\pi}{a}}$ (dont memorize this)

Identifying $a = \frac{m\omega}{\hbar}$ and using the identity above

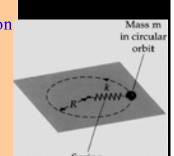
$\Rightarrow C_0 = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}}$

Hence the Complete NORMALIZED wave function is :

$\boxed{\psi_0(x) = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} e^{\frac{-m\omega x^2}{2\hbar}}}$ Ground State Wavefunction

has energy E = hf

Planck's Oscillators were electrons tied by the "spring" of the mutually attractive Coulomb Force



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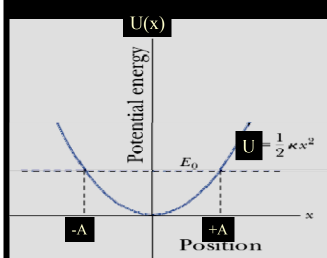
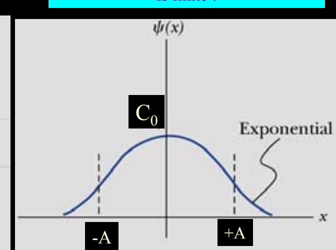
Quantum Oscillator In Pictures

$E = KE + U(x) > 0$ for n=0

Quantum Mechanical prob for particle To live outside classical turning points Is finite !





Classically particle most likely to be at the turning point (velocity=0)
Quantum Mechanically , particle most likely to be at $x=x_0$ for n=0

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Classical & Quantum Pictures of SHO compared

- Limits of classical vibration : Turning Points (do on Board)
- Quantum Probability for particle outside classical turning points P(|x|>A) =16% !!
  - Do it on the board (see Example problems in book)

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Excited States of The Quantum Oscillator

$\psi_n(x) = C_n H_n(x)\, e^{-\frac{m\omega x^2}{2\hbar}}$;

$H_n(x) =$ Hermite Polynomials

with

$H_0(x)=1$

$H_1(x)=2x$

$H_2(x)=4x^2-2$

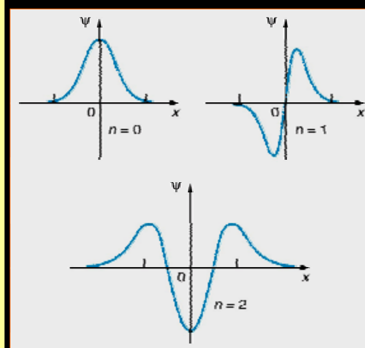
$H_3(x)=8x^3-12x$

$H_n(x)=(-1)^n e^{x^2}\frac{d^n e^{-x^2}}{dx^n}$

and

$$E_n=(n+\frac{1}{2})\hbar\omega=(n+\frac{1}{2})hf$$

Again n=0,1,2,3...∞ Quantum #



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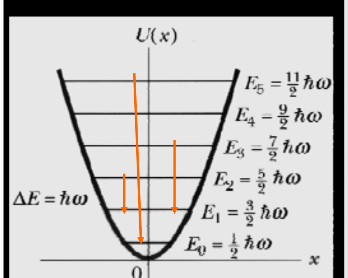
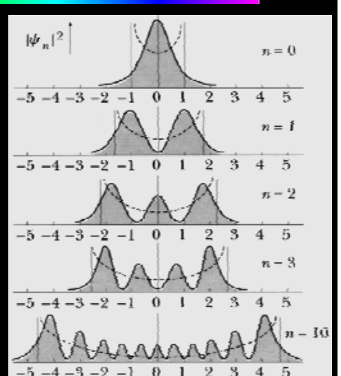
Excited States of The Quantum Oscillator





Ground State Energy >0 always

As n → ∞ classical and quantum probabilities become similar

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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 !

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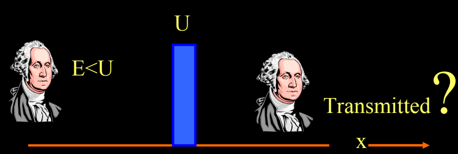
Potential Barrier



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

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

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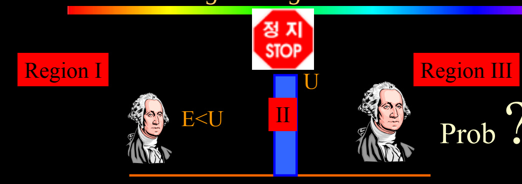
Tunneling Through A Potential Barrier



- 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

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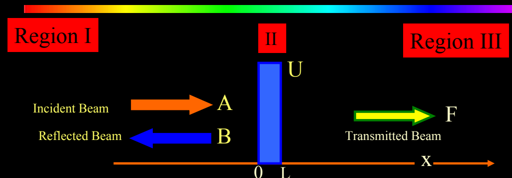
Beam Of Particles With E < U Incident On Barrier From Left



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

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

define Reflection Coefficient : $R = \dfrac{|B|^2}{|A|^2}$ = *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 $T = \dfrac{|F|^2}{|A|^2}$

Unitarity Condition ⇒ R + T= 1 (particle is either reflected or transmitted)

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

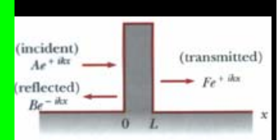
Solutions are of form $\psi(x) \propto e^{\pm\alpha x}$

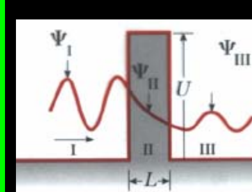
$\boxed{\Psi_{II}(x,t) = Ce^{+\alpha x - i\omega t} + De^{-\alpha x - i\omega t}}$ 0<x<L

To determine C & D ⇒ apply matching cond.

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

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





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

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

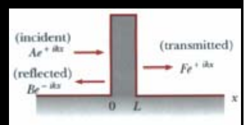
Four equations & four unknowns

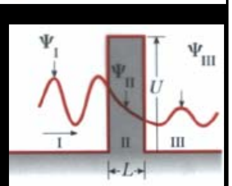
Cant determine A,B,C,D but if you

Divide thruout by A in all 4 equations :

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

That's what we need any way





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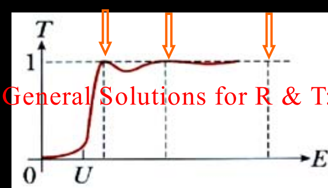
Potential Barrier when E < U

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 !!

[do the derivation on blackboard]

That's the Wave nature of the

Quantum particle

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A Special Case That is Instructive & Useful: U>>E

Given the 4 equations from Continuity Conditions: Solve for $\frac{A}{F}$

$$\frac{A}{F} = \left[\frac{1}{2} + \frac{i}{4}\left(\frac{\alpha}{k} - \frac{k}{\alpha}\right)\right]e^{(ik+\alpha)L} + \left[\frac{1}{2} - \frac{i}{4}\left(\frac{\alpha}{k} - \frac{k}{\alpha}\right)\right]e^{(ik-\alpha)L}$$

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

when U>>E, $\boxed{\alpha \gg k \ \& \ \frac{\alpha}{k} \gg \frac{k}{\alpha}}$ So $\frac{\alpha}{k} - \frac{k}{\alpha} \approx \frac{\alpha}{k}$; For large Barrier L, $\alpha L \gg 1$

$$\frac{A}{F} = \left[\frac{1}{2} + \frac{i}{4}\left(\frac{\alpha}{k}\right)\right]e^{(ik+\alpha)L}; \left(\frac{A}{F}\right)^* = \left[\frac{1}{2} - \frac{i}{4}\left(\frac{\alpha}{k}\right)\right]e^{(-ik+\alpha)L}$$

$$T^{-1} = \left(\frac{A}{F}\right)^* \frac{A}{F} = \left[\frac{1}{4} + \frac{1}{16}\left(\frac{\alpha^2}{k^2}\right)\right]e^{(2\alpha)L} = \frac{1}{T(E)};$$ now invert & consolidate

$$T = \left|\frac{F^*F}{A^*A}\right| = \left(\frac{16}{4 + \left(\frac{\alpha}{k}\right)^2}\right)e^{-2\alpha L}$$; now watch the variables employed

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A Special Case That is Instructive & Useful: U>>E

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

$$\left(\frac{\alpha}{k}\right)^2 = \frac{2m(U-E)/\hbar^2}{2mE/\hbar^2} = \frac{U}{E} - 1 \simeq \frac{U}{E}$$

$$\Rightarrow \left(\frac{16}{4 + \left(\frac{\alpha}{k}\right)^2}\right) = \left(\frac{16}{4 + \left(\frac{U}{E} - 1\right)}\right)$$ $\rightarrow$ varies slowly compared with $e^{-2\alpha L}$ *term*

keeing in mind only the Order of magnitude, I suggest

$$\left(\frac{16}{4 + \left(\frac{U}{E} - 1\right)}\right) \approx 1;$$ back to $T = \left(\frac{16}{4 + \left(\frac{\alpha}{k}\right)^2}\right)e^{-2\alpha L}$ substituting

So approximately $\boxed{T \approx e^{-2\alpha L}}$ Transmission Prob is fn of U,E,L

Why subject you to this TORTURE? $\rightarrow$ Estimate T for complicated Potentials

See next (example of Cu oxide layer, radioactivity, blackhole blowup etc)

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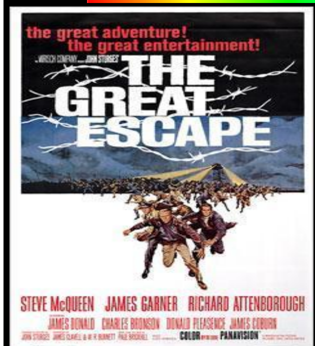
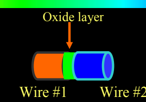
The Great Escape ! My Favorite Movie



Story involves an Allied plan for a massive breakout from a Nazi P.O.W. camp, during World War Two. The Nazis had created a high-security, escape -proof prisoner of war camp for those annoying detainees who have attempted escape from their other prison of war camps. These prisoners are not discouraged at all, as they plan a huge escape of 100 men.

Ceparated in Coppertino



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?

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

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

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

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

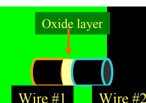
$$\Rightarrow \alpha = \frac{\sqrt{2m_e(U-E)}}{\hbar} = \frac{\sqrt{2\times 511 kev/c^2 (3.0\times 10^{-3} keV)}}{1.973 \text{ keV.Å/c}} = 0.8875 \text{Å}^{-1}$$

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; $T=0.657\times 10^{-7}$

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

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

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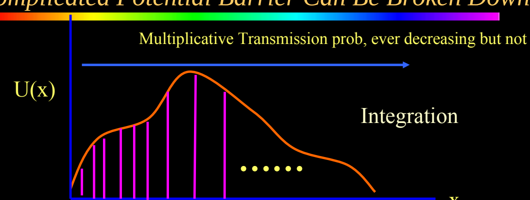
A Complicated Potential Barrier Can Be Broken Down



Can be broken down into a sum of successive Rectangular potential barriers for which we learnt to find the Transmission probability T_i

The Transmitted beam intensity thru one small barrier becomes incident beam intensity for the following one

So on & so forth …till the particle escapes with final Transmission prob T

$$T = \int T_i\ dx = e^{-2\left[\frac{\sqrt{2m}}{\hbar}\int\sqrt{U(x)-E}\,dx\right]}$$

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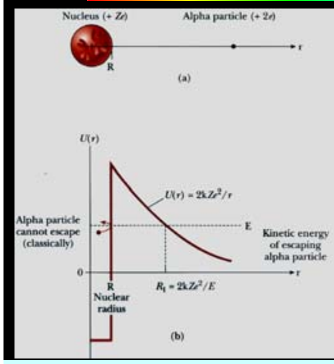
Radioactivity: The α-particle & Steve McQueen Compared



$$T = \int T_i \; dx = e^{-2\left[\frac{\sqrt{2m_\alpha}}{\hbar}\int\sqrt{\frac{2ke^2Z}{r} - E_\alpha}\,dx\right]}$$

- In a Nucleus such as Ra, Uranium etc α particle rattles around parent nucleus, "hitting"the nuclear walls with a very high frequency (probing the "fence"), if the Transmission prob T>0, then eventually particle escapes
- Within nucleus, α particle is virtually free but is trapped by the Strong nuclear force
- Once outside nucleus, the particle "sees" only the repulsive (+) columbic force (nuclear force too faint outside) which keeps it within nucleus
- Nuclear radius R = 10^{-14} m, E_α = 9MeV
- Coulomb barrier U(r) =kq_1q_2/r
  - At r=R, U(R) ≈ 30 MeV barrier
- α-particle, due to QM, tunnels thru
- It's the sensitivity of T on E_α that accounts for the wide range in half-lives of radioactive nuclei

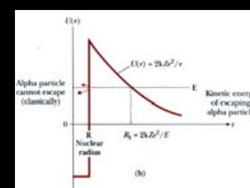
5

Radioactivity Explained Roughly (..is enough!)

- Protons and neutrons rattling freely inside radioactive nucleus (R≅10^{-15}m)
- Constantly morphing into clusters of protons and neutrons
- Proto-alpha particle =(2p+2n) of ≈ 9 MeV prevented from getting out by the imposing Coulombic repulsion of remaining charge (≈ 30MeV)
- Escapes by tunneling thru Coloumb potential…but some puzzling features:
- α particles emitted from all types of radioactive nuclei have roughly same KE ≅ 4-9 MeV
- In contrast, the half live T(N→ e^{-1} N) differ by more than 20 orders of magnitude !

$$T = \int T_i \; dx = e^{-2\left[\frac{\sqrt{2m_\alpha}}{\hbar}\int\sqrt{\frac{2ke^2Z}{r} - E_\alpha}\,dx\right]}$$

Element	KE of emitted α	Half Life
^{212}Po	8.95 MeV	3x10^{-7} s
^{240}Cm	6.40 MeV	27 days
^{226}Ra	4.90 MeV	1.60x10^{3} Yr
^{232}Th	4.05 MeV	1.41x10^{10} yr



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Radioactivity Explained Crudely

$$T(E) \approx e^{\left[\frac{-2}{\hbar}\sqrt{2m}\int\sqrt{U(x)-E}\;dx\right]}, U(x) = \frac{2e^2Z}{4\pi\varepsilon_0 r}$$

$$\ln T = \frac{-2}{\hbar}\int_0^b \sqrt{2m_\alpha\left(\frac{2e^2Z}{4\pi\varepsilon_0 r} - E_\alpha\right)}\,dr,$$

limits of integration correspond to values of r when $\boxed{E=U}$

$$\Rightarrow \frac{2e^2Z}{4\pi\varepsilon_0 b} = E \Rightarrow \boxed{b = \frac{2e^2Z}{4\pi\varepsilon_0 E_\alpha}}$$

$$\text{Define } \xi = \frac{r}{b}; = \frac{r}{2e^2Z/4\pi\varepsilon_0 E} \Rightarrow \ln T \cong \frac{-2\left(\sqrt{2m_\alpha E}\right)b}{\hbar}\int_0^1\sqrt{\frac{1}{\xi}-1}\;d\xi$$

Substitute $\xi = \sin^2\theta$ in integration, change limits ⇒

$$\ln T \cong \frac{-4\left(\sqrt{2m_\alpha E_\alpha}\right)b}{\hbar}\boxed{\int_0^{\pi/2}\cos^2\theta d\theta}; use \int_0^{\pi/2}\cos^2\theta d\theta = \pi/4 \;\&\; E_\alpha = \frac{m_\alpha V_\alpha^2}{2}$$

$$\ln T \cong \frac{-2\pi}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0}\sqrt{\frac{2m_\alpha}{E_\alpha}} = \frac{-4\pi}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{V_\alpha} \Rightarrow \boxed{T \cong e^{\left[\frac{-4\pi}{\hbar}\frac{Ze^2}{4\pi\varepsilon_0}\frac{1}{V_\alpha}\right]}}$$

$$\Rightarrow \boxed{T \propto e^{\frac{-1}{V_\alpha}} \text{ and } T \propto e^{-Z}}$$ ....SHARP DEPENDENCE!!

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Radioactivity

A more eloberate calculation (Bohm) yields $\boxed{T(E) = e^{\left\{-4\pi Z\sqrt{\frac{E_0}{E}}+8\sqrt{\frac{ZR}{r_0}}\right\}}}$

where $r_0 = \frac{\hbar^2}{m_\alpha ke^2} \simeq 8\text{fm}$ is the "Bohr Radius" of alpha particles

and $E_0 = \frac{ke^2}{2r_0} = 0.0993 MeV$ = Nuclear "Rydberg"

To obtain decay rates, need to multiply T(E) by the number of collisions α particle makes with the "walls" of the nuclear barrier. This collission frequency

$f = \frac{V_\alpha}{2R}$ = transit time for α particle crossing the nuclear barrier (rattle time)

Typically f =10^{21} collissions/second

Decay rate (prob. of α emission per unit time) $\lambda = f \bullet T(E)$

$$\lambda = 10^{21} e^{\left\{-4\pi Z\sqrt{\frac{E_0}{E_\alpha}}+8\sqrt{\frac{ZR}{r_0}}\right\}}$$

Definition : Half life $\boxed{t_{1/2} = \frac{\ln 2}{\lambda}}$

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Half Lives Compared: Sharp dependence on E_α

α particles emerge with (a) E=4.05 MeV in Thorium (b) E=8.95 MeV in Polonium. The Nuclear size R = 9 fm in both cases. Which one will outlive you ?

Thorium (Z=90) decays into Radium (Z=88)

$$T(E) = \exp\left\{-4\pi(\boxed{88})\sqrt{(0.0993/4.05)} + 8\sqrt{\boxed{88}(9.00/7.25)}\right\}$$

$$=1.3\times10^{-39}$$

Taking $f=10^{21}Hz \Rightarrow \lambda = 1.3\times10^{-18}$ α emission $\Rightarrow t_{1/2} = \frac{0.693}{1.3\times10^{-18}} = 1.7\times10^{10}\,yr$!!!

Polonium (Z=84) decays into Lead (Z=82)

$$T(E) = \exp\left\{-4\pi(\boxed{82})\sqrt{(0.0993/8.95)} + 8\sqrt{\boxed{82}(9.00/7.25)}\right\}$$

$$= 8.2\times10^{-13}$$

Taking $f=10^{21}Hz \Rightarrow \lambda = 8.2\times10^{-8}$ α emission $\Rightarrow t_{1/2} = \frac{0.693}{8.2\times10^{-8}} = 8.4\times10^{-10}\,s$!!!

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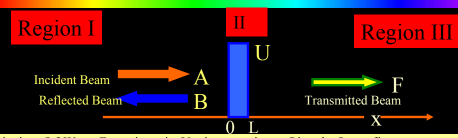
Potential Barrier : An Unintuitive Result When E>U



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

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

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

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

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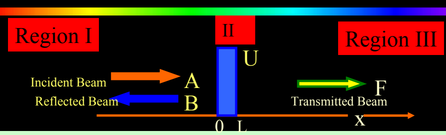
Potential Barrier : An Unintuitive Result When E>U



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

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

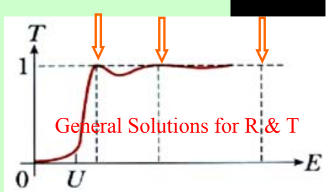
Since $k' = \sqrt{\frac{2m(E-U)}{\hbar^2}} \Rightarrow \sqrt{\frac{2m(E-U)}{\hbar^2}} = n\pi$

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



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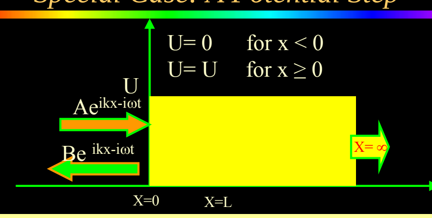
Special Case: A Potential Step



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

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

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

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

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

rewrite as ikδA - ikδB = - (A+B) $\Rightarrow$ A(1+ikδ) = -B(1-ikδ)

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

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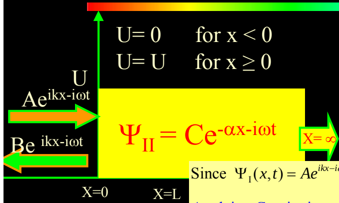
Transmission Probability in A Potential Step



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 :

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

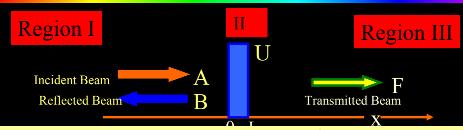
$\Rightarrow \frac{C}{A} = -\frac{2ik\delta}{1-ik\delta} \neq 0 \quad \Rightarrow \boxed{T = \left(\frac{C}{A}\right)\left(\frac{C}{A}\right)^* > 0!!!}$

The particle burrows into the skin of the step barrier. If one has a barrier of width $L=\delta$, 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 $\boxed{\Delta x = \frac{1}{2}\frac{\hbar}{\sqrt{2m(U-E)}}}$

Particle Beams and Flux Conservation



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

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

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

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

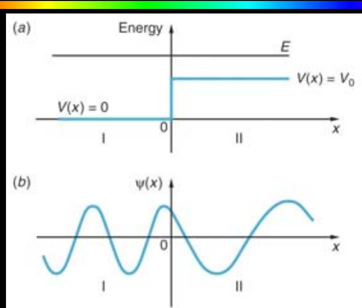
The general expression for flux probabilities : number of particles passing by any point per unit time:

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

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

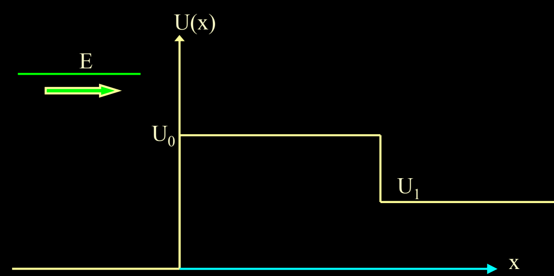
The general expression for conservation of particle flux remains: $\boxed{1=T+R}$

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?

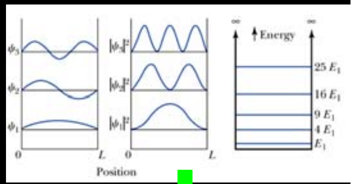


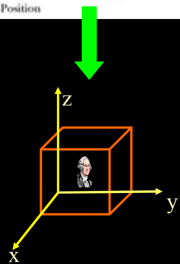
QM in 3 Dimensions

- 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)





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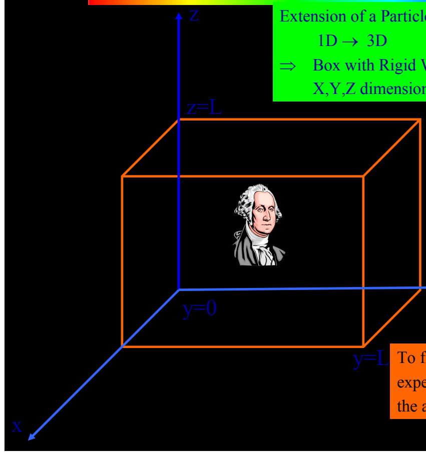
Quantum Mechanics In 3D: Particle in 3D Box

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

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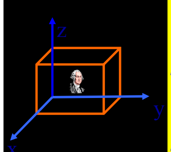
The Schrodinger Equation in 3 Dimensions: Cartesian Coordinates



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) ⇒

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

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

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

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

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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 ψ_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

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

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

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

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

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

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

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

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

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

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

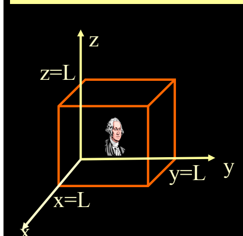
Particle in 3D Box : Energy Spectrum & Degeneracy

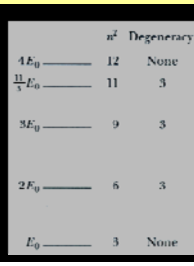
$$\boxed{E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2); \quad n_i = 1, 2, 3...\infty, n_i \neq 0}$$

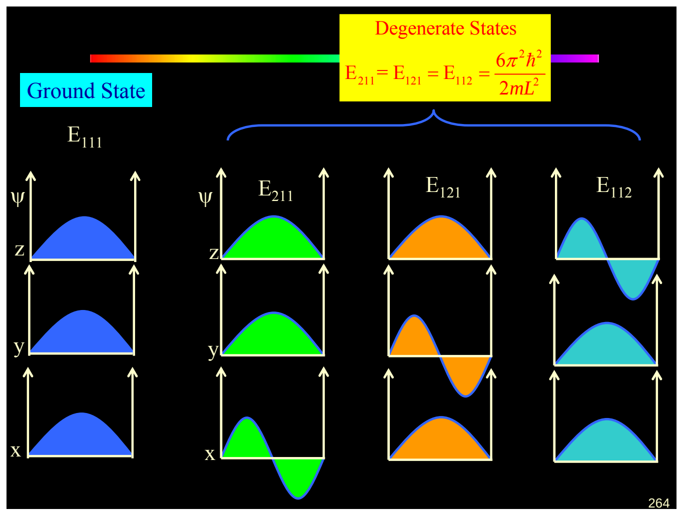
Ground State Energy $E_{111} = \frac{3\pi^2\hbar^2}{2mL^2}$

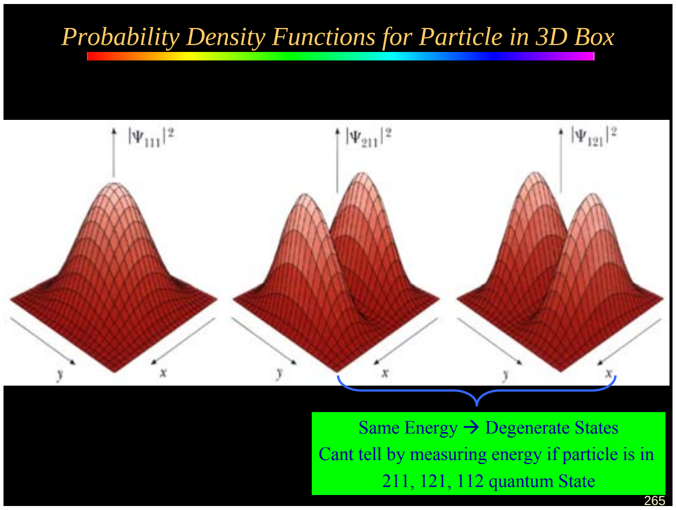
Next level $\Rightarrow$ 3 Excited states $E_{211} = E_{121} = E_{112} = \frac{6\pi^2\hbar^2}{2mL^2}$

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








Probability Density Functions for Particle in 3D Box
$|\Psi_{111}|^2$
$|\Psi_{211}|^2$
$|\Psi_{121}|^2$
y
x
Same Energy → Degenerate States
Cant tell by measuring energy if particle is in 211, 121, 112 quantum State
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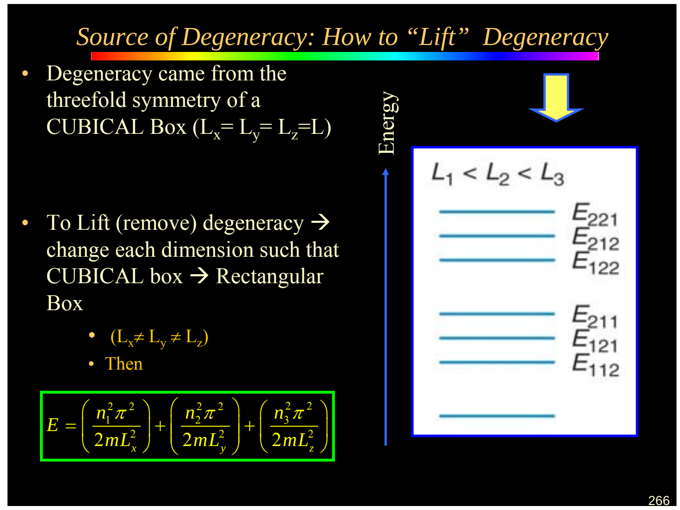
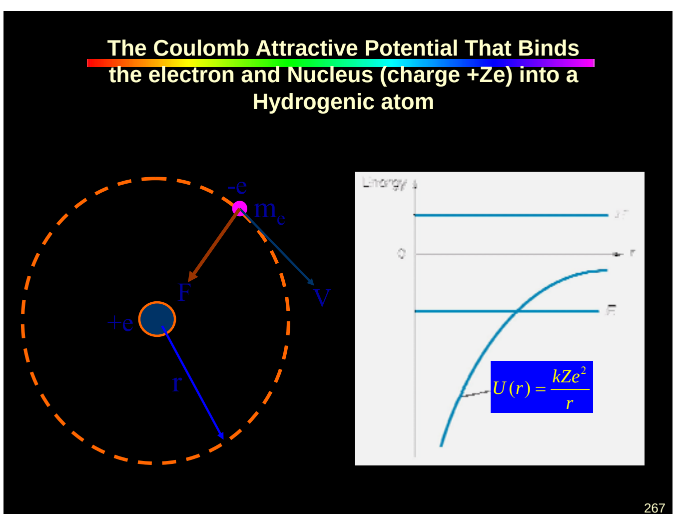

Source of Degeneracy: How to "Lift" Degeneracy
Degeneracy came from the threefold symmetry of a CUBICAL Box ($L_x = L_y = L_z = L$)
To Lift (remove) degeneracy → change each dimension such that CUBICAL box → Rectangular Box
($L_x \neq L_y \neq L_z$)
Then
$E = \left(\frac{n_1^2\pi^2}{2mL_x^2}\right) + \left(\frac{n_2^2\pi^2}{2mL_y^2}\right) + \left(\frac{n_3^2\pi^2}{2mL_z^2}\right)$
Energy
$L_1 < L_2 < L_3$
E_{221}
E_{212}
E_{122}
E_{211}
E_{121}
E_{112}
266


The Coulomb Attractive Potential That Binds the electron and Nucleus (charge +Ze) into a Hydrogenic atom
-e
m_e
F
V
+e
r
$U(r) = \frac{kZe^2}{r}$
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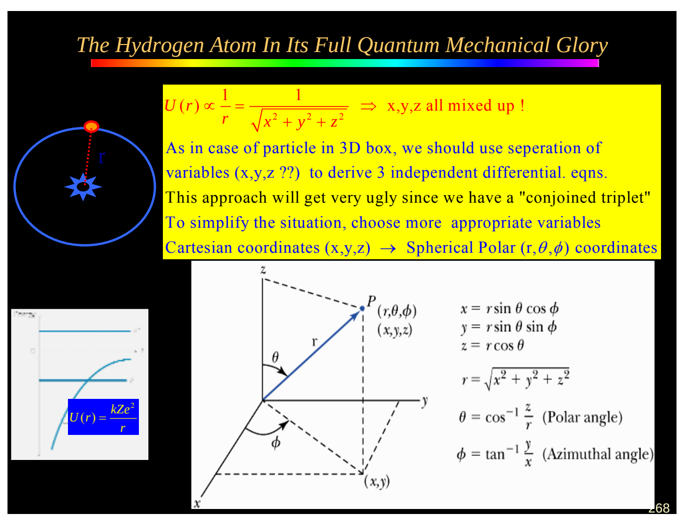
The Hydrogen Atom In Its Full Quantum Mechanical Glory
$U(r) \propto \frac{1}{r} = \frac{1}{\sqrt{x^2 + y^2 + z^2}} \Rightarrow$ x,y,z all mixed up !
As in case of particle in 3D box, we should use seperation of variables (x,y,z ??) to derive 3 independent differential. eqns.
This approach will get very ugly since we have a "conjoined triplet"
To simplify the situation, choose more appropriate variables
Cartesian coordinates (x,y,z) → Spherical Polar (r,θ,φ) coordinates
r
$U(r) = \frac{kZe^2}{r}$
P (r,θ,φ) (x,y,z)
$x = r \sin\theta \cos\phi$
$y = r \sin\theta \sin\phi$
$z = r \cos\theta$
$r = \sqrt{x^2 + y^2 + z^2}$
$\theta = \cos^{-1}\frac{z}{r}$ (Polar angle)
$\phi = \tan^{-1}\frac{y}{x}$ (Azimuthal angle)
(x,y)
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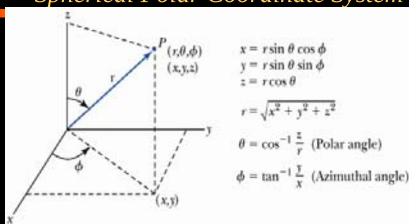
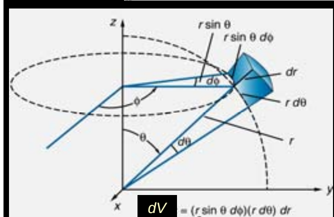
Spherical Polar Coordinate System

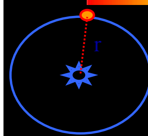


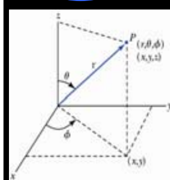


Volume Element dV

$$dV = (r\sin\theta d\phi)(rd\theta)(dr) = r^2\sin\theta dr d\theta d\phi$$

The Hydrogen Atom In Its Full Quantum Mechanical Glory





Instead of writing Laplacian $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$,

write ∇^2 for spherical polar coordinates:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi}$$

Thus the T.I.S.Eq. for $\psi(x,y,z) = \psi(r,\theta,\phi)$ becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi(r,\theta,\phi)}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi(r,\theta,\phi)}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi(r,\theta,\phi)}{\partial^2\phi} + \frac{2m}{\hbar^2}(E-U(r))\psi(r,\theta,\phi) = 0$$

with $U(r) \propto \frac{1}{r} = \frac{1}{\sqrt{x^2+y^2+z^2}}$

The Schrodinger Equation in Spherical Polar Coordinates *(is bit of a mess!)*

The TISE is :

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial^2\phi} + \frac{2m}{\hbar^2}(E-U(r))\psi(r,\theta,\phi) = 0$$

Try to free up second last term from all except ϕ

This requires multiplying thruout by $\boxed{r^2\sin^2\theta} \Rightarrow$

$$\sin^2\theta\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{\partial^2\psi}{\partial^2\phi} + \frac{2mr^2\sin^2\theta}{\hbar^2}(E+\frac{ke^2}{r})\psi = 0$$

For Seperation of Variables, Write $\psi(r,\theta,\phi) = R(r) . \Theta(\theta) . \Phi(\phi)$

Plug it into the TISE above & divide thruout by $\psi(r,\theta,\phi)=R(r).\Theta(\theta).\Phi(\phi)$

Note that :

$$\frac{\partial\Psi(r,\theta,\phi)}{\partial r} = \Theta(\theta).\Phi(\phi)\ \frac{\partial R(r)}{\partial r}$$
$$\frac{\partial\Psi(r,\theta,\phi)}{\partial\theta} = R(r)\Phi(\phi)\ \frac{\partial\Theta(\theta)}{\partial\theta}$$
$$\frac{\partial\Psi(r,\theta,\phi)}{\partial\theta} = R(r)\Theta(\theta)\ \frac{\partial\Phi(\phi)}{\partial\phi}$$

$\Rightarrow$ when substituted in TISE

Solving For the Hydrogen Atom: Separation of Variables

Don't Panic: Its simpler than you think !

$$\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial^2\phi} + \frac{2mr^2\sin^2\theta}{\hbar^2}(E+\frac{ke^2}{r}) = 0$$

Rearrange by taking the ϕ term on RHS

$$\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{2mr^2\sin^2\theta}{\hbar^2}(E+\frac{ke^2}{r}) = -\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial^2\phi}$$

LHS is fn. of r,θ & RHS is fn of ϕ only , for equality to be true for all r,θ,ϕ

$\Rightarrow$ $\boxed{\text{LHS= constant = RHS = } m_l^2}$

Deconstructing The Schrodinger Equation for Hydrogen

Now go break up LHS to seperate the r & θ terms.....

$$\text{LHS:}\frac{\sin^2\theta}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\frac{2mr^2\sin^2\theta}{\hbar^2}(E+\frac{ke^2}{r})=m_l^2$$

Divide Thruout by $\sin^2\theta$ and arrange all terms with r away from $\theta \Rightarrow$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right)+\frac{2mr^2}{\hbar^2}(E+\frac{ke^2}{r})=\frac{m_l^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)$$

Same argument : LHS is fn of r, RHS is fn of θ;

For them to be equal for all r, $\theta \Rightarrow$ $\boxed{\text{LHS} = \text{const} = \text{RHS} = l(l+1)}$

What is the mysterious $l(l+1)$? Just a number like 2(2+1)

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So What do we have after all the shuffling!

$$\frac{d^2\Phi}{d\phi^2}+m_l^2\Phi=0\text{..................(1)}$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m_l^2}{\sin^2\theta}\right]\Theta(\theta)=0\text{.....(2)}$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{\partial R}{\partial r}\right)+\left[\frac{2mr^2}{\hbar^2}(E+\frac{ke^2}{r})-\frac{l(l+1)}{r^2}\right]R(r)=0\text{....(3)}$$

These 3 "simple" diff. eqn describe the physics of the Hydrogen atom.

All we need to do now is guess the solutions of the diff. equations

Each of them, clearly, has a different functional form

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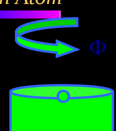
And Now the Solutions of The S. Eqns for Hydrogen Atom



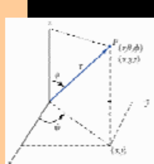
The Azimuthal Diff. Equation : $\boxed{\frac{d^2\Phi}{d\phi^2}+m_l^2\Phi=0}$

Solution : $\Phi(\phi)=A\,e^{im_l\phi}$ but need to check "Good Wavefunction Condition"

Wave Function must be Single Valued for all $\phi \Rightarrow \Phi(\phi)=\Phi(\phi+2\pi)$

$\Rightarrow \Phi(\phi)=A\,e^{im_l\phi}=A\,e^{im_l(\phi+2\pi)} \Rightarrow m_l=0,\pm1,\pm2,\pm3....$(*Magnetic* Quantum #)

The Polar Diff. Eq: $\boxed{\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left[l(l+1)-\frac{m_l^2}{\sin^2\theta}\right]\Theta(\theta)=0}$



Solutions : go by the name of "Associated Legendre Functions"

only exist when the integers l and m_l are related as follows

$m_l=0,\pm1,\pm2,\pm3....\pm l$; l = positive number

l: Orbital Quantum Number

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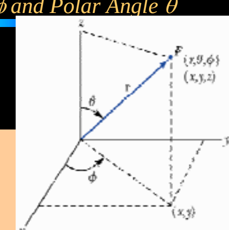
Wavefunction Along Azimuthal Angle ϕ and Polar Angle θ



For $l=0, m_l=0 \Rightarrow$ $\boxed{\Theta(\theta)=\frac{1}{\sqrt{2}}}$;

For $l=1, m_l=0,\pm1$ $\Rightarrow$ Three Possibilities for the Orbital part of wavefunction

$\boxed{[l=1,m_l=0]\Rightarrow\Theta(\theta)=\frac{\sqrt{6}}{2}\cos\theta}$ $\boxed{[l=1,m_l=\pm1]\Rightarrow\Theta(\theta)=\frac{\sqrt{3}}{2}\sin\theta}$

$[l=2,m_l=0]\Rightarrow\Theta(\theta)=\frac{\sqrt{10}}{4}(3\cos^2\theta-1)$

....*and* so on and so forth (see book for more Functions)

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Radial Differential Equations and Its Solutions

The Radial Diff. Eqn: $\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{\partial R}{\partial r}\right)+\left[\frac{2mr^2}{\hbar^2}(E+\frac{ke^2}{r})-\frac{l(l+1)}{r^2}\right]R(r)=0$

Solutions : Associated Laguerre Functions R(r), Solutions exist only if:

1. E>0 or has negtive values given by

$$E=-\frac{ke^2}{2a_0}\left(\frac{1}{n^2}\right); \quad \text{with } a_0=\frac{\hbar^2}{mke^2}=\text{Bohr Radius}$$

2. And when n = integer such that $l=0,1,2,3,4,.......(n-1)$

n = principal Quantum # or the "big daddy" quantum #

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The Hydrogen Wavefunction: $\psi(r,\theta,\phi)$ and $\Psi(r,\theta,\phi,t)$

To Summarize : The hydrogen atom is brought to you by the letters:

$n = 1,2,3,4,5,....\infty$
$l=0,1,2,3,,4....(n-1)$
$m_l=0,\pm1,\pm2,\pm3,...\pm l$

Quantum # appear only in Trapped systems

The Spatial part of the Hydrogen Atom Wave Function is:

$$\psi(r,\theta,\phi)=R_{nl}(r)\ .\ \Theta_{lm_l}(\theta)\ \ .\ \Phi_{m_l}(\phi)=R_{nl}Y_l^{m_l}$$

$Y_l^{m_l}$ are known as Spherical Harmonics. They define the angular structure in the Hydrogen-like atoms.

The Full wavefunction is $\Psi(r,\theta,\varphi,t)=\ \psi(r,\theta,\phi)e^{-\frac{iE}{\hbar}t}$

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Radial Wave Functions For n=1,2,3

n	l	m_l	R(r)=
1	0	0	$\frac{2}{a_0^{3/2}}e^{-r/a}$
2	0	0	$\frac{1}{2\sqrt{2}a_0^{3/2}}(2-\frac{r}{a_0})e^{-\frac{r}{2a_0}}$
3	0	0	$\frac{2}{81\sqrt{3}a_0^{3/2}}(27-18\frac{r}{a_0}+2\frac{r^2}{a_0^2})e^{-\frac{r}{3a_0}}$

n=1 → K shell
n=2 → L Shell
n=3 → M shell
n=4 → N Shell
……

l=0→ s(harp) sub shell
l=1→ p(rincipal) sub shell
l=2→ d(iffuse) sub shell
l=3→ f(undamental) ss
l=4→ g sub shell
…….

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Symbolic Notation of Atomic States in Hydrogen

$l\rightarrow$ / n ↓	$s\ (l=0)$	$p\ (l=1)$	$d\ (l=2)$	$f\ (l=3)$	$g(l=4)$	.....
1	1s					
2	2s	2p				
3	3s	3p	3d			
4	4s	4p	4d	4f		
5	5s	5p	5d	5f	5g	

Note that:

- n =1 is a non-degenerate system
- n>1 are all degenerate in l and m_l.
  All states have same energy
  But different angular configuration

$$E=-\frac{ke^2}{2a_0}\left(\frac{1}{n^2}\right)$$

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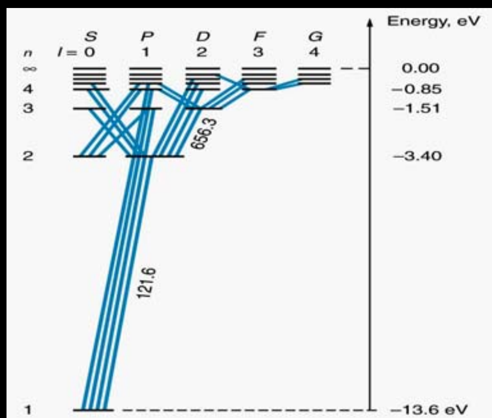
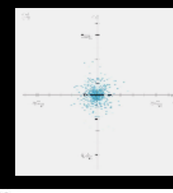
Energy States, Degeneracy & Transitions



Facts About Ground State of H Atom

$n=1,\ l=0,\ m_l=0 \Rightarrow R(r)=\frac{2}{a_0^{3/2}}\,e^{-r/a};\ \Theta(\theta)=\frac{1}{\sqrt{2\pi}};\ \Phi(\phi)=\frac{1}{\sqrt{2}}$

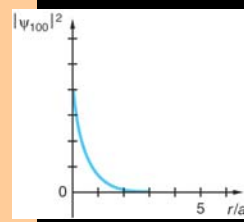
$$\boxed{\Psi_{100}(r,\theta,\phi)=\frac{1}{a_0\sqrt{\pi}}e^{-r/a}}$$ ......look at it carefully



1. Spherically symmetric $\Rightarrow$ no θ,ϕ dependence (structure)

2. Probability Per Unit Volume : $\left|\Psi_{100}(r,\theta,\phi)\right|^2=\frac{1}{\pi a_0^3}e^{-\frac{2r}{a}}$

Likelihood of finding the electron is same at all θ,ϕ and depends only on the radial seperation (r) between electron & the nucleus.



3 Energy of Ground State $=-\frac{ke^2}{2a_0}=-13.6eV$

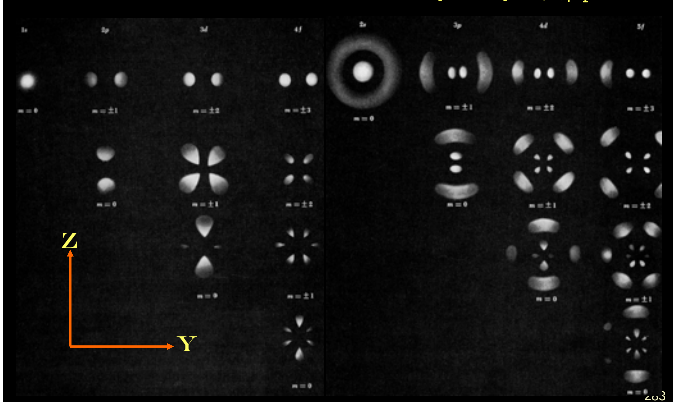
Overall The Ground state wavefunction of the hydrogen atom is quite *boring*

Not much chemistry or Biology could develop if there was only the ground state of the Hydrogen Atom!

We need structure, we need variety, we need some curves!

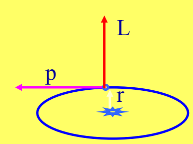
Cross Sectional View of Hydrogen Atom prob. densities in r,θ,ϕ
Birth of Chemistry (Can make Fancy Bonds→ Overlapping electron "clouds")

What's the electron "cloud" : Its the Probability Density in r, θ,ϕ space!



Interpreting Orbital Quantum Number (l)

Radial part of S.Eqn: $\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left[\frac{2m}{\hbar^2}(E+\frac{ke^2}{r})-\frac{l(l+1)}{r^2}\right]R(r)=0$



For H Atom: $E=K+U=K_{RADIAL}+K_{ORBITAL}-\frac{ke^2}{r}$; substitute this in E

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2m}{\hbar^2}\left[K_{RADIAL}+K_{ORBITAL}-\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]R(r)=0$$

Examine the equation, if we set $\boxed{K_{ORBITAL}=\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}}$ *then*

what remains is a differential equation in r

$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2m}{\hbar^2}\left[K_{RADIAL}\right]R(r)=0$ which depends only on radius r of orbit

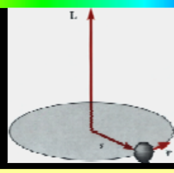
Further, we also know that $K_{ORBITAL}=\frac{1}{2}mv_{orbit}^2;\quad \vec{L}=\vec{r}\times\vec{p};\quad |L|=mv_{orb}r \Rightarrow \boxed{K_{ORBITAL}=\frac{L^2}{2mr^2}}$

Putting it all togather: $\boxed{K_{ORBITAL}=\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}=\frac{L^2}{2mr^2}} \Rightarrow$ magnitude of Ang. Mom $|L|=\sqrt{l(l+1)}\hbar$

Since $l=$ *positive* integer=0,1,2,3...(n-1) $\Rightarrow$ angular momentum $\boxed{|L|=\sqrt{l(l+1)}\hbar=\textit{discrete values}}$

$|L|=\sqrt{l(l+1)}\hbar$: QUANTIZATION OF Electron's Angular Momentum

Magnetic Quantum Number : m_l



$\vec{L} = \vec{r} \times \vec{p}$ (Right Hand Rule)

Classically, direction & Magnitude of $\vec{L}$ always well defined

QM: Can/Does $\vec{L}$ have a definite direction ? Proof by Negation:

Suppose $\vec{L}$ was precisely known/defined ($\vec{L} \parallel \hat{z}$)

Since $\vec{L} = \vec{r} \times \vec{p} \Rightarrow$ Electron MUST be in x-y orbit plane

$\Rightarrow \Delta z = 0$; $\Delta p_z \Delta z \sim \hbar \Rightarrow \Delta p_z \sim \infty; E = \dfrac{p^2}{2m} \sim \infty$!!!

So, in Hydrogen atom, $\vec{L}$ can not have precise measurable value

Uncertainty Principle & Angular Momentum : $\boxed{\Delta L_z \Delta\phi \sim \hbar}$

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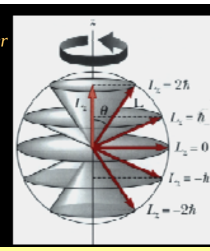
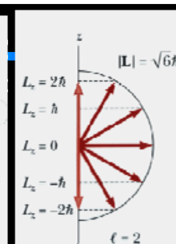
Magnetic Quantum Number m_l

Consider $\ell = 2$

$|L| = \sqrt{\ell(\ell+1)} = \sqrt{6}\hbar$





In Hydrogen atom, $\vec{L}$ can not have precise measurable value

Arbitararily picking Z axis as a reference direction:

$\vec{L}$ vector spins around Z axis (precesses).

The Z component of $\vec{L}$: $\boxed{|L_Z| = m_l\hbar; \quad m_l = \pm1, \pm2, \pm3 \ldots \pm l}$

Note: since $|L_Z| < |L|$ (always)

since $m_l\hbar < \sqrt{l(l+1)}\ \hbar$ It can never be that $|L_Z| = m_l\hbar = \sqrt{l(l+1)}\ \hbar$

(breaks Uncertainty Principle)

So......the Electron's dance has begun !

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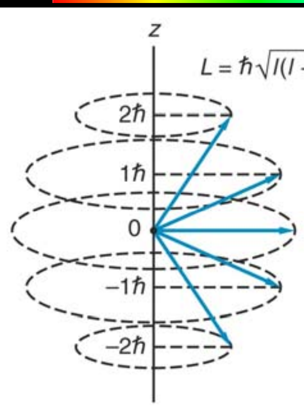
L=2, m_l=0,±1, ± 2 : Pictorially

$L = \hbar\sqrt{l(l+1)} = \hbar\sqrt{2(2+1)} = \hbar\sqrt{6}$



Electron "sweeps" conical paths of different ϑ:

Cos ϑ = L_Z/L

On average, the angular momentum component in x and y cancel out

$\langle L_X \rangle = 0$

$\langle L_Y \rangle = 0$

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Where is it likely to be ? → Radial Probability Densities

$\Psi(r,\theta,\phi) = R_{nl}(r)\ .\ \Theta_{lm_l}(\theta)\ \ .\ \Phi_{m_l}(\phi) = R_{nl} Y_l^{m_l}$

Probability Density Function in 3D:

$\boxed{P(r,\theta,\phi) = \Psi^*\Psi = |\Psi(r,\theta,\phi)|^2 = |R_{nl}|^2 . |Y_l^{m_l}|^2}$

Note : 3D Volume element $\boxed{dV = r^2.\sin\theta.dr.d\theta.d\phi}$

Prob. of finding particle in a tiny volume dV is

$P.dV = |R_{nl}|^2 . |Y_l^{m_l}|^2 .r^2.\sin\theta.dr.d\theta.d\phi$

The Radial part of Prob. distribution: P(r)dr

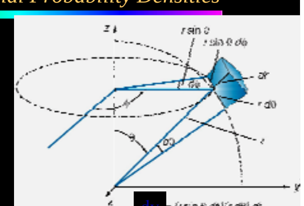
$P(r)dr = |R_{nl}|^2 .r^2 dr \int_0^{\pi} |\Theta_{lm_l}(\theta)|^2 d\theta \int_0^{2\pi} |\Phi_{m_l}(\phi)|^2\ d\phi$

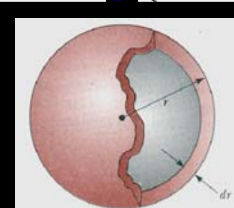
When $\Theta_{lm_l}(\theta)$ & $\Phi_{m_l}(\phi)$ are auto-normalized then

$P(r)dr = |R_{nl}|^2 .r^2 dr;$ in other words $\boxed{P(r) = r^2 |R_{nl}|^2}$

Normalization Condition: $\boxed{1 = \int_0^{\infty} r^2 |R_{nl}|^2 dr}$

Expectation Values $\boxed{\langle f(r) \rangle = \int_0^{\infty} f(r).P(r)dr}$





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Ground State: Radial Probability Density

$P(r)dr = |\psi(r)|^2 .4\pi r^2 dr$

$\Rightarrow \boxed{P(r)dr = \frac{4}{a_0^3} r^2 e^{-2\frac{r}{a_0}}}$

Probability of finding Electron for $r>a_0$

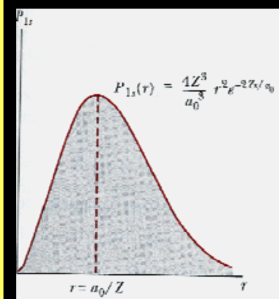
$P_{r>a_0} = \int_a^\infty \frac{4}{a_0^3} r^2 e^{-2\frac{r}{a_0}} dr$

To solve, employ change of variable

Define $z=\left[\frac{2r}{a_0}\right]$; *change* limits of integration

$P_{r>a_0} = \frac{1}{2}\int_2^\infty z^2 e^{-z} dz$ (such integrals called Error. Fn)

$= -\frac{1}{2}[z^2+2z+2]e^{-z} |_2^\infty = 5e^2 = 0.667 \Rightarrow$ 66.7% !!



Most Probable & Average Distance of Electron from Nucleus

Most Probable Distance:

In the ground state $(n=1, l=0, m_l=0)$ $\boxed{P(r)dr = \frac{4}{a_0^3} r^2 e^{-2\frac{r}{a_0}}}$

Most probable distance r from Nucleus $\Rightarrow$ What value of r is P(r) max?

$\Rightarrow \frac{dP}{dr}=0 \Rightarrow \frac{4}{a_0^3}.\frac{d}{dr}\left[r^2 e^{-2\frac{r}{a_0}}\right] = 0 \Rightarrow \left[\frac{-2r^2}{a_0} + 2r\right] e^{-2\frac{r}{a_0}} = 0$

$\Rightarrow \frac{2r^2}{a_0} + 2r = 0 \Rightarrow \boxed{r = 0 \text{ or } r = a_0}$... which solution is correct?

(see past quiz) : Can the electron BE at the center of Nucleus (r=0)?

$P(r=0) = \frac{4}{a_0^3} 0^2 e^{-2\frac{0}{a_0}} = 0! \Rightarrow$ $\boxed{\text{Most Probable distance } r = a_0}$ (Bohr guessed right)

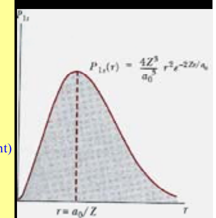
What about the AVERAGE location <r> of the electron in Ground state?

$<r> = \int_{r=0}^\infty rP(r)dr = \frac{4}{a_0^3}\int_0^\infty r r^2 e^{-2\frac{r}{a_0}} dr$ ...change of variable $z=\frac{2r}{a_0}$

$\Rightarrow <r> = \frac{a_0}{4}\int_{z=0}^\infty z^3 e^{-z} dz$....... $\boxed{\text{Use general form } \int_0^\infty z^n e^{-z} dz = n! = n(n-1)(n-2)...(1)}$

$\Rightarrow \boxed{<r> = \frac{a_0}{4} 3! = \frac{3a_0}{2} \neq a_0!}$ Average & most likely distance is not same. Why?

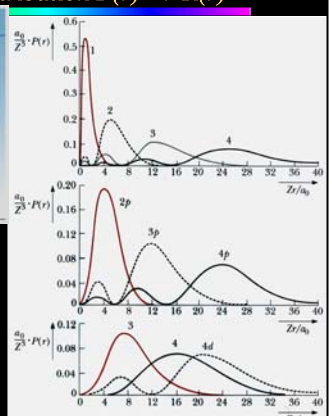
Asnwer is in the form of the radial Prob. Density: Not symmetric



Radial Probability Distribution $P(r)= r^2R(r)$

TABLE 7-2 Radial functions for hydrogen

$n=1$	$l=0$	$R_{10} = \frac{2}{\sqrt{a_0^3}} e^{-r/a_0}$
$n=2$	$l=0$	$R_{20} = \frac{1}{\sqrt{2a_0^3}}\left(1-\frac{r}{2a_0}\right)e^{-r/2a_0}$
	$l=1$	$R_{21} = \frac{1}{2\sqrt{6a_0^3}}\frac{r}{a_0}e^{-r/2a_0}$
$n=3$	$l=0$	$R_{30} = \frac{2}{3\sqrt{3a_0^3}}\left(1-\frac{2r}{3a_0}+\frac{2r^2}{27a_0^2}\right)e^{-r/3a_0}$
	$l=1$	$R_{31} = \frac{8}{27\sqrt{6a_0^3}}\frac{r}{a_0}\left(1-\frac{r}{6a_0}\right)e^{-r/3a_0}$
	$l=2$	$R_{32} = \frac{4}{8\sqrt{30a_0^3}}\frac{r^2}{a_0^2}e^{-r/3a_0}$



Because $P(r)=r^2R(r)$; No matter what R(r) is for some n,

The prob. Of finding electron inside the nucleus = 0 !!

Normalized Spherical Harmonics & Structure in H Atom

TABLE 7-1 Spherical harmonics

$l=0$	$m=0$	$Y_{00} = \sqrt{\frac{1}{4\pi}}$
$l=1$	$m=1$	$Y_{11} = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$
	$m=0$	$Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta$
	$m=-1$	$Y_{1-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}$
$l=2$	$m=2$	$Y_{22} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{2i\phi}$
	$m=1$	$Y_{21} = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$
	$m=0$	$Y_{20} = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$
	$m=-1$	$Y_{2-1} = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{-i\phi}$
	$m=-2$	$Y_{2-2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{-2i\phi}$

Excited States (n>1) of Hydrogen Atom : Birth of Chemistry !

Features of Wavefunction in θ & ϕ :

Consider $n = 2,\ l = 0 \Rightarrow \psi_{200}$ = Spherically Symmetric (last slide)

Excited States (3 & each with same E_n) :

$\psi_{211}, \psi_{210}, \psi_{21\text{-}1}$ are all 2p states

$$\psi_{211} = R_{21} Y_1^1 = \left(\frac{1}{\pi}\right)\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Z}{8}\right)\left(\frac{r}{a_0}\right) e^{\frac{-Zr}{a_0}} . \sin\theta . e^{i\phi}$$

$|\psi_{211}|^2 = |\psi^*_{211}\psi_{211}| \propto \sin^2\theta$ Max at $\theta = \frac{\pi}{2}$, min at $\theta = 0$; Symm in ϕ

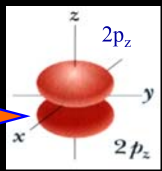
What about $(n=2, \ell=1, m_l = 0)$

$\psi_{210} = R_{21}(r)\ Y_1^0(\theta,\phi)$;

$Y_1^0(\theta,\phi) \propto \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$;

Function is max at $\theta=0$, min at $\theta = \frac{\pi}{2}$

We call this $2p_z$ state because of its extent in z



Excited States (n>1) of Hydrogen Atom : Birth of Chemistry !

Remember Principle of Linear Superposition

for the TISE which is basically a simple differential equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi$$

Principle of Linear Superposition $\Rightarrow$ If ψ_1 and ψ_2 are sol. of TISE then a "designer" wavefunction made of linear sum

$\psi' = a\psi_1 + b\psi_2$ is also a sol. of the diff. equation !

To check this, just substitute ψ' in place of ψ

& convince yourself that

$$-\frac{\hbar^2}{2m}\nabla^2\psi' + U\psi' = E\psi'$$

The diversity in Chemistry and Biology DEPENDS on this superposition rule

Designer Wave Functions: Solutions of S. Eq !

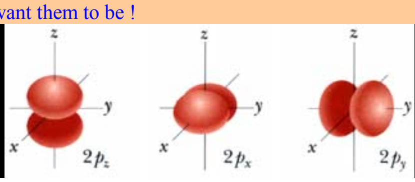
Linear Superposition Principle means allows me to "cook up" wavefunctions

$$\psi_{2p_x} = \frac{1}{\sqrt{2}}\left[\psi_{211} + \psi_{21-1}\right]$$ ......has electron "cloud" oriented along x axis

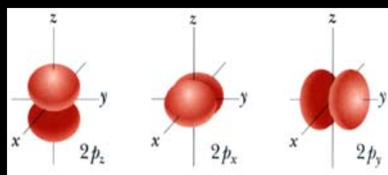
$$\psi_{2p_y} = \frac{1}{\sqrt{2}}\left[\psi_{211} - \psi_{21-1}\right]$$ ......has electron "cloud" oriented along y axis

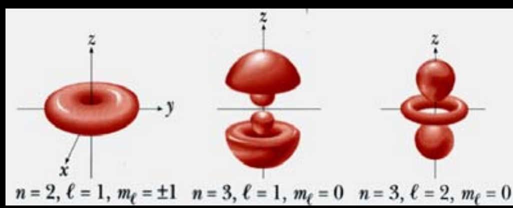
So from 4 solutions $\psi_{200}, \psi_{210}, \psi_{211}, \psi_{21-1} \rightarrow 2s, 2p_x, 2p_y, 2p_z$

Similarly for n=3 states ...and so on ...can get very complicated structure in θ & ϕ.......which I can then mix & match to make electrons "most likely" to be where I want them to be !



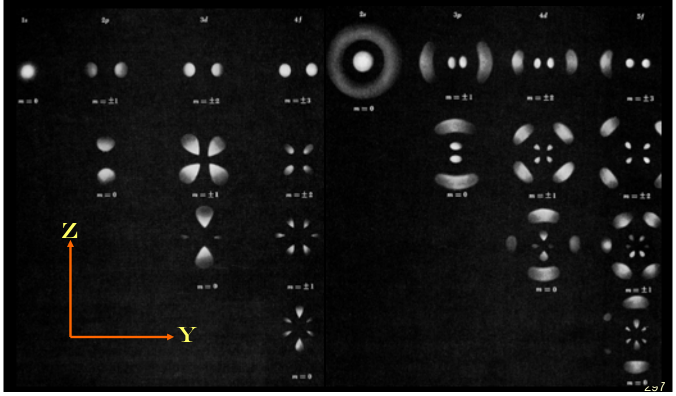
Designer Wave Functions: Solutions of S. Eq !



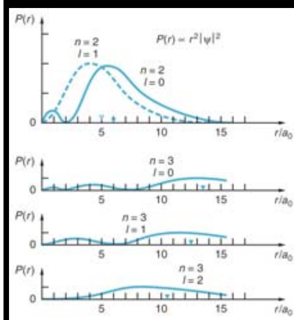


Cross Sectional View of Hydrogen Atom prob. densities in r,θ,φ
Birth of Chemistry (Can make Fancy Bonds→ Overlapping electron "clouds")

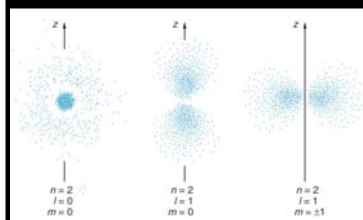
What's the electron "cloud" : Its the Probability Density in r, θ,φ space!



More Radial Probabilities P(r) Vs. r/a_0



Net Prob. densities for n=2 states



spherically symmetric | dumbbell | Doughnut (toroid)

Transition Between States In Quantum Systems

In formulating the Hydrogen Atom, Bohr was obliged to postulate that the frequency of radiation emitted by an atom dropping from energy level E_m to a lower level E_n is:

$$\boxed{f = \frac{E_m - E_n}{h}}$$

This relationship rises naturally in Quantum Mechanics, consider for simplicity a system in which an electron only in the x direction:The time-dependent Wavefunction $\Psi_n(x,t)=\psi_n(x)e^{-i\frac{E_n}{\hbar}t}$;

$<x>=\int_{-\infty}^{\infty} x\ \psi_n^*\psi_n dx =$ constant in time, does not oscillate, no radiation occurs

But, due to an external perturbation lasting some time, electron shifts from one state (m) to another(n)
In this period wavefunction of electron is a linear superposition of two possible states

$\Psi = a\Psi_n + b\Psi_m$; a^*a= prob. of electron in state n and b^*b= prob. of electron in state m; $\boxed{a^*a+b^*b=1}$

Initially a=1,b=0 and finally a=0,b=1. While the electron is in either state there is no radiation but when it is in the midst of transition from m → n, both a and b have non-vanishing values and radiation is produced.

Expectation value for compostive wavefunction $<x> = \int x\Psi^*\Psi dx$;

$$<x>=\int_{-\infty}^{\infty} x(a^2\Psi_n^*\Psi_n + b^*a\Psi_m^*\Psi_n + a^*b\Psi_n^*\Psi_m + b^2\Psi_m^*\Psi_m)dx$$

Transition Between States In Quantum Systems

$$<x>=\int_{-\infty}^{\infty} x(a^2\Psi_n^*\Psi_n + b^*a\Psi_m^*\Psi_n + a^*b\Psi_n^*\Psi_m + b^2\Psi_m^*\Psi_m)dx$$

$$<x>= a^2\int x\psi_n^*\psi_n dx + b^2\int x\psi_m^*\psi_m dx$$
$$+ ab^*\int x\psi_m^* e^{+i(E_m/\hbar)t}\psi_n e^{-i(E_n/\hbar)t}dx + a^*b\int x\psi_n^* e^{+i(E_n/\hbar)t}\psi_m e^{-i(E_m/\hbar)t}dx$$

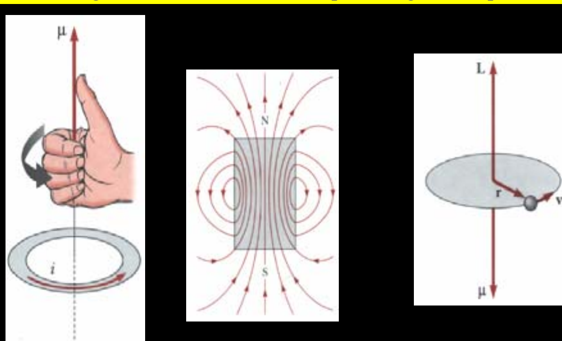
Use $e^{i\theta} = \cos\theta + i\sin\theta$ and $e^{-i\theta} = \cos\theta - i\sin\theta$ in the above and consider just the REAL part of expression for the last two terms, it varies with time as

$$\cos\left(\frac{E_m - E_n}{\hbar}\right)t = \cos 2\pi\left(\frac{E_m - E_n}{h}\right)t = \cos 2\pi ft$$

So the <x> of the electron oscillates with frequency f and one has a nice electric dipole analogy ⇒ Hence radiative transtions !
Similarly for particle in an infinite well or harmonic oscillator ...

What's So "Magnetic" about m_l ?

Precessing electron → Current in loop → Magnetic Dipole moment μ



The electron's motion → hydrogen atom is a dipole magnet

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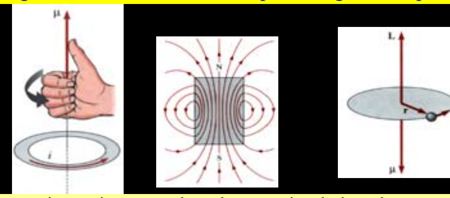
The "Magnetism" of an Orbiting Electron

Precessing electron → Current in loop → Magnetic Dipole moment μ



Electron in motion around nucleus ⇒ circulating charge ⇒ curent i

$i = \frac{-e}{T} = \frac{-e}{\frac{2\pi r}{v}} = \frac{-ep}{2\pi m r}$; Area of current loop $A = \pi r^2$

Magnetic Moment $|\mu| = iA = \left(\frac{-e}{2m}\right) rp$; $\vec{\mu} = \left(\frac{-e}{2m}\right) \vec{r} \times \vec{p} = \left(\frac{-e}{2m}\right) \vec{L}$

Like the $\vec{L}$, magnetic moment $\vec{\mu}$ also precesses about "z" axis

z component, $\mu_z = \left(\frac{-e}{2m}\right) L_z = \left(\frac{-e\hbar}{2m}\right) m_l = -\mu_B m_l$ = *quantized !*

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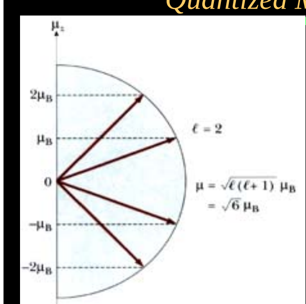
Quantized Magnetic Moment



$$\mu_z = \left(\frac{-e}{2m}\right) L_z = \left(\frac{-e\hbar}{2m}\right) m_l$$
$$= -\mu_B m_l$$
$$\mu_B = \text{Bohr Magnetron}$$
$$= \left(\frac{e\hbar}{2m_e}\right)$$

Why all this ? Need to find a way to break the Energy Degeneracy & get electron in each (n, l, m_l) state to identify itself, so we can "talk" to it and make it do our bidding:
" Walk this way, talk this way!"

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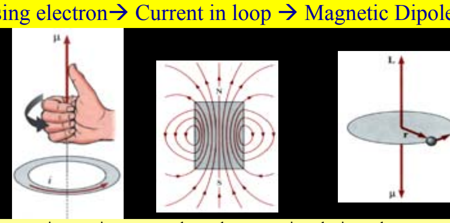
The "Magnetism" of an Orbiting Electron

Precessing electron → Current in loop → Magnetic Dipole moment μ



Electron in motion around nucleus ⇒ circulating charge ⇒ curent i

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Magnetic Moment $|\mu| = iA = \left(\frac{-e}{2m}\right) rp$; $\vec{\mu} = \left(\frac{-e}{2m}\right) \vec{r} \times \vec{p} = \left(\frac{-e}{2m}\right) \vec{L}$

Like the $\vec{L}$, magnetic moment $\vec{\mu}$ also precesses about "z" axis

z component, $\mu_z = \left(\frac{-e}{2m}\right) L_z = \left(\frac{-e\hbar}{2m}\right) m_l = -\mu_B m_l$ = *quantized !*

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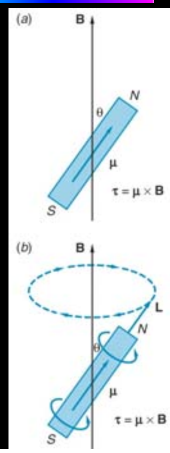
Bar Magnet Model of Magnetic Moment

In external B field, magnet experiences a torque which tends to align it with the field direction

If the magnet is spinning, torque causes magnet to precess around the ext. B field with a constant frequency: Larmor frequency



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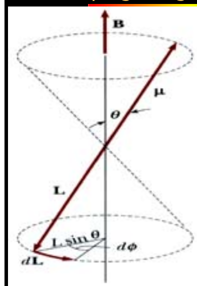
"Lifting" Degeneracy : Magnetic Moment in External B Field



Apply an External $\vec{B}$ field on a Hydrogen atom (viewed as a dipole)

Consider $\vec{B} \parallel \vec{Z}$ axis (could be any other direction too)

The dipole moment of the Hydrogen atom (due to electron orbit)

experiences a Torque $\vec{\tau} = \vec{\mu} \times \vec{B}$ which does work to align $\vec{\mu} \parallel \vec{B}$

but this can not be (same Uncertainty principle argument)

$\Rightarrow$ So, Instead, $\vec{\mu}$ precesses (dances) around $\vec{B}$... like a spinning top

The Azimuthal angle ϕ changes with time : calculate frequency

Look at Geometry: |projection along x-y plane : $|dL| = L\sin\theta . d\phi$

$\Rightarrow d\phi = \frac{|dL|}{L\sin\theta}$; Change in Ang Mom. $|dL| = |\tau|\, dt = \left|\frac{q}{2m} LB\sin\theta\right| dt$

$\Rightarrow \boxed{\omega_L = \frac{d\phi}{dt} = \frac{1}{L\sin\theta}\frac{|dL}{dt} = \frac{1}{L\sin\theta}\frac{q}{2m} LB\sin\theta = \frac{qB}{2m_e}}$ Larmor Freq

ω_L depends on B, the applied external magnetic field

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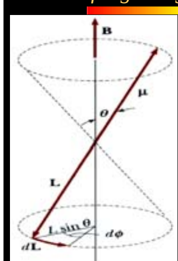
"Lifting" Degeneracy : Magnetic Moment in External B Field



WORK done to reorient $\vec{\mu}$ against $\vec{B}$ field: $\boxed{dW = \tau d\theta = -\mu B\sin\theta d\theta}$

$dW = d(\mu B\cos\theta)$: This work is stored as orientational Pot. Energy U

$dW = -dU$

Define Magnetic Potential Energy $U = -\vec{\mu}.\vec{B} = -\mu\cos\theta.B = -\mu_z B$

Change in Potential Energy $U = \frac{e\hbar}{2m_e} m_l B = \boxed{\hbar\omega_L m_l}$

Zeeman Effect in Hydrogen Atom

In presence of External B Field, Total energy of H atom changes to

$$\boxed{E = E_0 + \hbar\omega_L m_l}$$

So the Ext. B field can break the E degeneracy "organically" inherent in the H atom. The Energy now depends not just on n but also m_l

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4E : The Quantum Universe

Lecture 29, May 24

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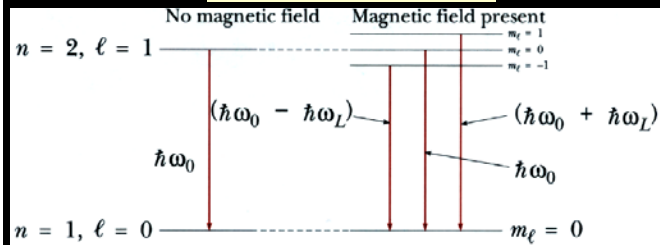
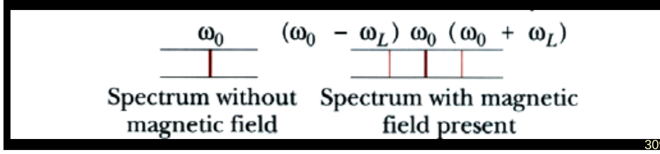
Zeeman Effect Due to Presence of External B field

Energy Degeneracy Is Broken





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Electron has "Spin": An additional degree of freedom

Electron possesses additional "hidden" degree of freedom : "Spinning around itself" !

Spin Quantum # $s = \frac{1}{2}$ (either Up or Down)

How do we know this ? $\Rightarrow$ Stern-Gerlach expt

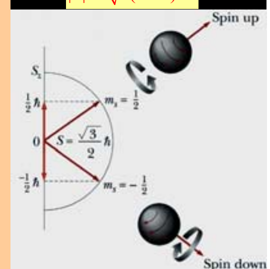
Spin Vector $\vec{S}$ (a form of angular momentum) is also Quantized

$$|\vec{S}| = \sqrt{s(s+1)}\ \hbar = \sqrt{\frac{3}{4}}\ \hbar$$

& $S_z = m_s\hbar;\ m_s = \pm\frac{1}{2}$

Spinning electron is an entitity defying any simple classical description. ....hidden D.O.F

$|\vec{S}| = \sqrt{s(s+1)}\ \hbar$



Spin angular momentum S also exhibits Space quantization

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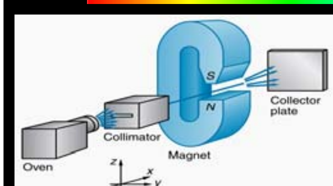
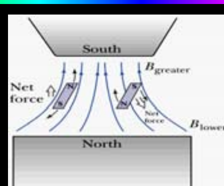
Stern-Gerlach Expt$\Rightarrow$An additional degree of freedom: "Spin"





In an inhomogeneous field perpendicular to beam direction, magnetic moment μ experiences a force F_z whose direction depends on Z component of the net magnetic moment & inhomogeneity dB/dz. The force deflects magnetic moment up or down. **Space Quantization means expect *(2l+1)* deflections**. For l =0, expect ***all*** electrons to arrive on the screen at the center (no deflection)

$\vec{\mu}$ in inhomogenous $\vec{B}$ field, experiences force $\vec{F}$

$\vec{F} = -\nabla U_B = -\nabla(-\vec{\mu}.\vec{B})$

When gradient only along z, $\frac{\partial B}{\partial z} \neq 0; \frac{\partial B}{\partial x} = \frac{\partial B}{\partial y} = 0$

$F_z = m\mu_B(\frac{\partial B}{\partial z})$ moves particle up or down

(in addition to torque causing magnetic moment $\vec{\mu}$ to precess about B field direction

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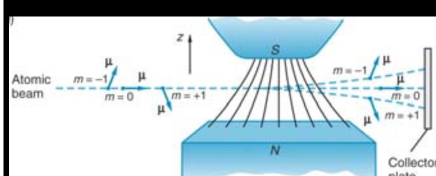
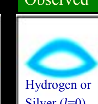
An Additional degree of freedom: "Spin" for lack of a better name !



Expected

Observed



!

This was a big surprise for Stern-Gerlach ! They had accidentally Discovered a new degree of freedom for electron : "spin" which Can take only two orientations for angular momentum S : up or down Leads to a new quantum number *s=1/2*. As a result:

Z Component of Spin Angular Momentum $S_z = m_s\hbar$

The magnitude $|S| = \sqrt{s(s+1)}\ \hbar$ is FIXED, never changes !

Allowed orientations are $s(s+1) = 2$

$\vec{S} \Rightarrow \vec{\mu}_S$; The corresponding Spin Magnetic Moment

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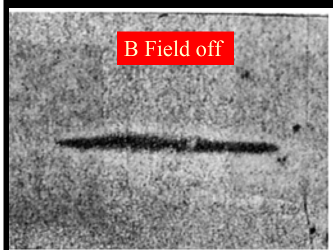
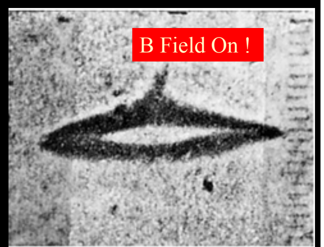
What Stern&Gerlach Saw in l=0 Silver Atoms

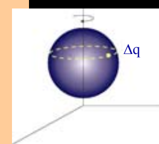




Picture changes instantaneously as the external Field is switched off or on….discovery !

Four (not 3) Numbers Describe Hydrogen Atom → n, l, m_l, m_s

"Spinning" charge gives rise to a dipole moment $\vec{\mu}_s$:



Imagine (semi-clasically, incorrectly!) electron as sphere: charge q, radius r

Total charge uniformly distributed: $q = \sum_i \Delta q_i$;

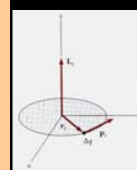
as electron spins, each "chargelet" rotates ⇒ current ⇒ dipole moment $\vec{\mu}_{s_i}$

$$\vec{\mu}_s = \left(\frac{q}{2m_e}\right)\sum_i \vec{\mu}_{s_i} = g\left(\frac{q}{2m_e}\right)\vec{S}; g = 2$$

In a Magnetic Field $\vec{B}$ ⇒ magnetic energy due to spin $U_s = \vec{\mu}_s.\vec{B}$

Net Angular Momentum in H Atom $\vec{J} = \vec{L} + \vec{S}$

Net Magnetic Moment of H atom: $\vec{\mu} = \vec{\mu}_0 + \vec{\mu}_s = \left(\frac{-e}{2m_e}\right)(\vec{L} + g\vec{S})$



Notice that since g=2, net dipole moment vector $\vec{\mu}$ is not || to $\vec{J}$

(There are many such "ubiquitous" quantum numbers for elementary particles!)

Magnetic Energy in an External B Field

Contributions from Orbital and Spin motions. Defining Z axis to be the orientation of the B field:

$$U = -\vec{\mu}.\vec{B} = \frac{e}{2m}B\{L_z + gS_z\} = \frac{e\hbar}{2m}B\{m_l + gm_s\}$$

Example: Zeeman spectrum in B=1T produced by Hydrogen initially in n=2 state

after taking spin into account: n=2 ⇒ $E_2 = -13.6eV/2^2 = -3.40eV$

Since $m_l = 0, \pm 1$, orbital contribution to Magnetic energy $U_0 = m_l\hbar\omega_L$

This splits energy levels to $E = E_2 \pm \hbar\omega_L$; for $m_l = \pm 1$ states

These states get further split in pairs due to spin magnetic moment

Since g=2 and $m_s = \pm\frac{1}{2}$; spin energy is again Zeeman energy=$\hbar\omega_L$

As a result electrons in this shell have one of the following energies

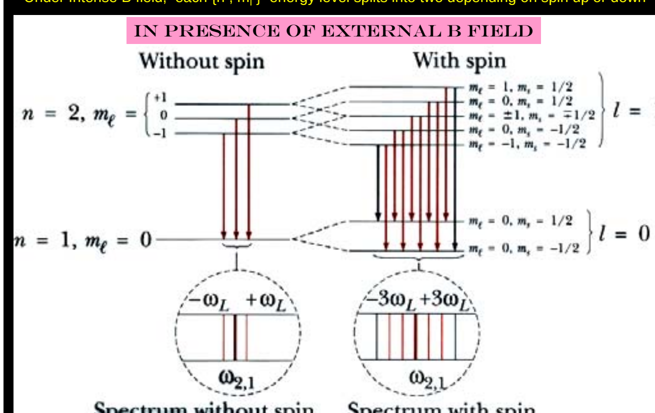
E_2 $E_2 \pm \hbar\omega_L$ $E_2 \pm 2\hbar\omega_L$

This leads to a variety of allowed ($\Delta(m_l + m_s) = 0, \pm 1$) energy transitions with different intensities (Principal and satellites) which are visible when B field is large (ignore LS coupling

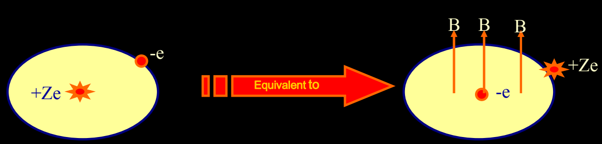
See energy level diagram on next page

Doubling of Energy Levels Due to Spin Quantum Number

Under Intense B field, each {n , m_l } energy level splits into two depending on spin up or down



Spin-Orbit Interaction: L and S Momenta are Linked Magnetically



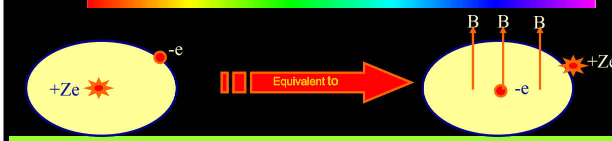
Electron revolving around Nucleus finds itself in a "internal" B field because in its frame of reference, the nucleus is orbiting around it

This B field, due to orbital motion, interacts with electron's spin dipole moment $\vec{\mu}_s$

$U_m = -\vec{\mu}.\vec{B} \Rightarrow$ Energy larger when $\vec{S} \parallel \vec{B}$, smaller when anti-parallel

$\Rightarrow$ States with same (n, l, m_l) but diff. spins $\Rightarrow$ energy level splitting/doubling due to $\vec{S}$

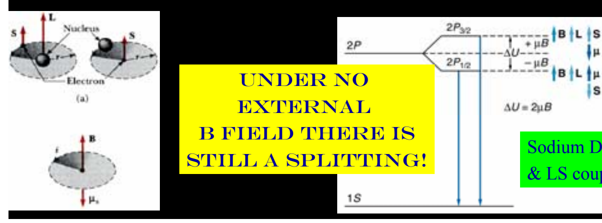
Spin-Orbit Interaction: Angular Momenta are Linked Magnetically



This B field, due to orbital motion, interacts with electron's spin dipole moment $\vec{\mu}_s$

$U_m = -\vec{\mu}.\vec{B} \Rightarrow$ Energy larger when $\vec{S} \parallel \vec{B}$, smaller when anti-parallel

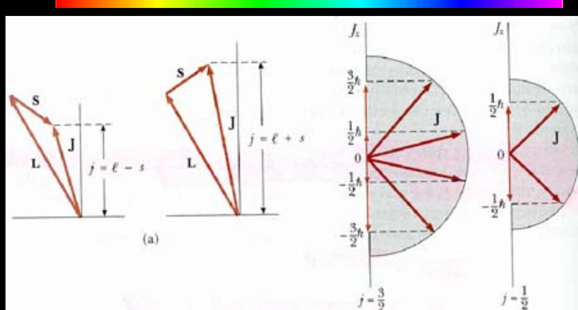
$\Rightarrow$ States with same (n, l, m_l) but diff. spins $\Rightarrow$ energy level splitting/doubling due to $\vec{S}$

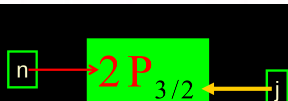


UNDER NO EXTERNAL B FIELD THERE IS STILL A SPLITTING!

Sodium Doublet & LS coupling

Vector Model For Total Angular Momentum *J*





Vector Model For Total Angular Momentum *J*

Coupling of Orbital & Spin magnetic moments $\Rightarrow$

Neither Orbital nor Spin angular Momentum are conserved seperately!

$\vec{J} = \vec{L} + \vec{S}$ is conserved so long as there are no external torques present

Rules for Total Angular Momentum Quantization :

$|J| = \sqrt{j(j+1)}\,\hbar$ with $j = |l+s|,\ l+s-1,\ l+s-2 \ldots\ldots, \ldots\ldots, |l-s|$

$J_z = m_j \hbar$ with $m_j = j, j-1, j-2 \ldots\ldots, -j$

Example: state with $(l = 1, s = \frac{1}{2})$

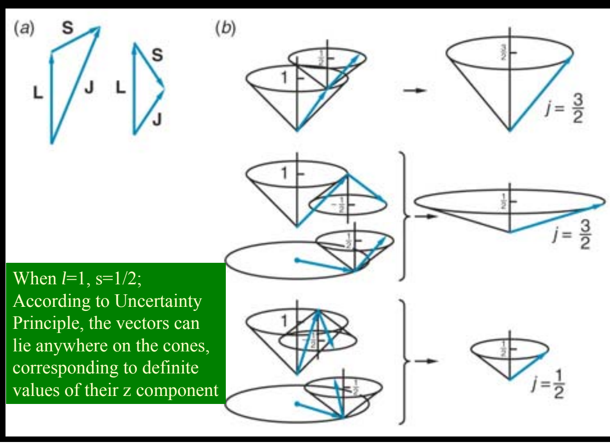
$j = 3/2 \Rightarrow m_j = -3/2, -1/2, 1/2, 3/2$

$j = 1/2 \Rightarrow m_j = \pm 1/2$

In general m_j takes $(2j+1)$ values

$\Rightarrow$ Even # of orientations

Addition of Orbital and Spin Angular Momenta



When l=1, s=1/2;
According to Uncertainty Principle, the vectors can lie anywhere on the cones, corresponding to definite values of their z component

Complete Description of Hydrogen Atom

Full description of the Hydrogen atom:

$\{n, l, m_l, m_s\}$

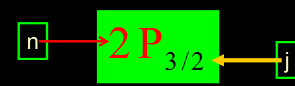
$\Downarrow$

LS Coupling

$\Downarrow$

$\{n, l, j, m_s\}$

corresponding to 4 D.O.F.

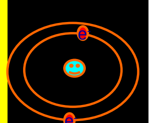


How to describe multi-electrons atoms like He, Li etc?
How to order the Periodic table?

- Four guiding principles:
  - Indistinguishable particle & Pauli Exclusion Principle
  - Independent particle model (ignore inter-electron repulsion)
  - Minimum Energy Principle for atom
  - Hund's "rule" for order of filling vacant orbitals in an atom

Multi-Electron Atoms : >1 electron in orbit around Nucleus

In Hydrogen Atom $\psi(r,\theta,\phi)=R(r).\Theta(\theta).\Phi(\phi) \equiv \{n, l, j, m_j\}$

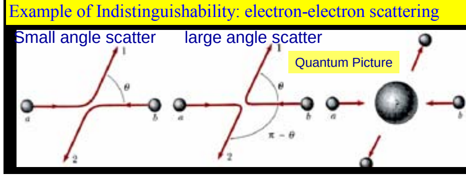


In n-electron atom, to simplify, ignore electron-electron interactions
complete wavefunction, in "independent"particle approx" :

$$\psi(1,2,3,..n)=\psi(1).\psi(2).\psi(3)...\psi(n) \quad ???$$

Complication $\rightarrow$ Electrons are identical particles, labeling meaningless!
Question: How many electrons can have same set of quantum #s?
Answer: No two electrons in an atom can have SAME set of quantum#s
(if not, all electrons would occupy 1s state (least energy)... no structure!!

Example of Indistinguishability: electron-electron scattering

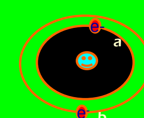


If we cant follow electron path, don't know between which of the two scattering events actually happened

Helium Atom: Two electrons around a Nucleus

In Helium, each electron has : kinetic energy + electrostatic potential energy
If electron "1" is located at r_1 & electron "2"is located at r_2 then TISE has terms like:

$$H_1 = -\frac{\hbar^2}{2m}\nabla_1^2 + k\frac{(2e)(-e)}{r_1};\ H_2 = -\frac{\hbar^2}{2m}\nabla_2^2 + k\frac{(2e)(-e)}{r_2} \quad \text{such that}$$



$\boxed{H_1\psi + H_2\psi = E\psi}$; H_1 & H_2 are same except for "label"

Independent Particle Approx $\Rightarrow$ ignore repulsive $U=k\frac{e^2}{|r_2 - r_1|}$ term

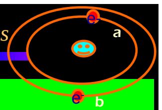
Helium WaveFunction: $\psi=\psi(r_1,r_2)$; Probability $P=\psi^*(r_1,r_2)\psi(r_1,r_2)$
But if we exchange location of (identical, indistinguishable) electrons $\Rightarrow |\psi(r_1,r_2)|=|\psi(r_2,r_1)|$
In general, when $\psi(r_1,r_2)=\psi(r_2,r_1)$......................Bosonic System (made of photons, e.g)
when $\psi(r_1,r_2)=-\psi(r_2,r_1)$....................fermionic System (made of electron, proton e.g)
$\Rightarrow$ Helium wavefunction must be ODD; if electron "1" is in state a & electron "2" is in state b
Then the net wavefunction $\psi_{ab}(r_1,r_2)=\psi_a(r_1).\psi_b(r_2)$ satisfies

$$H_1\psi_a(r_1).\psi_b(r_2) = E_a\psi_a(r_1).\psi_b(r_2)$$
$$H_2\psi_a(r_1).\psi_b(r_2) = E_b\psi_a(r_1).\psi_b(r_2)$$

and the sum $\quad [H_1+H_2]\psi_a(r_1).\psi_b(r_2) = (E_a + E_b)\psi_a(r_1).\psi_b(r_2)$

Total Helium Energy $E \simeq E_a + E_b$ =sum of Hydrogen atom like E

Helium Atom: Two electrons around a Nucleus



Helium wavefunction must be ODD ⇒ anti-symmetric: $\psi_{ab}(r_1,r_2)=-\psi_{ab}(r_2,r_1)$

So it must be that $\psi_{ab}(r_1,r_2)=\psi_a(r_1).\psi_b(r_2)-\psi_a(r_2).\psi_b(r_1)$

It is impossible to tell, by looking at probability or energy which particular electron is in which state

If both are in the same quantum state ⇒ a=b & $\psi_{aa}(r_1,r_2)=\psi_{bb}(r_1,r_2)=0$... Pauli Exclusion principle

General Principles for Atomic Structure for n-electron system:

1. n-electron system is stable when its total energy is minimum
2. Only one electron can exist in a particular quantum state in an atom...not 2 or more !
3. Shells & SubShells In Atomic Structure:

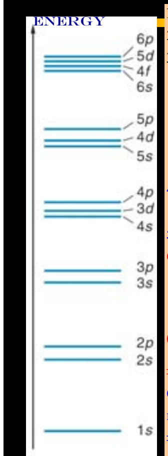
(a) ignore inter-electron repulsion (crude approx.)
(b) think of each electron in a constant "effective" mean Electric field
(Effective field: "Seen" Nuclear charge (+Ze) reduced by partial screening due to other electrons "buzzing" closer (in r) to Nucleus)

Electrons in a SHELL: have same n, are at similar <r> from nucleus, have similar energies

Electons in a SubShell: have same principal quantum number n

- Energy depends on l, those with lower l closer to nucleus, more tightly bound
- all electrons in sub-shell have same energy, with minor dependence on m_l, m_s

Shell & Sub-Shell Energies & Capacity



1. Shell & subshell capacity limited due to Pauli Exclusion principle
2. Shell is made of sub-shells (of same principal quantum # n)
3. Subshell $\Leftarrow (n,l)$, given $n \Rightarrow l = 0,1,2,3,..(n-1)$,

   for any $l \Rightarrow m_l = 0,\pm 1,\pm 2,.. \Rightarrow (2l+1), m_s = \pm\frac{1}{2}$

   $\Rightarrow$ Max. # of electrons in a shell = $\sum$ subshell capacity

   $$N_{MAX} = \sum_{l=0}^{n-1} 2.(2l+1) = 2[1+3+5+..2(n-1)+1] = 2(n)\left[\frac{1}{2}(1+(2n-1))\right] = 2n^2$$

4. The "K" Shell (n=1) holds 2 electrons, "L" Shell (n=1) holds 8 electrons,
   M shell (n=3) holds 18 electrons ......
5. Shell is closed when fully occupied
6. Sub-Shell closed when
   (a) $\sum_i \vec{L}_i = 0, \sum_i \vec{S}_i = 0, \Rightarrow$ Effective charge distribution= symmetric
   (b) Electrons are tightly bound since they "see" large nuclear charge

(c) Because $\sum_i \vec{L}_i = 0 \Rightarrow$ No dipole moment $\Rightarrow$ No ability to attract electrons

$\Rightarrow$ *Inert*! *Noble* gas!

6.Alkali Atoms: have a single "s" electron in outer orbit;
nuclear charge heavily shielded by inner shell electrons
$\Rightarrow$ very small binding energy of "valence"electron
$\Rightarrow$ large orbital radius of valence electron

Electronic Configurations of elements from Lithium to Neon

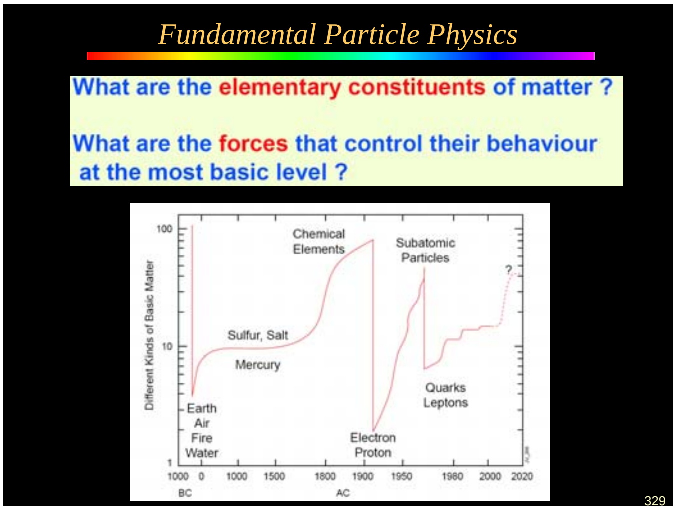
Hund's Rule: Whenever possible
-electron in a sub-shell remain unpaired
- States with spins parallel occupied first
- Because electrons repel when close together
- → electrons in same sub-shell (l) and same spin
  -Must have diff. m_l
  -(very diff. angular distribution)
- Electrons with parallel spin are further apart
  -Than when anti-parallel⇒ lesser E state
  - Get filled first

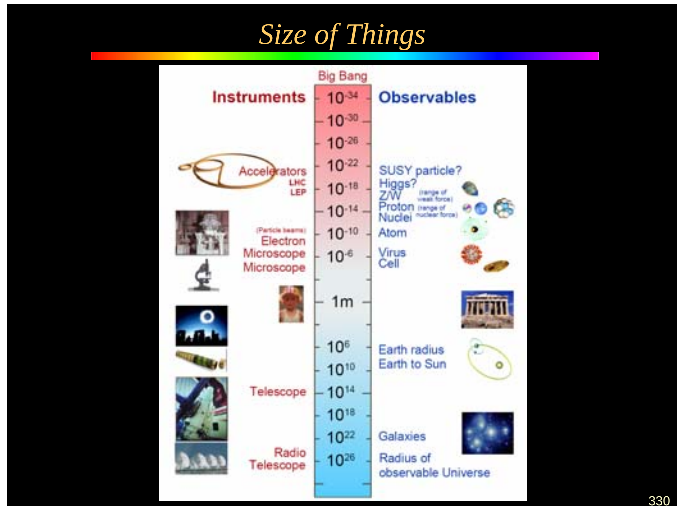
Periodic table is formed

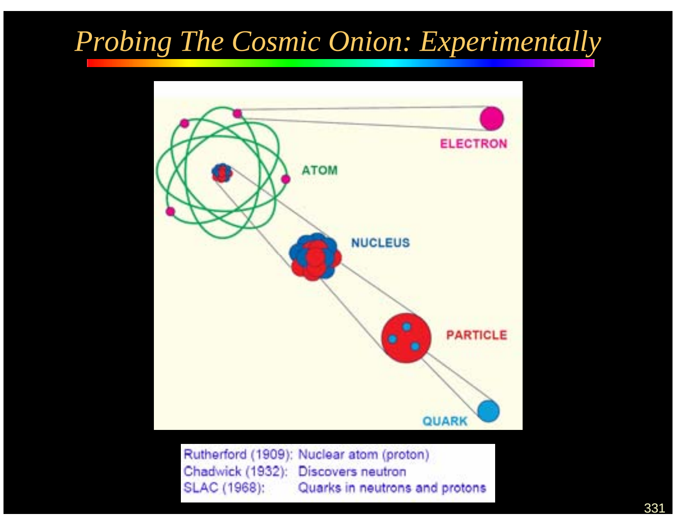
Atom	1s	2s	2p			Electron configuration
Li	↑↓	↑				$1s^2 2s^1$
Be	↑↓	↑↓				$1s^2 2s^2$
B	↑↓	↑↓	↑			$1s^2 2s^2 2p^1$
C	↑↓	↑↓	↑	↑		$1s^2 2s^2 2p^2$
N	↑↓	↑↓	↑	↑	↑	$1s^2 2s^2 2p^3$
O	↑↓	↑↓	↑↓	↑	↑	$1s^2 2s^2 2p^4$
F	↑↓	↑↓	↑↓	↑↓	↑	$1s^2 2s^2 2p^5$
Ne	↑↓	↑↓	↑↓	↑↓	↑↓	$1s^2 2s^2 2p^6$

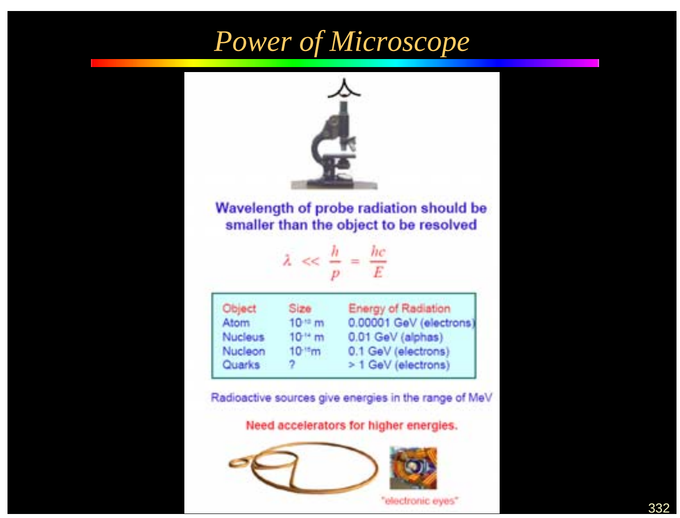
Topics In Particle Physics

- Cosmic Messengers!
  - Dirac, Anderson and the Positron !
    - antimatter
- Fundamental forces in nature
- How elementary particles are produced: Accelerators
- Classification of Particle and How we know this
  - Conservation laws
- Colored Quarks and Quantum Chromodynamics!
- Electroweak theory and Standard model
- The Higgs Particle and Large Hadron Collider
- Beyond the Standard model : Supersymmetry & Strings


Fundamental Particle Physics
What are the elementary constituents of matter ?
What are the forces that control their behaviour at the most basic level ?
Different Kinds of Basic Matter
Chemical Elements
Subatomic Particles
Sulfur, Salt
Mercury
Earth
Air
Fire
Water
Electron
Proton
Quarks
Leptons
?
1000 0 1000 1500 1800 1900 1950 1980 2000 2020
BC
AC
329

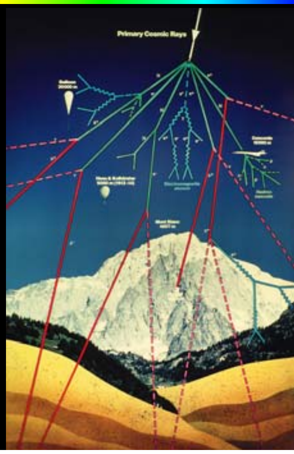

Size of Things
Big Bang
Instruments
Observables
Accelerators
LHC
LEP
Electron Microscope
Microscope
Telescope
Radio Telescope
SUSY particle?
Higgs?
Z/W
Proton
Nuclei
Atom
Virus
Cell
1m
Earth radius
Earth to Sun
Galaxies
Radius of observable Universe
330


Probing The Cosmic Onion: Experimentally
ELECTRON
ATOM
NUCLEUS
PARTICLE
QUARK
Rutherford (1909): Nuclear atom (proton)
Chadwick (1932): Discovers neutron
SLAC (1968): Quarks in neutrons and protons
331


Power of Microscope
Wavelength of probe radiation should be smaller than the object to be resolved
$\lambda << \frac{h}{p} = \frac{hc}{E}$
Object Size Energy of Radiation
Atom 0.00001 GeV (electrons)
Nucleus 0.01 GeV (alphas)
Nucleon 0.1 GeV (electrons)
Quarks ? > 1 GeV (electrons)
Radioactive sources give energies in the range of MeV
Need accelerators for higher energies.
"electronic eyes"
332

Cosmic Messengers

High energy particles bombard the earth at large rate



Discovery of new subatomic particles: Muon and positron !

333

Relativity, Dirac and Anti-matter

$$E^2 = (pc)^2 + (mc^2)^2 \Rightarrow E = \pm\sqrt{(pc)^2 + (mc^2)^2}$$

What does the negative energy solution imply ??!

- Dirac postulated that all negative energy states were filled with electrons. They exert no net force on any thing and thus are unobservable
- Used Pauli Excl. principle to claim that only "holes" in this infinite sea of negative energy states observable
- Holes would act as positive charge with positive energy
  - Anderson's discovery of positron !

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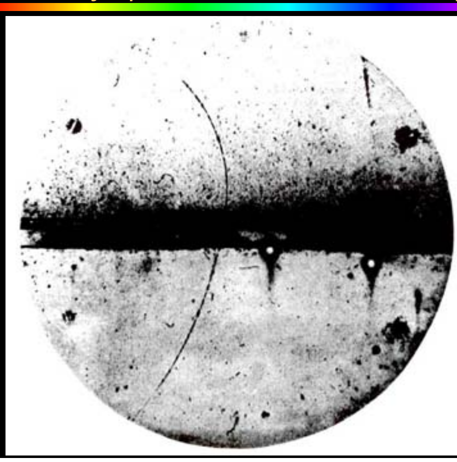
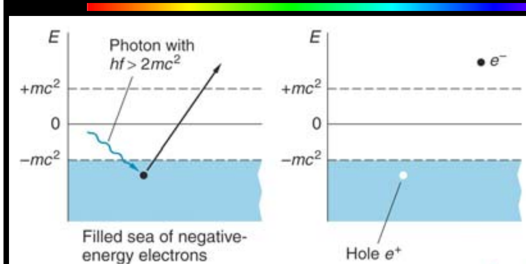
Discovery of Positron From Cosmic Rays

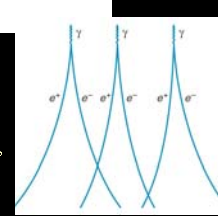


335

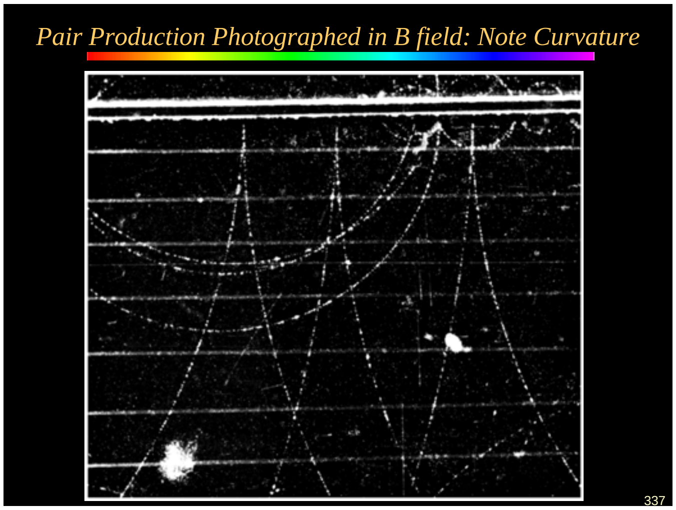
Pair Production: Photoelectric effect with a negative energy electron !

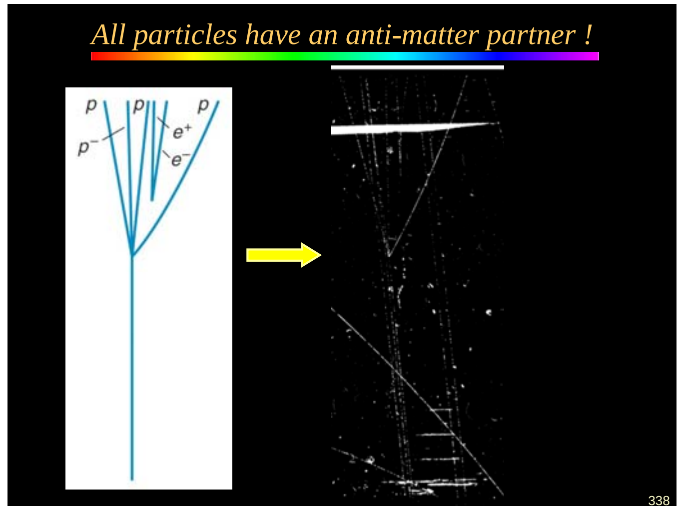


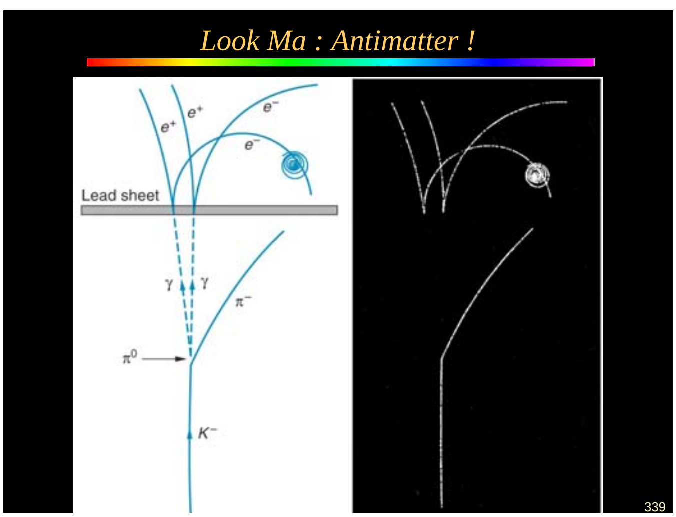
Photon collides with the negative energy Electron and excites it to positive energy state, leaving a "hole" that appears as positron

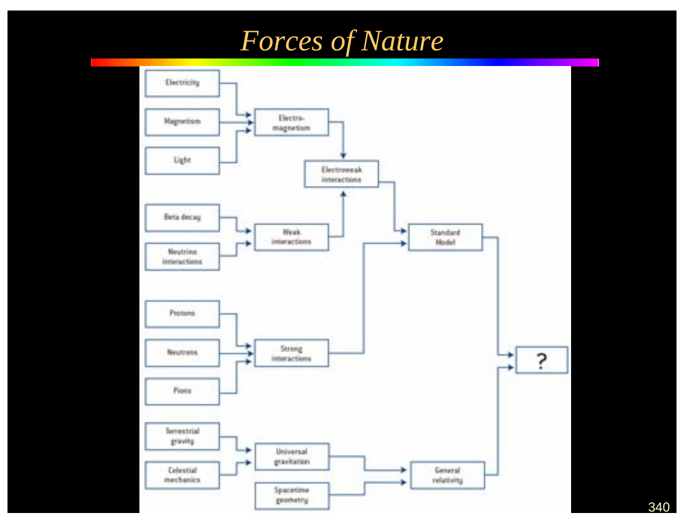


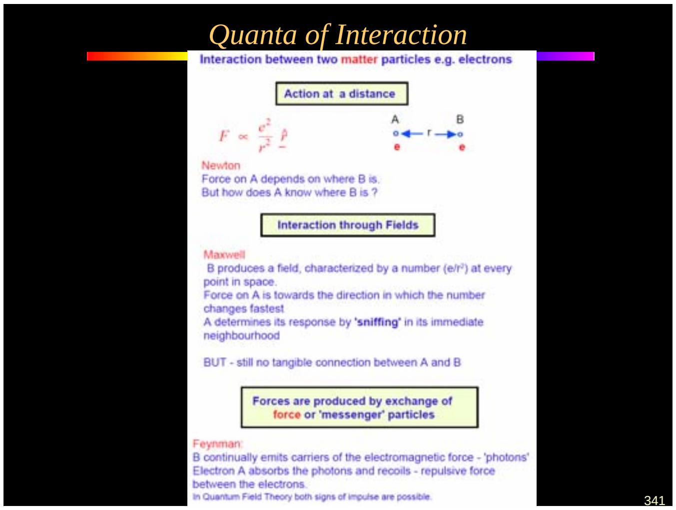
36

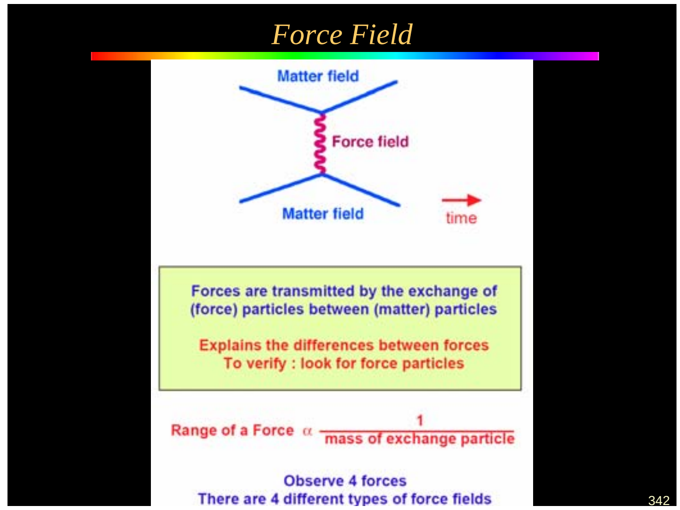

Pair Production Photographed in B field: Note Curvature
337

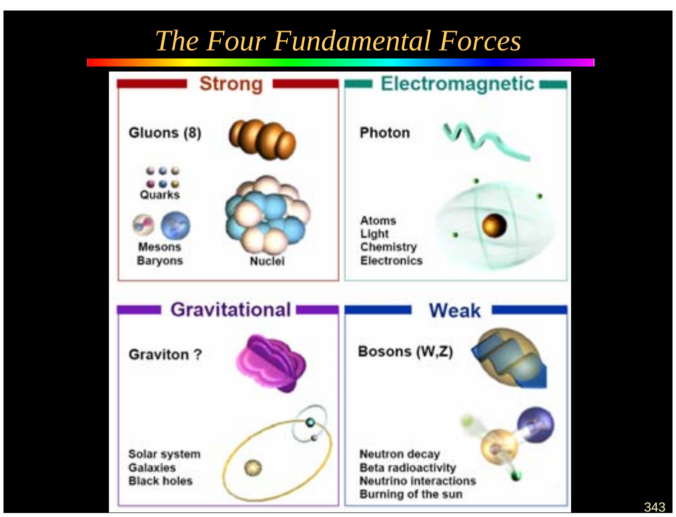

All particles have an anti-matter partner !
p
p
p
p^-
e^+
e^-
338


Look Ma : Antimatter !
e^+
e^+
e^-
e^-
Lead sheet
γ
γ
π^-
π^0
K^-
339


Forces of Nature
Electricity
Magnetism
Light
Electro-magnetism
Electroweak interactions
Beta decay
Neutrino interactions
Weak interactions
Standard Model
Protons
Neutrons
Pions
Strong interactions
?
Terrestrial gravity
Celestial mechanics
Universal gravitation
Spacetime geometry
General relativity
340







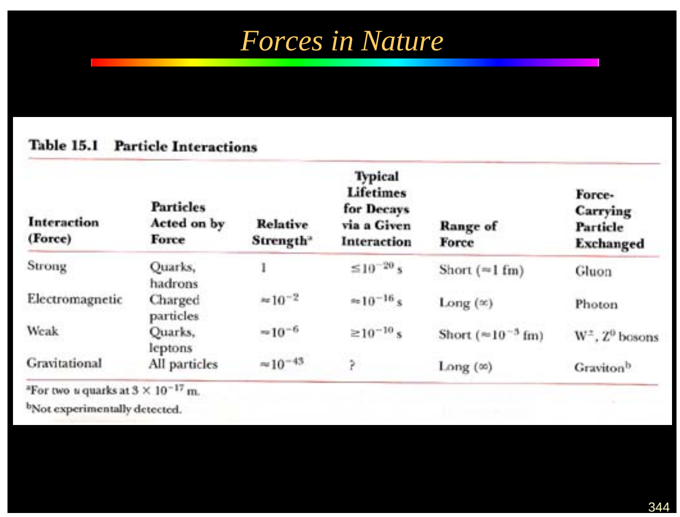
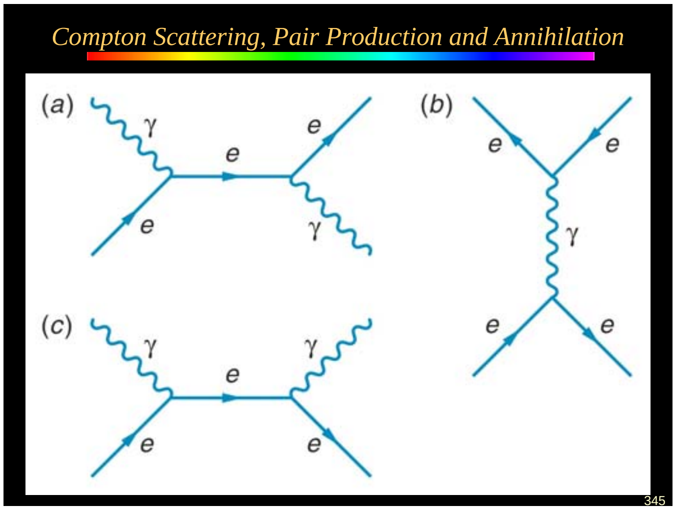
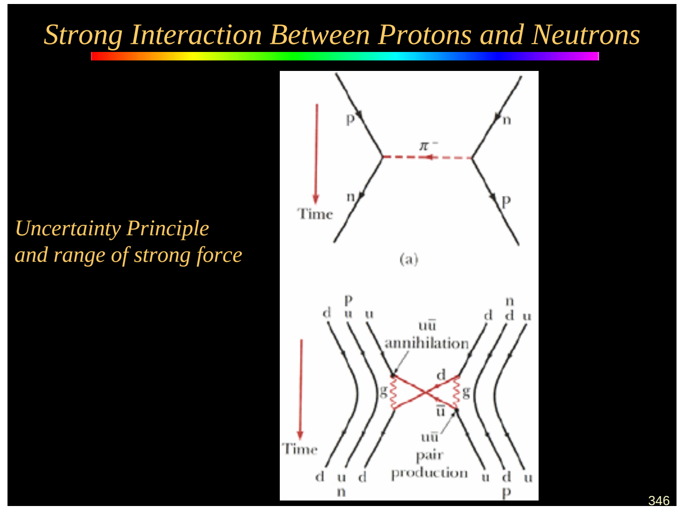


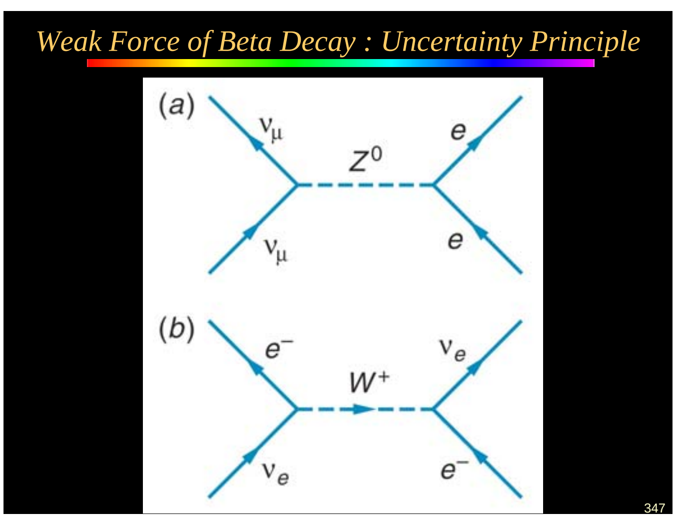
Table 15.1 Particle Interactions

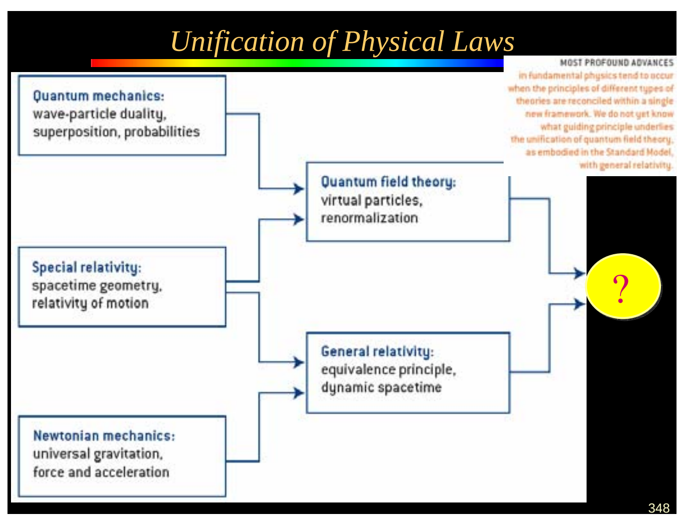
Interaction (Force)	Particles Acted on by Force	Relative Strength[a]	Typical Lifetimes for Decays via a Given Interaction	Range of Force	Force-Carrying Particle Exchanged
Strong	Quarks, hadrons	1	$\leq 10^{-20}$ s	Short ($\approx$1 fm)	Gluon
Electromagnetic	Charged particles	$\approx 10^{-2}$	$\approx 10^{-16}$ s	Long (∞)	Photon
Weak	Quarks, leptons	$\approx 10^{-6}$	$\geq 10^{-10}$ s	Short ($\approx 10^{-3}$ fm)	$W^{\pm}$, Z^0 bosons
Gravitational	All particles	$\approx 10^{-43}$	?	Long (∞)	Graviton[b]

[a]For two u quarks at 3×10^{-17} m.
[b]Not experimentally detected.


Compton Scattering, Pair Production and Annihilation
(a)
γ
e
e
e
γ
(b)
e
e
γ
e
e
(c)
γ
e
γ
e
e
345


Strong Interaction Between Protons and Neutrons
Uncertainty Principle
and range of strong force
p
n
π⁻
n
p
Time
(a)
uū
annihilation
uū
pair
production
Time
346


Weak Force of Beta Decay : Uncertainty Principle
(a)
νμ
Z0
e
νμ
e
(b)
e⁻
W+
νe
νe
e⁻
347


Unification of Physical Laws
MOST PROFOUND ADVANCES
in fundamental physics tend to occur when the principles of different types of theories are reconciled within a single new framework. We do not yet know what guiding principle underlies the unification of quantum field theory, as embodied in the Standard Model, with general relativity.
Quantum mechanics:
wave-particle duality,
superposition, probabilities
Special relativity:
spacetime geometry,
relativity of motion
Newtonian mechanics:
universal gravitation,
force and acceleration
Quantum field theory:
virtual particles,
renormalization
General relativity:
equivalence principle,
dynamic spacetime
?
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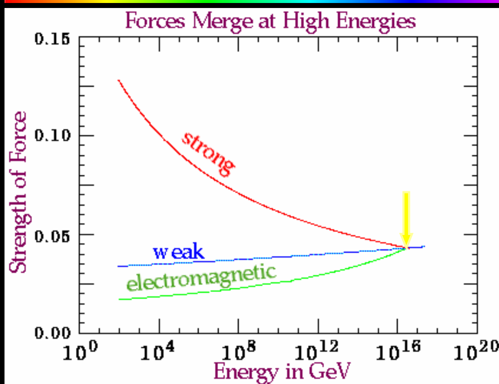
Unification of Forces



Analogy: Are steam, water and ice manifestation of the same thing ?

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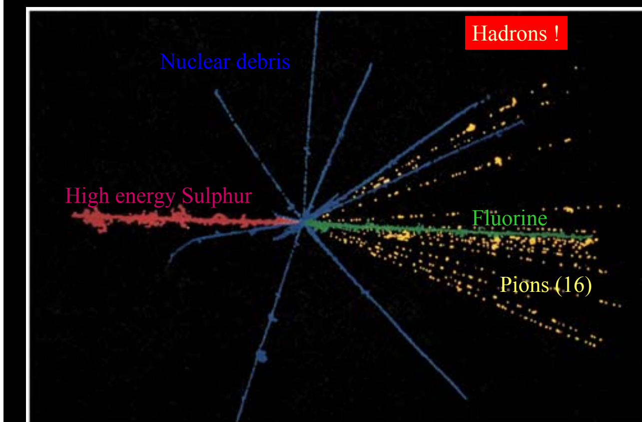
Cosmic Ray Smashing Through Nucleus



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Particle Categories: Hadrons & Leptons

Category	Particle Name	Symbol	Anti-particle	Mass (MeV/c^2)	B	L_e	L_μ	L_τ	S	Lifetime (s)	Principal Decay Modes*
Leptons	Electron	e^-	e^+	0.511	0	+1	0	0	0	Stable	
	Electron-neutrino	ν_e	$\bar{\nu}_e$	$<2.8 \times 10^{-6}$	0	+1	0	0	0	Stable	
	Muon	μ^-	μ^+	105.7	0	0	+1	0	0	2.19×10^{-6}	$e^- \bar{\nu}_e \nu_\mu$
	Muon-neutrino	ν_μ	$\bar{\nu}_\mu$	$<3.5 \times 10^{-6}$	0	0	+1	0	0	Stable	
	Tau	τ^-	τ^+	1784	0	0	0	+1	0	3.3×10^{-13}	$\mu^- \bar{\nu}_\mu \nu_\tau$, $e^- \bar{\nu}_e \nu_\tau$
	Tau-neutrino	ν_τ	$\bar{\nu}_\tau$	$<8.4 \times 10^{-6}$	0	0	0	+1	0	Stable	
Hadrons											
Mesons	Pion	π^+	π^-	139.6	0	0	0	0	0	2.60×10^{-8}	$\mu^+ \nu_\mu$
		π^0	Self	135.0	0	0	0	0	0	0.83×10^{-16}	2γ
	Kaon	K^+	K^-	493.7	0	0	0	0	+1	1.24×10^{-8}	$\mu^+ \nu_\mu$ $\pi^+ \pi^0$
		K^0_S	$\bar{K}^0_S$	497.7	0	0	0	0	+1	0.89×10^{-10}	$\pi^+ \pi^-$ $2\pi^0$
		K^0_L	$\bar{K}^0_L$	497.7	0	0	0	0	+1	5.2×10^{-8}	$\pi^\pm e^\mp \bar{\nu}_e$ $3\pi^0$ $\pi^\pm \mu^\mp \bar{\nu}_\mu$
	Eta	η	Self	548.8	0	0	0	0	0	$<10^{-18}$	2γ, $3\pi^0$
		η'	Self	958	0	0	0	0	0	2.2×10^{-21}	$\eta \pi^+ \pi^-$
Baryons	Proton	p	$\bar{p}$	938.3	+1	0	0	0	0	Stable	
	Neutron	n	$\bar{n}$	939.6	+1	0	0	0	0	624	$p e^- \bar{\nu}_e$
	Lambda	Λ^0	$\bar{\Lambda}^0$	1115.6	+1	0	0	0	−1	2.6×10^{-10}	$p\pi^-$, $n\pi^0$
	Sigma	Σ^+	$\bar{\Sigma}^-$	1189.4	+1	0	0	0	−1	0.80×10^{-10}	$p\pi^0$, $n\pi^+$
		Σ^0	$\bar{\Sigma}^0$	1192.5	+1	0	0	0	−1	6×10^{-20}	$\Lambda^0 \gamma$
		Σ^-	$\bar{\Sigma}^+$	1197.3	+1	0	0	0	−1	1.5×10^{-10}	$n\pi^-$
	Delta	Δ^{++}	$\bar{\Delta}$	1230	+1	0	0	0	0	6×10^{-24}	$p\pi^+$
		Δ^+	$\bar{\Delta}^-$	1231	+1	0	0	0	0	6×10^{-24}	$p\pi^0$, $n\pi^+$
		Δ^0	$\bar{\Delta}^0$	1232	+1	0	0	0	0	6×10^{-24}	$n\pi^0$, $p\pi^-$
		Δ^-	$\bar{\Delta}^+$	1234	+1	0	0	0	0	6×10^{-24}	$n\pi^-$
	Xi	Ξ^0	$\bar{\Xi}^0$	1315	+1	0	0	0	−2	2.9×10^{-10}	$\Lambda^0 \pi^0$
		Ξ^-	Ξ^+	1321	+1	0	0	0	−2	1.64×10^{-10}	$\Lambda^0 \pi^-$
	Omega	Ω^-	Ω^+	1672	+1	0	0	0	−3	0.82×10^{-10}	$\Xi^- \pi^0$, $\Xi^0 \pi^-$, $\Lambda^0 K^-$

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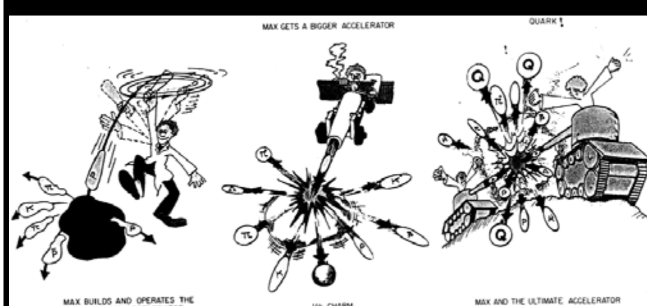
Particle Accelerators

$$\lambda = \frac{h}{p} \quad , \quad E = \sqrt{(pc)^2 + \left(mc^2\right)^2}$$



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Relativistic Force & Acceleration

$$\vec{p} = \frac{m\vec{u}}{\sqrt{1-(u/c)^2}} = \gamma m \vec{u}$$

Relativistic Force And Acceleration

$$\vec{F} = \frac{d\vec{p}}{dt} = \frac{d}{dt}\left(\frac{m\vec{u}}{\sqrt{1-(u/c)^2}}\right)$$

$$F = \left[\frac{m}{\left(1-(u/c)^2\right)^{3/2}}\right]\frac{du}{dt}$$: Relativistic Force

Since Acceleration $\vec{a} = \frac{d\vec{u}}{dt}$, [rate of change of velocity]

$$\Rightarrow \vec{a} = \frac{\vec{F}}{m}\left[1-(u/c)^2\right]^{3/2}$$

Reason why you cant quite get up to the speed of light no matter how hard you try!

Note: As $u/c \to 1$, $\vec{a} \to 0$!!!!
Its harder to accelerate when you get closer to speed of light

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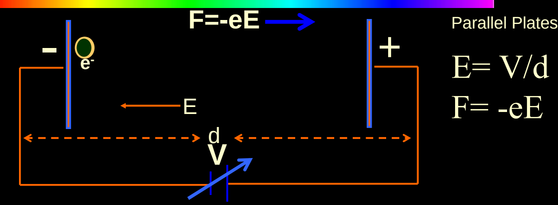
Linear Particle Accelerator : Parallel Plates With Potential Difference



Parallel Plates

$E = V/d$

$F = -eE$

Charged particle q moves in straight line in a uniform electric field $\vec{E}$ with speed $\vec{u}$ accelarates under force $\vec{F}=q\vec{E}$

$$|\vec{a}| = \left|\frac{d\vec{u}}{dt}\right| = \left|\frac{\vec{F}}{m}\right|\left(1-\frac{u^2}{c^2}\right)^{3/2} = \left|\frac{q\vec{E}}{m}\right|\left(1-\frac{u^2}{c^2}\right)^{3/2}$$

larger the potential difference V across plates, larger the force on particle

Under force, work is done on the particle, it gains Kinetic energy

New Unit of Energy

1 eV = 1.6×10^{-19} Joules
1 MeV = 1.6×10^{-13} Joules
1 GeV = 1.6x10-10 Joules

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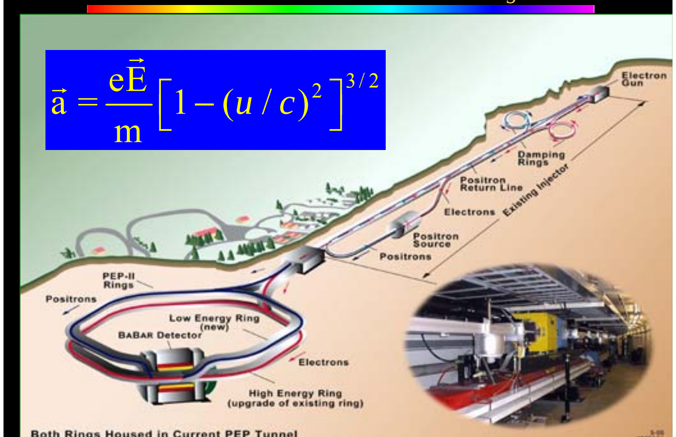
Linear Accelerator : 50 Billion Volts Accelerating Potential

$$\vec{a} = \frac{e\vec{E}}{m}\left[1-(u/c)^2\right]^{3/2}$$



PEP-II accelerator schematic and tunnel view

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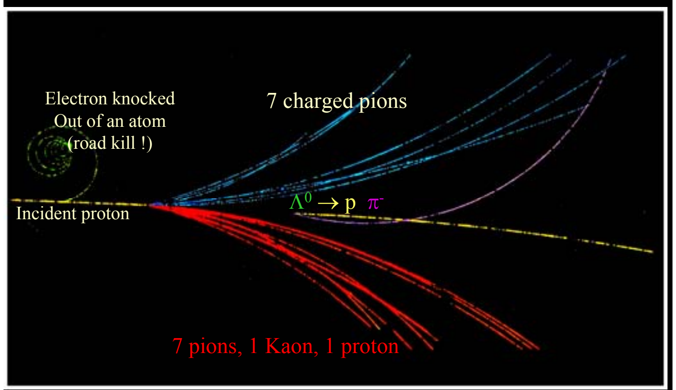
Discovery of Quarks: Constituents of Proton

High Energy Proton smashing into a Proton Rich Target



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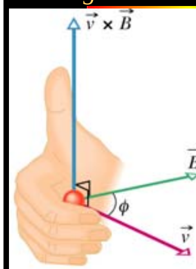
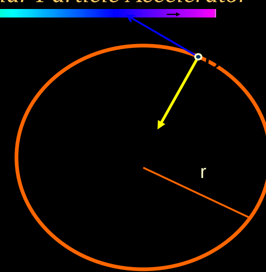
Magnetic Confinement & Circular Particle Accelerator



Classically

$$F = m\frac{v^2}{r}$$

$$qvB = m\frac{v^2}{r}$$



$$F = \frac{dp}{dt} = \frac{d(\gamma m u)}{dt} = \gamma m \frac{du}{dt} = quB$$

$$\frac{du}{dt} = \frac{u^2}{r} \text{ (Centripetal accelaration)}$$

$$\gamma m \frac{u^2}{r} = quB \quad \Rightarrow \gamma m u = qBr \Rightarrow p = qBr$$

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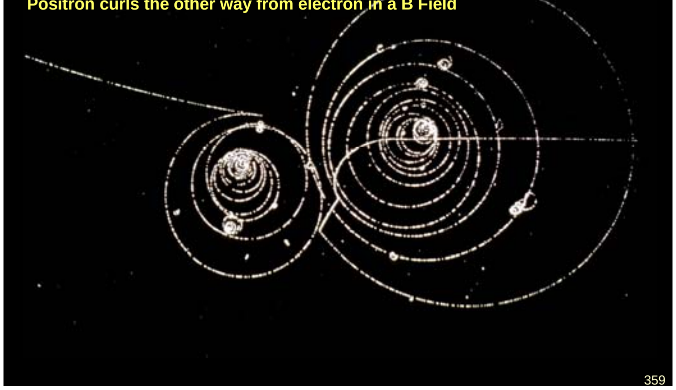
Charged Form of Matter & Anti-Matter in a B Field

Antimatter form of electron = Positron (e⁺)
Same Mass but opposite Charge
Positron curls the other way from electron in a B Field



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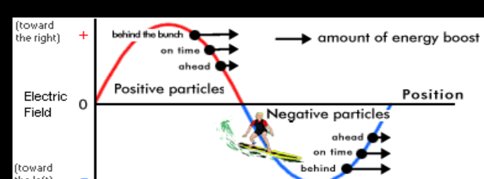
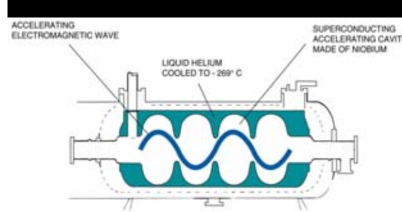
Accelerating Electrons Thru RF Cavities





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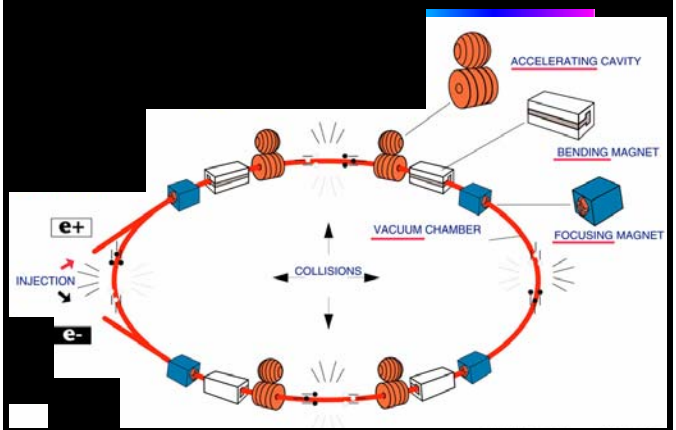
A Circular Accelerator : Using B Field to Confine the electron and RF cavity to power it



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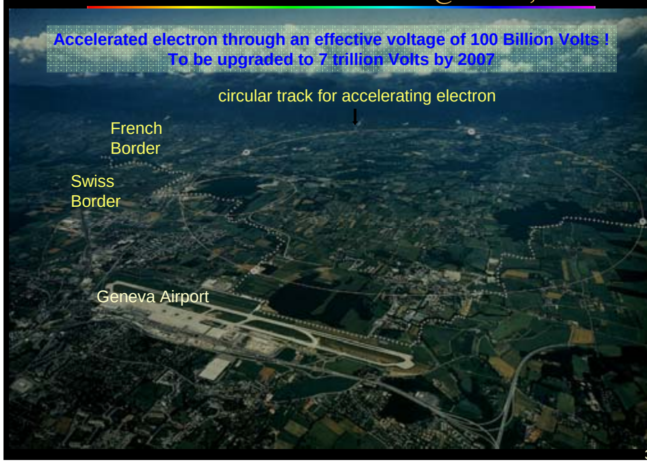
Circular Particle Accelerator: LEP @ CERN, Geneve



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Inside A Circular Particle Accelerator Tunnel : Monorail !

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In Tunnel 150m underground, 27km ring of Magnets Keep electron in Circular Orbit

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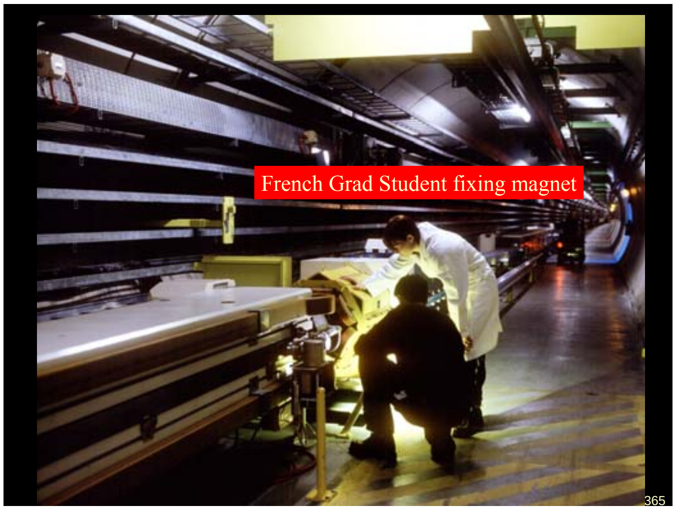
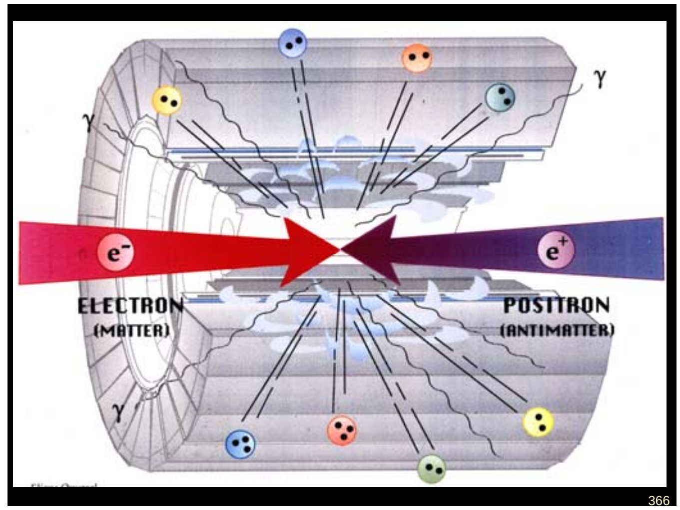
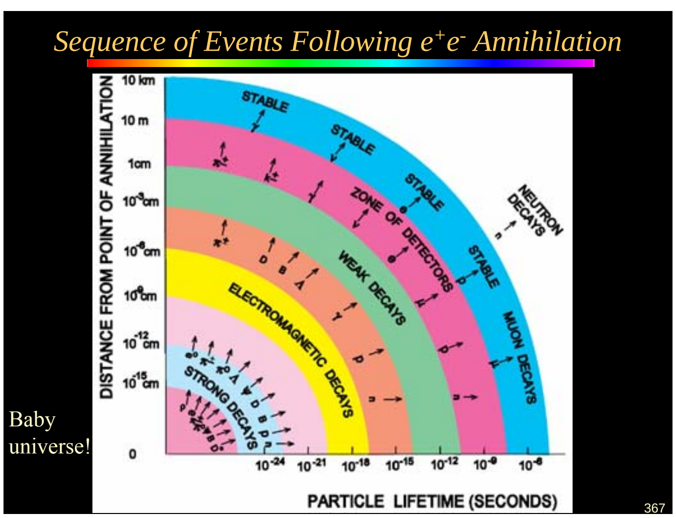

French Grad Student fixing magnet
365


γ
γ
γ
e⁻
e⁺
ELECTRON
(MATTER)
POSITRON
(ANTIMATTER)
366


Sequence of Events Following e⁺e⁻ Annihilation
DISTANCE FROM POINT OF ANNIHILATION
10 km
10 m
1cm
10⁻³cm
10⁻⁶cm
10⁻⁹cm
10⁻¹²cm
10⁻¹⁵cm
0
STABLE
STABLE
STABLE
STABLE
NEUTRON DECAYS
ZONE OF DETECTORS
WEAK DECAYS
MUON DECAYS
ELECTROMAGNETIC DECAYS
STRONG DECAYS
10⁻²⁴
10⁻²¹
10⁻¹⁸
10⁻¹⁵
10⁻¹²
10⁻⁹
10⁻⁶
PARTICLE LIFETIME (SECONDS)
Baby universe!
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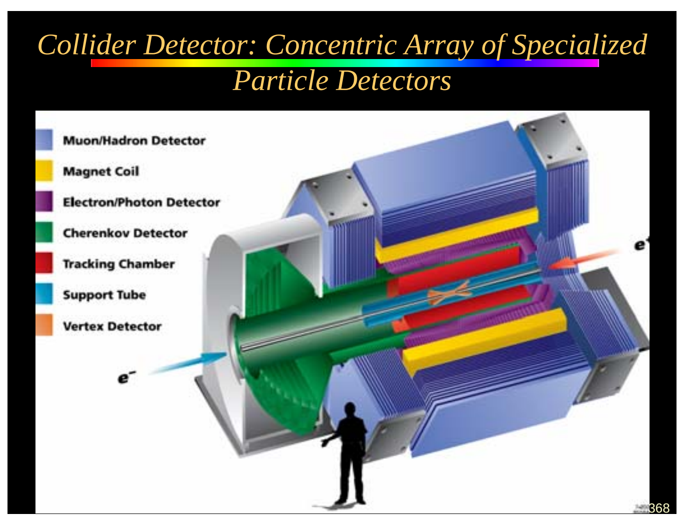
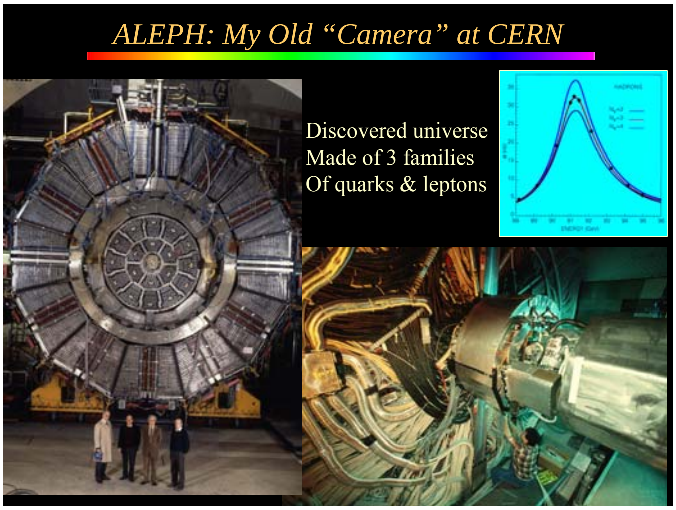
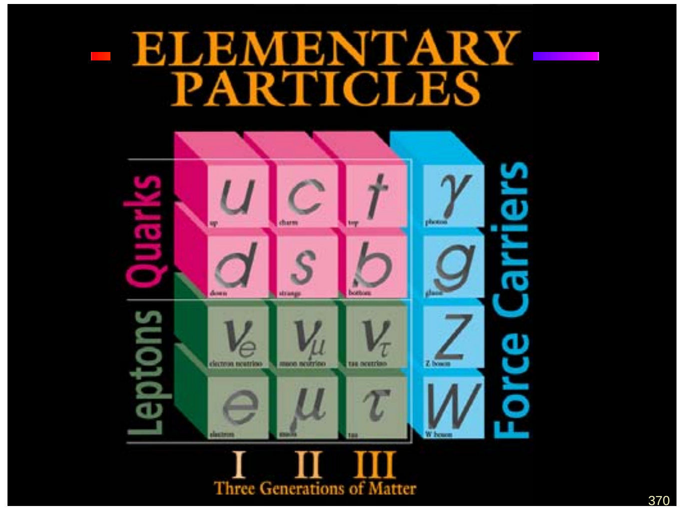
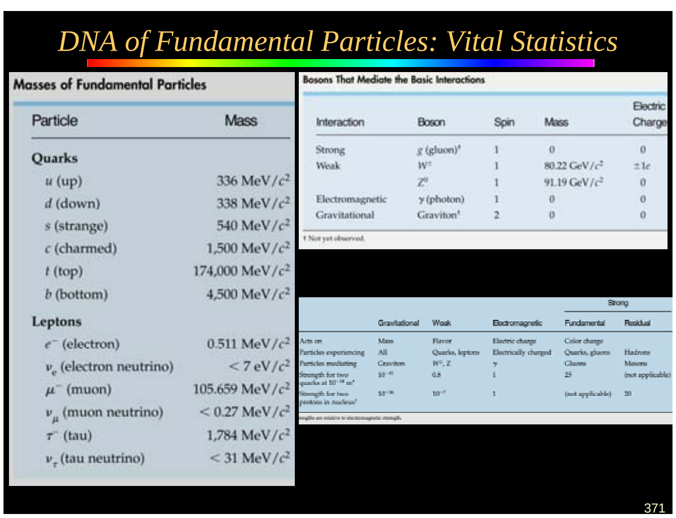

Collider Detector: Concentric Array of Specialized Particle Detectors
Muon/Hadron Detector
Magnet Coil
Electron/Photon Detector
Cherenkov Detector
Tracking Chamber
Support Tube
Vertex Detector
e⁻
e⁺
368







Masses of Fundamental Particles

Particle	Mass
Quarks	
u (up)	336 MeV/c^2
d (down)	338 MeV/c^2
s (strange)	540 MeV/c^2
c (charmed)	1,500 MeV/c^2
t (top)	174,000 MeV/c^2
b (bottom)	4,500 MeV/c^2
Leptons	
e^- (electron)	0.511 MeV/c^2
ν_e (electron neutrino)	< 7 eV/c^2
μ^- (muon)	105.659 MeV/c^2
ν_μ (muon neutrino)	< 0.27 MeV/c^2
τ^- (tau)	1,784 MeV/c^2
ν_τ (tau neutrino)	< 31 MeV/c^2

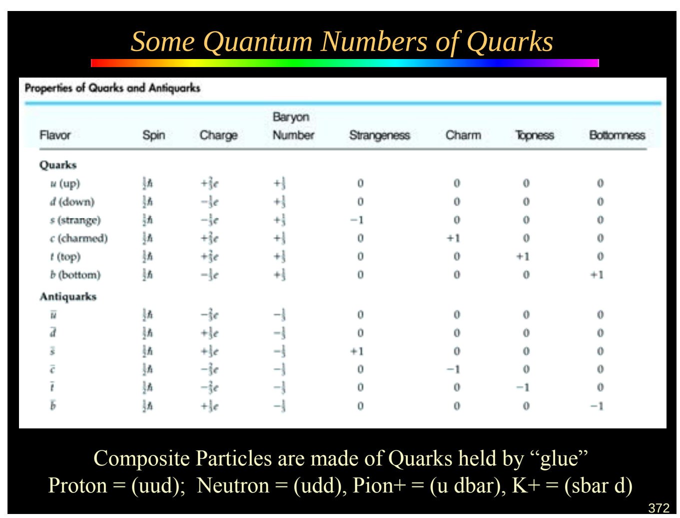
Bosons That Mediate the Basic Interactions

Interaction	Boson	Spin	Mass	Electric Charge
Strong	g (gluon)†	1	0	0
Weak	$W^\pm$	1	80.22 GeV/c^2	±1e
	Z^0	1	91.19 GeV/c^2	0
Electromagnetic	γ (photon)	1	0	0
Gravitational	Graviton†	2	0	0

† Not yet observed.

	Gravitational	Weak	Electromagnetic	Strong: Fundamental	Strong: Residual
Acts on	Mass	Flavor	Electric charge	Color charge	
Particles experiencing	All	Quarks, leptons	Electrically charged	Quarks, gluons	Hadrons
Particles mediating	Graviton	$W^\pm$, Z	γ	Gluons	Mesons
Strength for two quarks at 10^{-18} m*	10^{-41}	0.8	1	25	(not applicable)
Strength for two protons in nucleus*	10^{-36}	10^{-7}	1	(not applicable)	20

...ngths are relative to electromagnetic strength.



Properties of Quarks and Antiquarks

Flavor	Spin	Charge	Baryon Number	Strangeness	Charm	Topness	Bottomness
Quarks							
u (up)	$\frac{1}{2}\hbar$	$+\frac{2}{3}e$	$+\frac{1}{3}$	0	0	0	0
d (down)	$\frac{1}{2}\hbar$	$-\frac{1}{3}e$	$+\frac{1}{3}$	0	0	0	0
s (strange)	$\frac{1}{2}\hbar$	$-\frac{1}{3}e$	$+\frac{1}{3}$	−1	0	0	0
c (charmed)	$\frac{1}{2}\hbar$	$+\frac{2}{3}e$	$+\frac{1}{3}$	0	+1	0	0
t (top)	$\frac{1}{2}\hbar$	$+\frac{2}{3}e$	$+\frac{1}{3}$	0	0	+1	0
b (bottom)	$\frac{1}{2}\hbar$	$-\frac{1}{3}e$	$+\frac{1}{3}$	0	0	0	+1
Antiquarks							
$\bar{u}$	$\frac{1}{2}\hbar$	$-\frac{2}{3}e$	$-\frac{1}{3}$	0	0	0	0
$\bar{d}$	$\frac{1}{2}\hbar$	$+\frac{1}{3}e$	$-\frac{1}{3}$	0	0	0	0
$\bar{s}$	$\frac{1}{2}\hbar$	$+\frac{1}{3}e$	$-\frac{1}{3}$	+1	0	0	0
$\bar{c}$	$\frac{1}{2}\hbar$	$-\frac{2}{3}e$	$-\frac{1}{3}$	0	−1	0	0
$\bar{t}$	$\frac{1}{2}\hbar$	$-\frac{2}{3}e$	$-\frac{1}{3}$	0	0	−1	0
$\bar{b}$	$\frac{1}{2}\hbar$	$+\frac{1}{3}e$	$-\frac{1}{3}$	0	0	0	−1

Some Open Questions In Particle Physics

- How do particles get the masses they have?
  - Physicists believe particle masses are generated by interaction with a mysterious field that permeates the entire universe
    - Stronger the particle interacts with the field, the more massive it is
  - It could be a new fundamental field called HIGGS field
  - Or it may be a composite object made of new particles (techniquarks) tightly bound together by a new force (technicolor!)
- Whatever the nature of this mass mechanism, odds are solid that it will be produced when beams of protons with energy of 7 TRILLION eV collide at the LHC accelerator
  - Could be seen as one or many new Higgs particle
- If the Universe is made of >4 dimensions, some of the extra dimensions could "pop" out in these violent collisions
- Little blackholes could also be produced in these high energy interactions….and the detector will catch them in action !!

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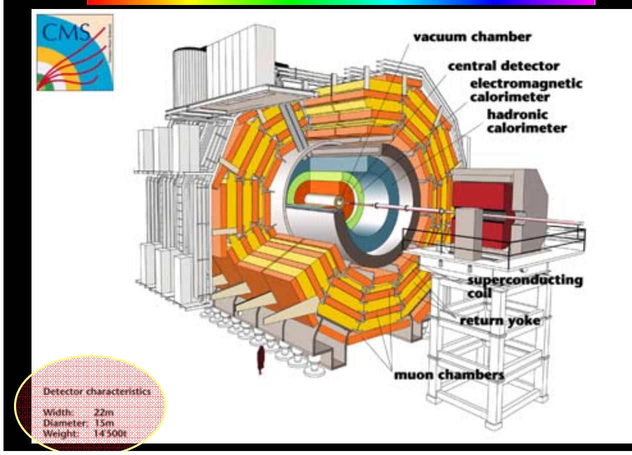
Hunting for Higgs Particle With CMS Detector



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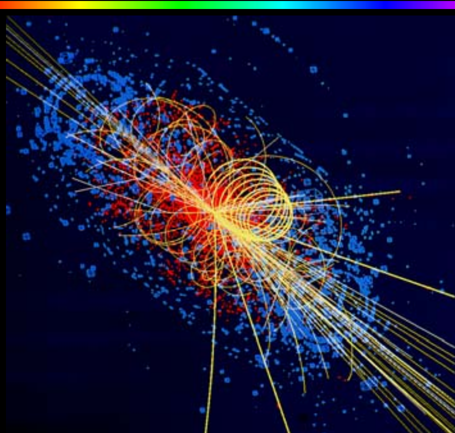
Setting the Trap for Higgs Particle



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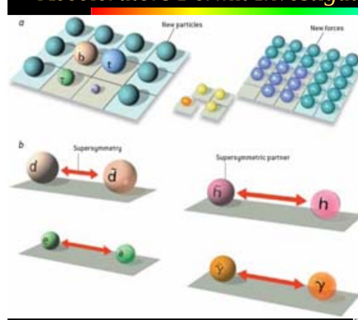
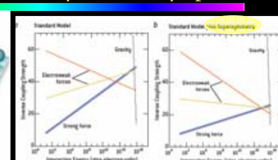
Accelerators Permit Investigations of Fabric of Spacetime





Is String theory the ultimate answer?

Dr. Brian Wecht will tell you about String theory next week