PHYS 3313 – Section 001
Lecture #11

Monday, Oct. 8, 2012

Dr. Jaehoon Yu

- Midterm Exam Review

Announcements

- Quiz results
  - Class average: 40.4/60
    - Equivalent to: 67.3/100
  - How did you do last time?: 27.4/100
  - Top score: 60/60
- Mid-term exam
  - In class on Wednesday, Oct. 10, in PKH107
  - Covers: CH1.1 to CH5.8
  - Style: Mixture of multiple choices and free response problems which are more heavily weighted
  - Mid-term exam constitutes 20% of the total
  - **Please do NOT miss the exam! You will get an F if you miss it.**
- Homework #4
  - End of chapter problems on CH5: 8, 10, 16, 24, 26, 36 and 47
  - Due: Wednesday, Oct. 17
- Colloquium this week
  - 4pm, Wednesday, Oct. 10, SH101
  - Dr. Marco Nadeli of UNT

Physics Department
The University of Texas at Arlington
COLLOQUIUM

First principles theory of charge mobility and heat transport in graphene-based systems.

Dr. Marco Nardelli

Department of Physics and Department of Chemistry
University of North Texas

4:00 pm Wednesday October 10, 2012 room 101 SH

Abstract:

Graphitic nanostructures such as graphene, nanoribbons and carbon nanotubes have shown to be potential candidates for device applications that may revolutionize the future of nanoelectronics. However, very little is known about their thermal properties. In fact, understanding the heat transfer at the nanoscale is essential for optimal thermal management, heat removal in device applications and the design of novel thermoelectric materials. In this talk I will discuss the development of a theoretical and computational tool-set for the first principles determination of charge mobility and heat transport in novel carbon-based materials and devices for anoelectronic applications. In particular, I will describe the effect of electron-phonon interactions in mono- and bi-layer graphene in determining the intrinsic carrier-phonon scattering properties of this material and thus the ultimate limit of any electronic device; I will consider the thermal and thermoelectric behavior of graphene nanoribbons, and show how the geometry of the systems can be exploited to design unique behaviors at the nanoscale, and, finally, I will briefly discuss the thermal properties of the graphene/SiC interface, since understanding of the heat transfer properties is essential for optimal thermal management and heat removal in device applications.

Refreshments will be served at 3:30p.m in the Physics Lounge

Triumph of Classical Physics: The Conservation Laws

- **Conservation of energy**: The total sum of energy (in all its forms) is conserved in all interactions.
- **Conservation of linear momentum**: In the absence of external forces, linear momentum is conserved in all interactions.
- **Conservation of angular momentum**: In the absence of external torque, angular momentum is conserved in all interactions.
- **Conservation of charge**: Electric charge is conserved in all interactions.

Isaac Newton (1642-1727)

Three laws describing the relationship between mass and acceleration.

- **Newton's first law** (*law of inertia*): An object in motion with a constant velocity will continue in motion unless acted upon by some net external force.
- **Newton's second law**: Introduces force (F) as responsible for the the change in linear momentum (p):

$$\vec{F} = m\vec{a} \quad \text{or} \quad \vec{F} = \frac{d\vec{p}}{dt}$$

- **Newton's third law** (*law of action and reaction*): The force exerted by body 1 on body 2 is equal in magnitude and opposite in direction to the force that body 2 exerts on body 1.

$$\vec{F}_{21} = -\vec{F}_{12}$$

Maxwell's Equations for EM Radiation

- In the absence of dielectric or magnetic materials, the four equations developed by Maxwell are:

$$\oint \vec{E} \cdot d\vec{A} = \frac{Q_{encl}}{\varepsilon_0}$$

Gauss' Law for electricity

A generalized form of Coulomb's law relating electric field to its sources, the electric charge

$$\oint \vec{B} \cdot d\vec{A} = 0$$

Gauss' Law for magnetism

A magnetic equivalent of Coulomb's law relating magnetic field to its sources. This says there are no magnetic monopoles.

$$\oint \vec{E} \cdot d\vec{l} = -\frac{d\Phi_B}{dt}$$

Faraday's Law

An electric field is produced by a changing magnetic field

$$\oint \vec{B} \cdot d\vec{l} = \mu_0 I_{encl} + \mu_0 \varepsilon_0 \frac{d\Phi_E}{dt}$$

Generalized Ampére's Law

A magnetic field is produced by an electric current or by a changing electric field

The Laws of Thermodynamics

- **First law**: The change in the internal energy ΔU of a system is equal to the heat Q added to a system plus the work W done by the system ➔ Generalization of conservation of energy including heat

$$\Delta U = Q + W$$

- **Second law**: It is not possible to convert heat completely into work without some other change taking place.
- **The "zeroth" law**: Two systems in thermal equilibrium with a third system are in thermal equilibrium with each other.
  - Explicitly stated only in early 20th century
- **Third law**: It is not possible to achieve an absolute zero temperature.

Primary Results of Statistical Interpretation

- Culminates in the **ideal gas equation** for *n* moles of a "simple" gas:

$$PV = nRT$$

(where R is the ideal gas constant, 8.31 J/mol · K)

- Average molecular kinetic energy directly related to absolute temperature
- **Internal energy** U directly related to the average molecular kinetic energy
- Internal energy equally distributed among the number of degrees of freedom (f) of the system

$$U = nN_A \langle K \rangle = \frac{f}{2} nRT$$

(N_A = Avogadro's Number)

- And many others

Particles vs. Waves

- Two distinct phenomena describing physical interactions
  - Both required Newtonian mass
  - Particles in the form of point masses and waves in the form of perturbation in a mass distribution, i.e., a material medium
  - The distinctions are observationally quite clear; however, not so for the case of visible light
  - Thus by the 17th century begins the major disagreement concerning the nature of light

The Nature of Light

- Isaac Newton promoted the corpuscular (particle) theory
  - Published a book "Optiks" in 1704
  - Particles of light travel in straight lines or rays
  - Explained sharp shadows
  - Explained reflection and refraction
- Christian Huygens (1629 -1695) promoted the wave theory
  - Presented theory in 1678
  - Light propagates as a wave of concentric circles from the point of origin
  - Explained reflection and refraction
  - Did not explain sharp shadows
- Thomas Young (1773 -1829) & Augustin Fresnel (1788 – 1829) ➔ Showed in 1802 and afterward that light clearly behaves as wave through two slit interference and other experiments
- In 1850 Foucault showed that light travel slowly in medium, the final blow to the corpuscular theory in explaining refraction

The Electromagnetic Spectrum

- Visible light covers only a small range of the total electromagnetic spectrum
- All electromagnetic waves travel in vacuum with a speed *c* given by:

$$c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}} = \lambda f$$

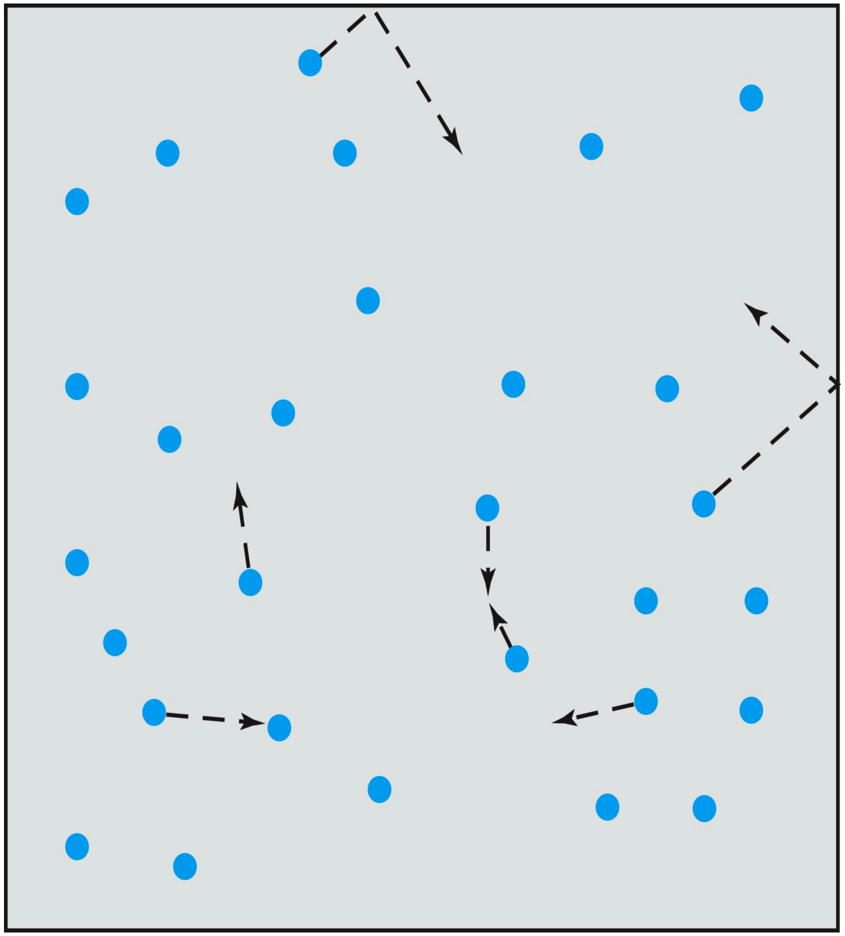
(where μ_0 and ε_0 are the respective permeability and permittivity of "free" space)

Also in the Modern Context…

- The three fundamental forces are introduced
  - **Gravitational**: $\vec{F}_g = -G\frac{m_1 m_2}{r^2}\hat{r}$
    - Responsible for planetary motions, holding things on the ground, etc
  - **Electroweak**
    - **Weak**: Responsible for nuclear beta decay and effective only over distances of ~10^{-15} m
    - **Electromagnetic**: Responsible for all non-gravitational interactions, such as all chemical reactions, friction, tension….
    - $\vec{F}_C = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2}\hat{r}$ (Coulomb force)
  - **Strong**: Responsible for "holding" the nucleus together and effective less than ~10^{-15} m

Relevance of Gas Concept to Atoms

- The idea of gas (17th century) as a collection of small particles bouncing around with kinetic energy enabled concept of small, unseen objects
- This concept formed the bases of existence something small that make up matter



The Atomic Theory of Matter

- Concept initiated by Democritus and Leucippus (~450 B.C.) (first to us the Greek *atomos*, meaning "indivisible")
- In addition to fundamental contributions by Boyle, Charles, and Gay-Lussac, Proust (1754 – 1826) proposes the **law of definite proportions**
- Dalton advances the **atomic theory of matter** to explain the law of definite proportions
- Avogadro proposes that all gases at the same temperature, pressure, and volume contain the ***same number of molecules (atoms)***; viz. 6.02×10^{23} atoms
- Cannizzaro (1826 – 1910) makes the distinction between atoms and molecules advancing the ideas of Avogadro.
- Maxwell derives the speed distribution of atoms in a gas
- Robert Brown (1753 – 1858) observes microscopic "random" motion of suspended grains of pollen in water
- Einstein in the 20th century explains this random motion using atomic theory

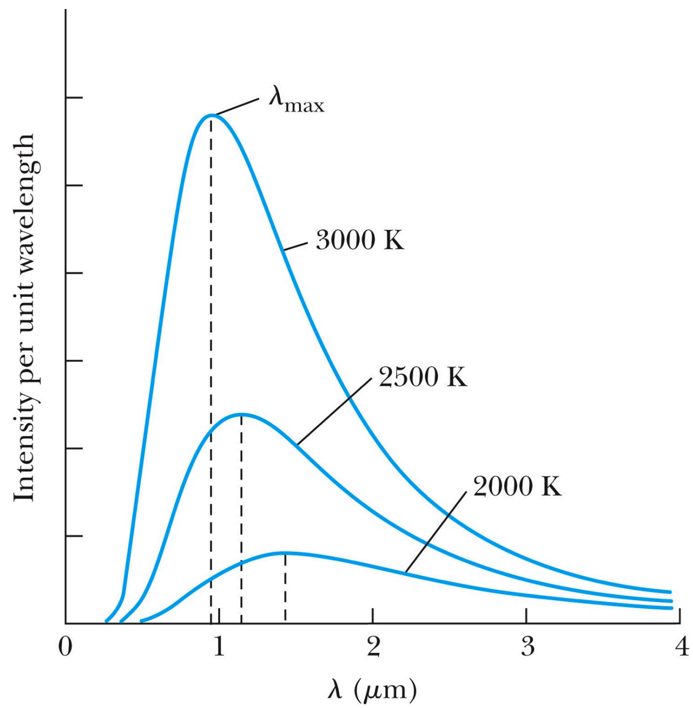
Overwhelming Evidence for Existence of Atoms

- Max Planck (1858 – 1947) advances the concept to explain blackbody radiation by use of submicroscopic "quanta"
- Boltzmann requires existence of atoms for his advances in statistical mechanics
- Albert Einstein (1879 – 1955) uses molecules to explain Brownian motion and determines the approximate value of their size and mass
- Jean Perrin (1870 – 1942) experimentally verifies Einstein's predictions

Further Complications

Three fundamental problems:

- The (non) existence of an EM medium that transmits light from the sun
- The observed differences in the electric and magnetic field between stationary and moving reference systems
- The failure of classical physics to explain blackbody radiation in which characteristic spectra of radiation that cover the entire EM wavelengths were observed depending on temperature not on the body itself



Additional Discoveries Contribute to the Complications

- Discovery of x-rays (1895, Rontgen)
- Discovery of radioactivity (1896, Becquerel)
- Discovery of the electron (1897, Thompson)
- Discovery of the Zeeman effect (1896, Zeeman) dependence of spectral frequency on magnetic field

Newtonian (Classical) Relativity

- It is assumed that Newton's laws of motion must be measured with respect to (relative to) some reference frame.
- A reference frame is called an **inertial frame** if Newton laws are valid in that frame.
- Such a frame is established when a body, not subjected to net external forces, is observed to move in rectilinear motion at constant velocity
- ➔ Newtonian Principle of Relativity (Galilean Invariance): If Newton's laws are valid in one reference frame, then they are also valid in another reference frame moving at a uniform velocity relative to the first system.

Conditions of the Galilean Transformation

- Parallel axes between the two inertial reference frames
- K' has a constant relative velocity in the *x*-direction with respect to K

$$x' = x - \vec{v}t$$

$$y' = y$$

$$z' = z$$

$$t' = t$$

- **Time** (*t*) for all observers is a *Fundamental invariant*, i.e., the same for all inertial observers
  - Space and time are separate!!

The Inverse Relations

Step 1. Replace $\vec{v}$ with $-\vec{v}$

Step 2. Replace "primed" quantities with "unprimed" and "unprimed" with "primed"

$$x = x' + \vec{v}t$$

$$y = y'$$

$$z = z'$$

$$t = t'$$

Ether as the Absolute Reference System

- In Maxwell's theory, the speed of light is given by

$$v = c = 1/\sqrt{\mu_0 \varepsilon_0}$$

  – The velocity of light between moving systems must be a constant.
  – Needed a system of medium that keeps this constant!
- Ether proposed as the absolute reference system in which the speed of light is constant and from which other measurements could be made.
- The Michelson-Morley experiment was an attempt to show the existence of ether.

Conclusions of Michelson Experiment

- Michelson noted that he should be able to detect a phase shift of light due to the time difference between path lengths but found none.
- He thus concluded that the hypothesis of the stationary ether must be incorrect.
- After several repeats and refinements with assistance from Edward Morley (1893-1923), again *a null result.*
- ***Thus, ether does not seem to exist!***
- Many explanations ensued afterward but none worked out!
- This experiment shattered the popular belief of light being waves

Einstein's Postulates

- Fundamental assumption: Maxwell's equations must be valid in all inertial frames
- **The principle of relativity**: The laws of physics are the same in all inertial systems. There is no way to detect absolute motion, and no preferred inertial system exists
  - Published a paper in 1905 at the age 26
  - Believed to be fundamental
- **The constancy of the speed of light**: Observers in all inertial systems measure the same value for the speed of light in a vacuum.

The complete Lorentz Transformations

$$x' = \frac{x - vt}{\sqrt{1-\beta^2}} \qquad x = \frac{x' + vt'}{\sqrt{1-\beta^2}}$$

$$y' = y \qquad y = y'$$

$$z' = z \qquad z = z'$$

$$t' = \frac{t - (vx/c^2)}{\sqrt{1-\beta^2}} \qquad t = \frac{t' + \frac{vx'}{c^2}}{\sqrt{1-\beta^2}}$$

- Where $\beta = v/c$ and $\gamma = 1/\sqrt{1-\beta^2}$
- Some things to note
  - What happens when β~0 (or v~0)?
    - The Lorentz x-formation becomes Galilean x-formation
  - Space–time are not separated
  - For non-imaginary x-formations, the frame speed cannot exceed c!

Time Dilation and Length Contraction

Direct consequences of the Lorentz Transformation:

- **Time Dilation**:

  Clocks in a moving inertial reference frame K' run slower with respect to stationary clocks in K.

- **Length Contraction**:

  Lengths measured in a moving inertial reference frame K' are shorter with respect to the same lengths stationary in K.

Time Dilation: Moving Clocks Run Slow

$$T' = \frac{T_0}{\sqrt{1 - v^2/c^2}} = \gamma T_0$$

1) $T' > T_0$ or the time measured between two events at *different positions* is greater than the time between the same events at *one position:* ***time dilation.***

   The proper time is always the shortest time!!

2) The events do not occur at the same space and time coordinates in the two system

3) System K requires 1 clock and K' requires 2 clocks.

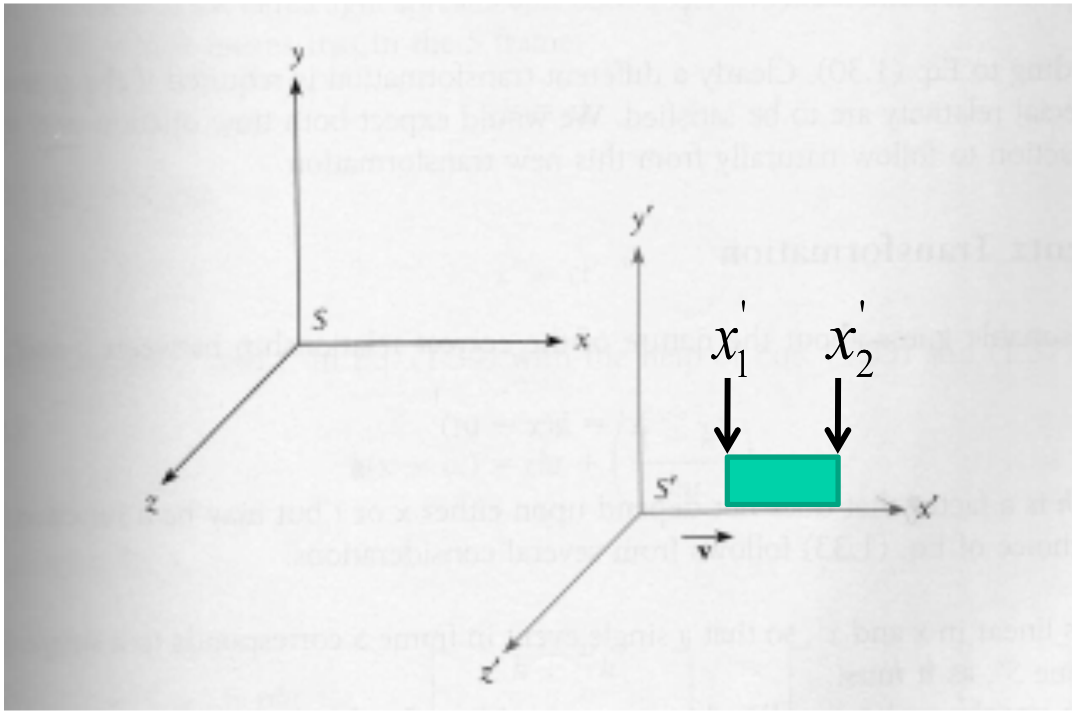
Time Dilation Example: muon lifetime

- Muons are essentially heavy electrons (~200 times heavier)
- Muons are typically generated in collisions of cosmic rays in upper atmosphere and, unlike electrons, decay ($t_0 = 2.2$ μsec)
- For a muon incident on Earth with v=0.998c, an observer on Earth would see what lifetime of the muon?
- 2.2 μsec?

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}} \approx 16$$

- t=35 μsec
- Moving clocks run slow so when an outside observer measures, they see a longer time than the muon itself sees.

Length Contraction



- Proper length (length of an object in its own frame:

$$L_0 = x_2' - x_1'$$

- Length of an object in observer's frame:

$$L = x_2 - x_1$$

$$L_0' = L_0 = x_2' - x_1' = \gamma(x_2 - vt) - \gamma(x_1 - vt) = \gamma(x_2 - x_1)$$

$L_0 = \gamma L$ $\quad$ $L = L_0 / \gamma$ $\quad$ $\gamma>1$ so the length is shorter in the direction of motion (length contraction!)

The Lorentz Velocity Transformations

In addition to the previous relations, the **Lorentz velocity transformations** for u'_x, u'_y, and u'_z can be obtained by switching primed and unprimed and changing v to $-v$:

$$u'_x = \frac{u_x - v}{1-(v/c^2)u_x}$$

$$u'_y = \frac{u_y}{\gamma\left[1-(v/c^2)u_x\right]}$$

$$u'_z = \frac{u_z}{\gamma\left[1-(v/c^2)u_x\right]}$$

Velocity Addition Summary

- Galilean Velocity addition $v_x = v_x^{'} + v$ where $v_x = \frac{dx}{dt}$ and $v_x^{'} = \frac{dx^{'}}{dt^{'}}$
- From inverse Lorentz transform $dx = \gamma(dx^{'} + v dt^{'})$ and $dt = \gamma(dt^{'} + \frac{v}{c^2} dx^{'})$
- So $$v_x = \frac{dx}{dt} = \frac{\gamma(dx^{'} + v dt^{'})}{\gamma(dt^{'} + \frac{v}{c^2} dx^{'})} \div \frac{dt^{'}}{dt^{'}} = \frac{\frac{dx^{'}}{dt^{'}} + v}{1 + \frac{v}{c^2}\frac{dx^{'}}{dt^{'}}} = \frac{v_x^{'} + v}{1 + \frac{v v_x^{'}}{c^2}}$$
- Thus $$\boxed{v_x = \frac{v_x^{'} + v}{1 + \frac{v v_x^{'}}{c^2}}}$$
- What would be the measured speed of light in S frame?
  - Since $v_x^{'} = c$ we get $$v_x = \frac{c + v}{1 + \frac{cv}{c^2}} = \frac{c^2(c + v)}{c(c + v)} = c$$

Observer in S frame measures c too! Strange but true!

Velocity Addition Example

- Lance is riding his bike at 0.8c relative to observer. He throws a ball at 0.7c in the direction of his motion. What speed does the observer see?

$$\boxed{v_x = \frac{v_x' + v}{1 + \frac{v v_x'}{c^2}}}$$

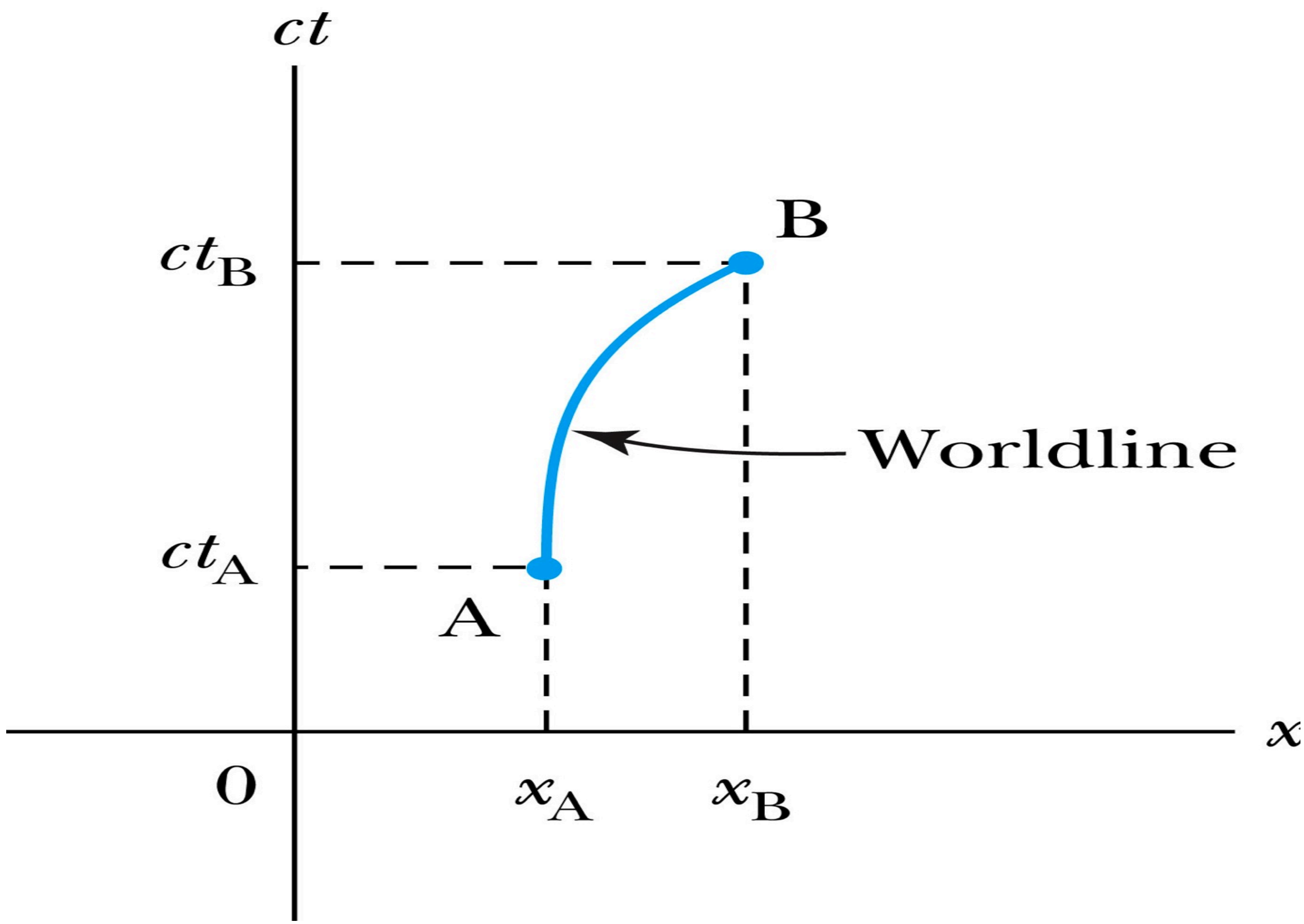
$$v_x = \frac{.7c + .8c}{1 + \frac{.7 \times .8c^2}{c^2}} = 0.962c$$

- What if he threw it just a bit harder?
- Doesn't help—asymptotically approach c, can't exceed (it's not just a postulate it's the law)

Spacetime

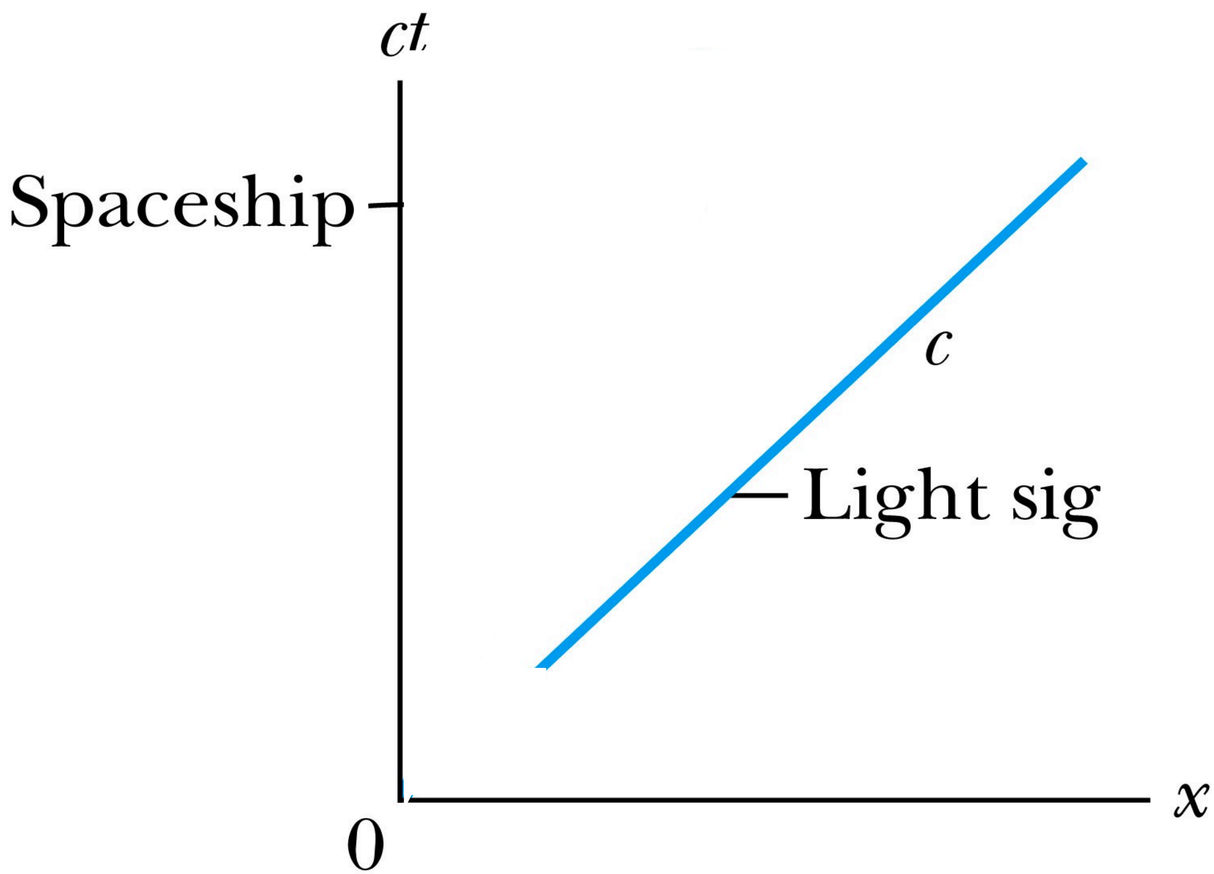
- When describing events in relativity, it is convenient to represent events on a **spacetime** diagram.
- In this diagram one spatial coordinate *x* specifies position and instead of time *t*, *ct* is used as the other coordinate so that both coordinates will have dimensions of length.
- Spacetime diagrams were first used by H. Minkowski in 1908 and are often called **Minkowski diagrams**. Paths in Minkowski spacetime are called **worldlines**.

Spacetime Diagram

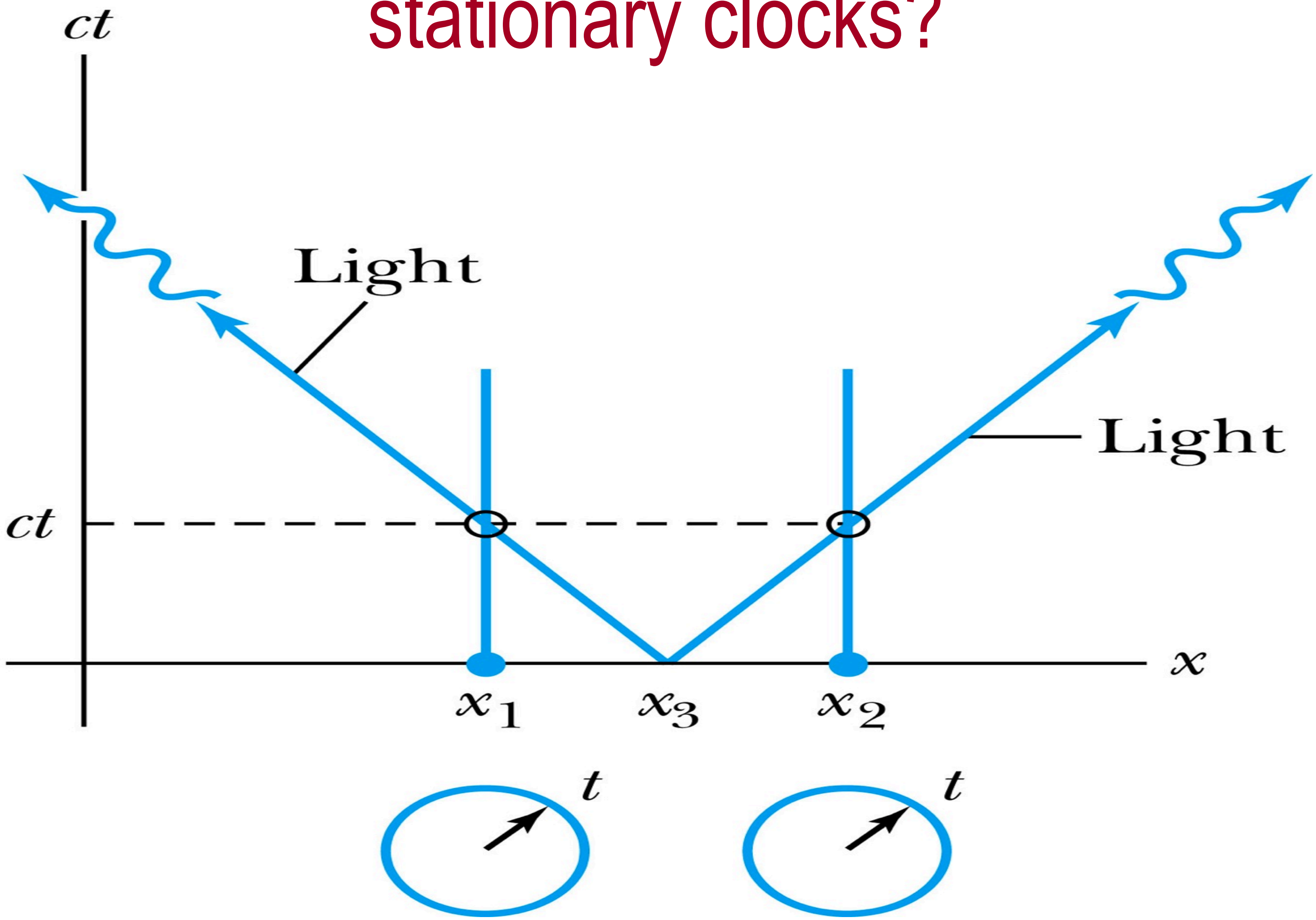


Particular Worldlines

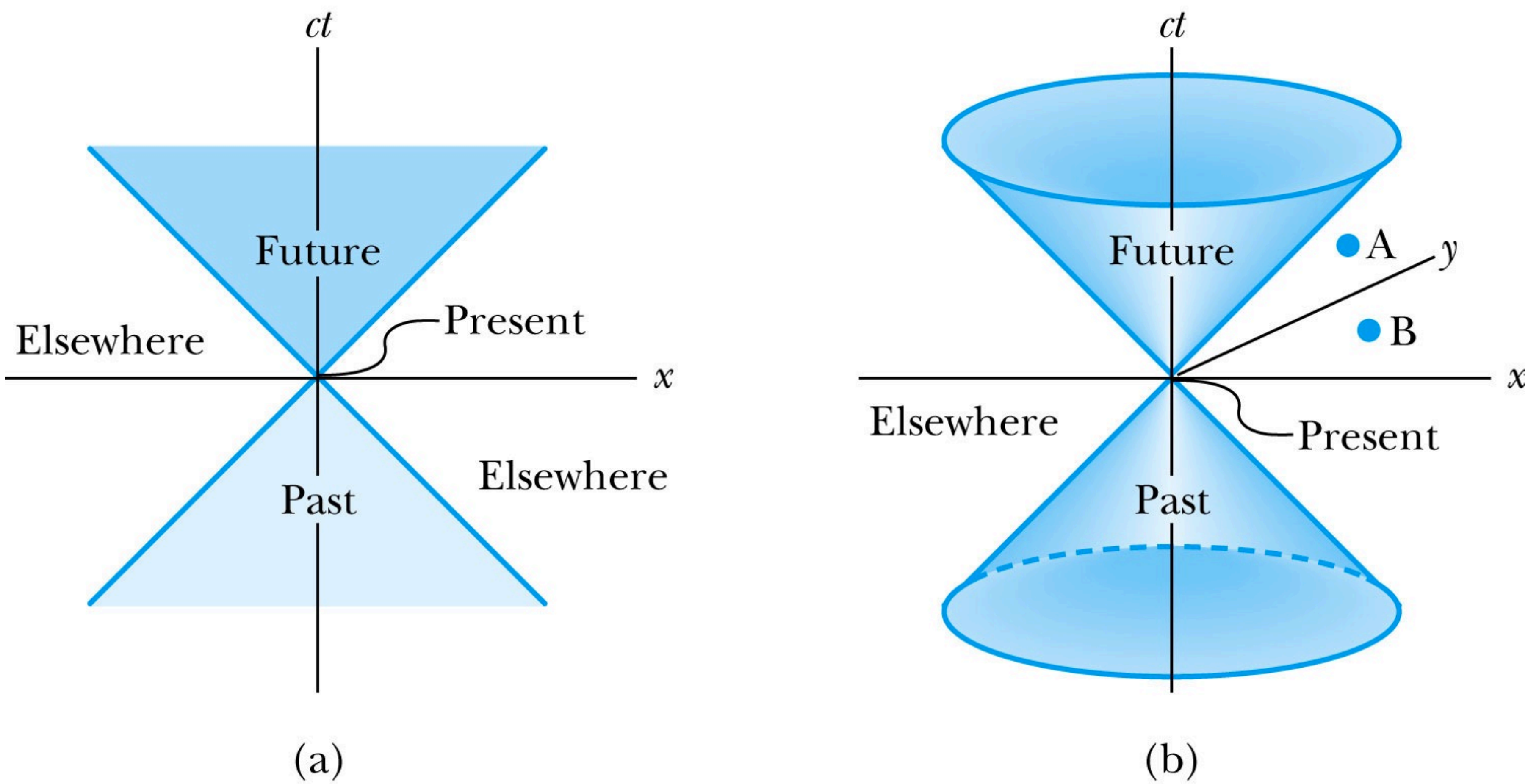
- How does the worldline for a spaceship running at the velocity v(<c) look?
- How does the worldline for light signal look?



How about time measured by two stationary clocks?



The Light Cone



Spacetime Invariants

There are three possibilities for the invariant quantity Δs^2:

$$\Delta s^2=\Delta x^2-\Delta(ct)^2$$

1) $\Delta s^2 = 0$: $\Delta x^2 = c^2\Delta t^2$: **lightlike** separation
   – Two events can be connected only by a light signal.
2) $\Delta s^2 > 0$: $\Delta x^2 > c^2\Delta t^2$: **spacelike** separation
   – No signal can travel fast enough to connect the two events. The events are not causally connected!!
3) $\Delta s^2 < 0$: $\Delta x^2 < c^2\Delta t^2$: **timelike** separation
   – Two events can be causally connected.
   – These two events cannot occur simultaneously!

Relativistic Doppler Effect

When source/receiver is approaching with $\beta = v/c$ the resulting frequency is

$$f = \frac{\sqrt{1+\beta}}{\sqrt{1-\beta}} f_0$$

Higher than the actual source's frequency, blue shift!!

When source/receiver is receding with $\beta = v/c$ the resulting frequency is

$$f = \frac{\sqrt{1-\beta}}{\sqrt{1+\beta}} f_0$$

Lower than the actual source's frequency, red shift!!

If we use $+\beta$ for approaching source/receiver and $-\beta$ for receding source/receiver, relativistic Doppler Effect can be expressed

$$\boxed{f = \frac{\sqrt{1+\beta}}{\sqrt{1-\beta}} f_0}$$

What can we use this for?

Relativistic Momentum, total Energy and Rest Energy

relativistic definition of the momentum:

$$\vec{p} = m\frac{d\vec{r}}{d\tau} = m\frac{d\vec{r}}{dt}\frac{dt}{d\tau} = m\vec{u}\gamma = \frac{1}{\sqrt{1-u^2/c^2}}m\vec{u}$$

Rewriting the relativistic kinetic energy: $\gamma mc^2 = \frac{mc^2}{\sqrt{1-u^2/c^2}} = K + mc^2$

The term mc^2 is called the rest energy and is denoted by E_0.

$$E_0 = mc^2$$

The sum of the kinetic energy and rest energy is interpreted as the total energy of the particle.

$$E = \gamma mc^2 = \frac{mc^2}{\sqrt{1-u^2/c^2}} = \frac{E_0}{\sqrt{1-u^2/c^2}} = K + E_0$$

$$K = E - E_0 = mc^2(\gamma - 1)$$

Relationship of Energy and Momentum

$$p = \gamma m u = \frac{mu}{\sqrt{1 - u^2 / c^2}}$$

We square this result, multiply by c^2, and rearrange the result.

$$p^2 c^2 = \gamma^2 m^2 u^2 c^2 = \gamma^2 m^2 c^4 \left(\frac{u^2}{c^2} \right) = \gamma^2 m^2 c^4 \beta^2$$

$$\beta^2 = 1 - \frac{1}{\gamma^2} \Rightarrow p^2 c^2 = \gamma^2 m^2 c^4 \left(1 - \frac{1}{\gamma^2} \right) = \gamma^2 m^2 c^4 - m^2 c^4$$

Rewrite

$$p^2 c^2 = E^2 - E_0^2$$

Rewrite

$$E^2 = p^2 c^2 + E_0^2 = p^2 c^2 + m^2 c^4$$

Units of Work, Energy and Mass

- The work done in accelerating a charge through a potential difference is $W = qV$.
  - For a proton, with the charge $e = 1.602 \times 10^{-19}$ C being accelerated across a potential difference of 1 V, the work done is

    1 eV = 1.602×10^{-19} J

    $W = (1.602 \times 10^{-19})(1\ \text{V}) = 1.602 \times 10^{-19}$ J

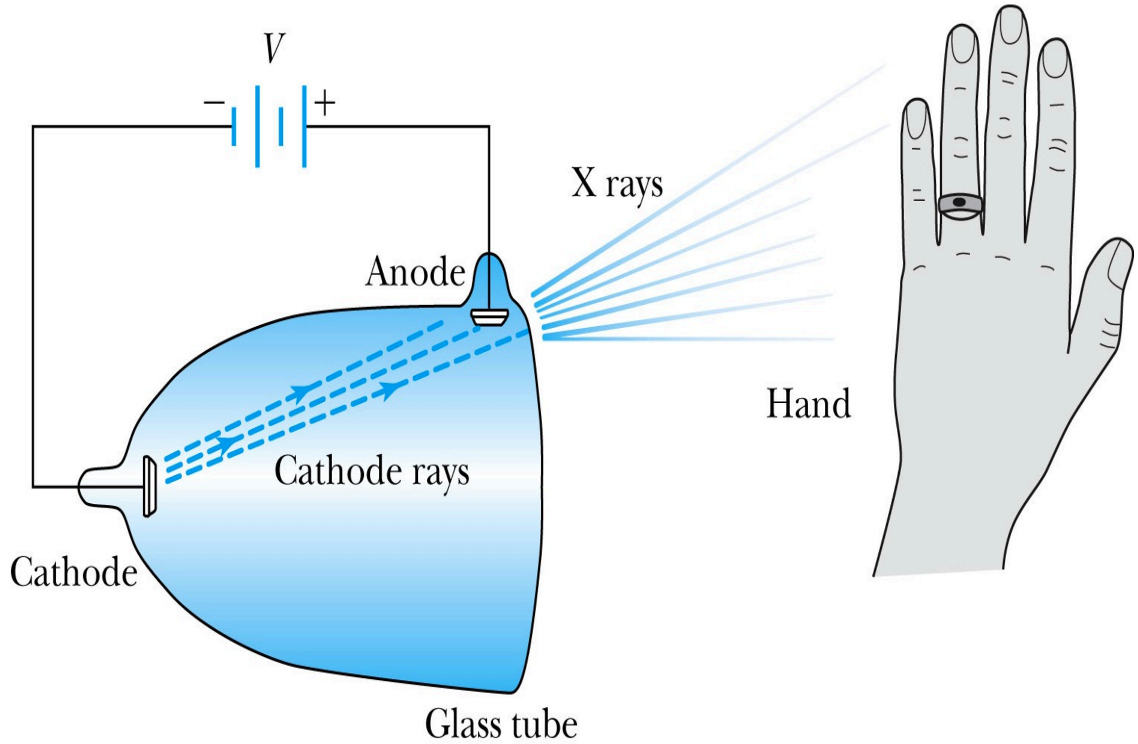
- eV is also used as a unit of energy.

What does the word “Quantize” mean?

- Dictionary: To restrict to discrete values
- To consist of indivisible discrete quantities instead of continuous quantities
  - Integer is a quantized set with respect to real numbers
- Some examples of quantization?
  - Digital photos
  - Lego blocks
  - Electric charge
  - Photon (a quanta of light) energy
  - Angular momentum
  - Etc…

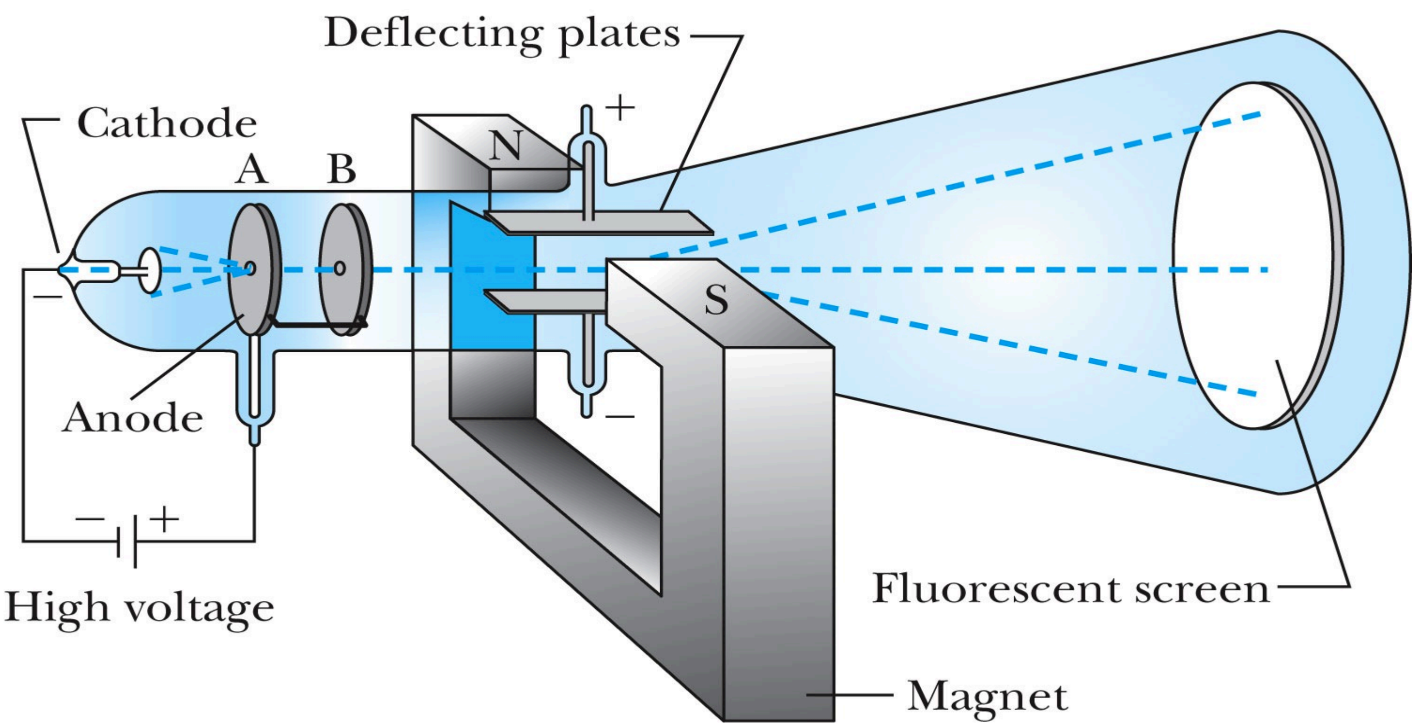
Röntgen's X Ray Tube

- Röntgen produced x-ray by allowing cathode rays to impact the glass wall of the tube.
- Took image the bones of a hand on a phosphorescent screen.



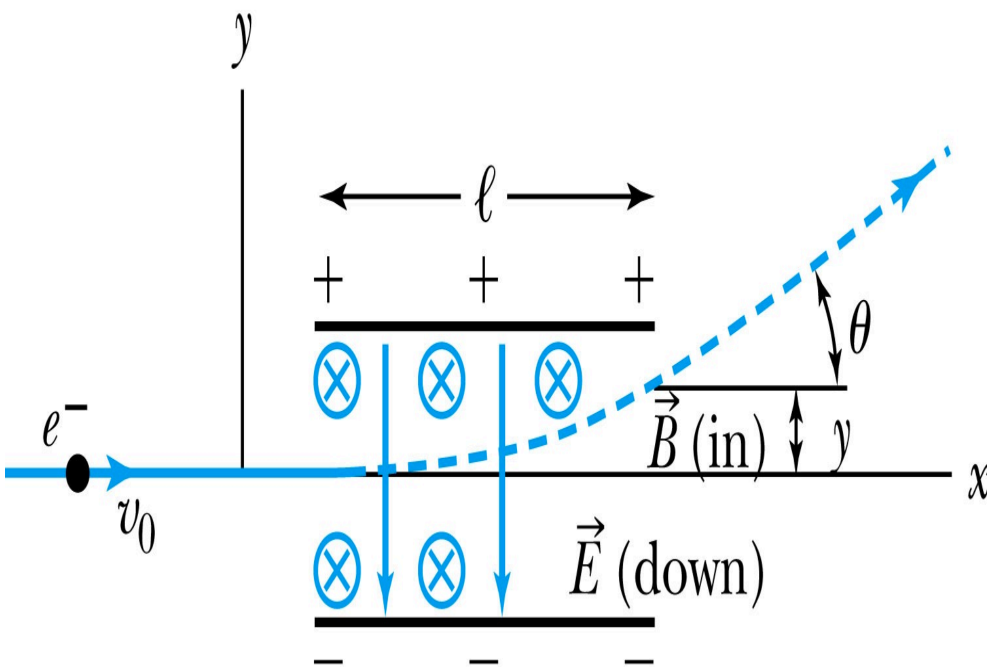
J.J. Thomson's Cathode-Ray Experiment

- Thomson showed that the cathode rays were negatively charged particles (electrons)! How?
  - By deflecting them in electric and magnetic fields.



Thomson's Experiment

- Thomson measured the ratio of the electron's charge to mass by sending electrons through a region containing a magnetic field perpendicular to an electric field.



- Measure the deflection angle with only E!
- Turn on and adjust B field till no deflection!

- What do we know?
  - l, B, E and θ
- What do we not know?
  - v_0, q and m

Ex 3.1: Thomson's experiment

- In an experiment similar to Thomson's, we use deflecting plates 5.0cm in length with an electric field of 1.2×10^4 V/m. Without the magnetic field, we find an angular deflection of 30^o, and with a magnetic field of 8.8×10^{-4} T we find no deflection. What is the initial velocity of the electron and its q/m?

- First v_0 using E and B, we obtain:

$$v_0 = v_x = \frac{E}{B} = \frac{1.2 \times 10^4}{8.8 \times 10^{-4}} = 1.4 \times 10^7 \, m/s$$

- q/m is then

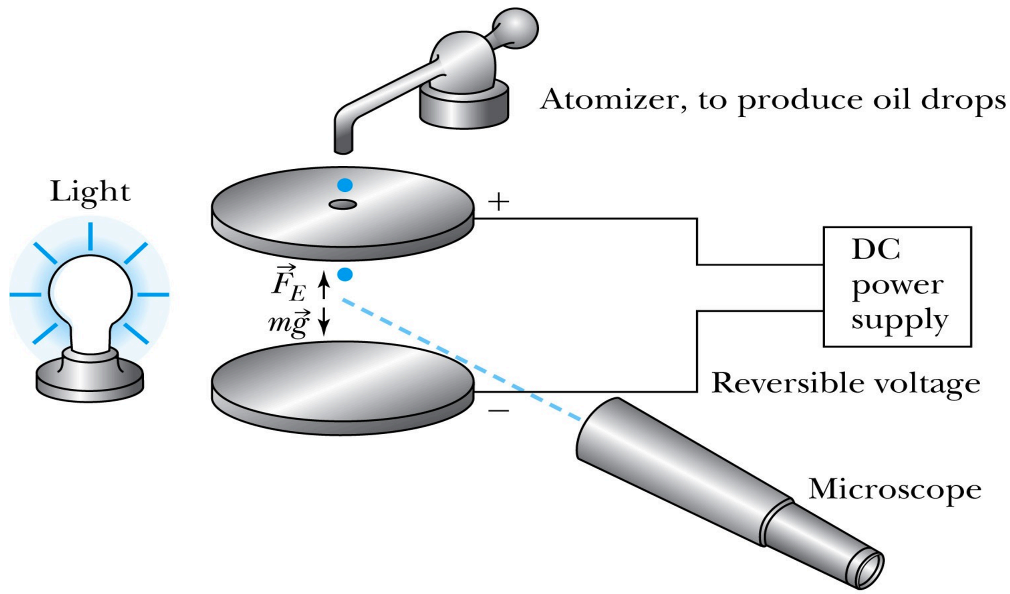
$$\frac{q}{m} = \frac{E \tan\theta}{B^2 l} = \frac{1.2 \times 10^4 \tan 30^\circ}{\left(8.8 \times 10^{-4}\right)^2 \cdot 0.5} = 1.8 \times 10^{11} \, C/kg$$

- What is the actual value of q/m using the known quantities?

$$\frac{q}{m} = \frac{1.6022 \times 10^{-19}}{9.1094 \times 10^{-31}} = 1.759 \times 10^{-11} \, C/kg$$

Determination of Electron Charge

- Millikan (and Fletcher) in 1909 measured charge of electron, showed that free electric charge is in multiples of the basic charge of an electron



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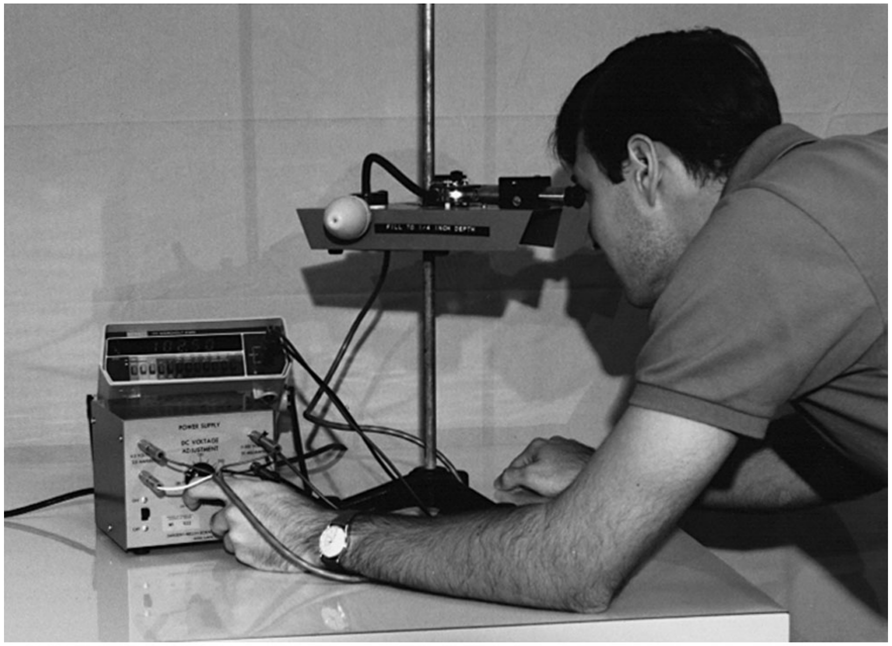


Line Spectra

- Chemical elements produce unique wavelengths of light when burned or excited in an electrical discharge.
- Collimated light is passed through a diffraction grating with thousands of ruling lines per centimeter.
  - The diffracted light is separated at an angle θ according to its wavelength λ by the equation:

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

where d is the distance between rulings and n is an integer called the order number

Rydberg Equation

- Several more series of emission lines at infrared and ultraviolet wavelengths were discoverd, the Balmer series equation was extended to the Rydberg equation:

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n^2} - \frac{1}{k^2} \right) \qquad R_H = 1.096776 \times 10^7 \text{ m}^{-1} \quad (n = 2)$$

Table 3.2 Hydrogen Series of Spectral Lines

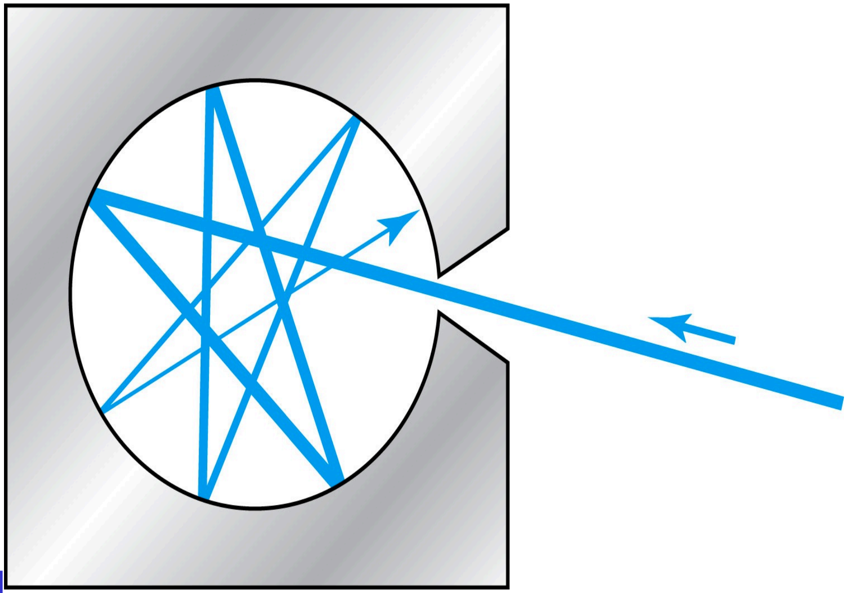
Discoverer (year)	**Wavelength**	***n***	***k***
Lyman (1916)	Ultraviolet	1	>1
Balmer (1885)	Visible, ultraviolet	2	>2
Paschen (1908)	Infrared	3	>3
Brackett (1922)	Infrared	4	>4
Pfund (1924)	Infrared	5	>5

Quantization

- Current theories predict that charges are quantized in units (**quarks**) of $\pm e/3$ and $\pm 2e/3$, but quarks are not directly observed experimentally.
- The charges of particles that have been directly observed are always quantized in units of $\pm e$.
- The measured atomic weights are not continuous—they have only discrete values, which are close to integral multiples of a unit mass.

Blackbody Radiation

- When matter is heated, it emits radiation.
- A blackbody is an ideal object that has 100% absorption and 100% emission without a loss of energy
- A cavity in a material that only emits thermal radiation can be considered as a black-body. Incoming radiation is fully absorbed in the cavity.



- Blackbody radiation is theoretically interesting because
  - Radiation properties are independent of the particular material.
  - Properties of intensity versus wavelength at fixed temperatures can be studied

Stefan-Boltzmann Law

- The total power radiated increases with the temperature: $$R(T) = \int_0^\infty \mathcal{I}(\lambda, T)\, d\lambda = \epsilon\,\sigma T^4$$
- This is known as the **Stefan-Boltzmann law**, with the constant σ experimentally measured to be 5.6705×10^{-8} W / ($m^2 \cdot K^4$).
- The **emissivity** ε (ε = 1 for an idealized blackbody) is the ratio of the emissive power of an object to that of an ideal blackbody and is always less than 1.

Planck's Radiation Law

- Planck assumed that the radiation in the cavity was emitted (and absorbed) by some sort of "oscillators" that were contained in the walls. He used Boltzman's statistical methods to arrive at the following formula that fit the blackbody radiation data.

$$\mathcal{I}(\lambda,T)=\frac{2\pi c^2 h}{\lambda^5}\frac{1}{e^{hc/\lambda kT}-1}$$ Planck's radiation law

- Planck made two modifications to the classical theory:
  1) The oscillators (of electromagnetic origin) can only have certain discrete energies determined by $E_n = nhf$, where n is an integer, f is the frequency, and h is called Planck's constant. $h = 6.6261 \times 10^{-34}$ J·s.
  2) **<u>The oscillators can absorb or emit energy ONLY in discrete multiples of the fundamental quantum of energy</u>** given by

$$\Delta E = hf = \frac{hc}{\lambda}$$

Photoelectric Effect

Definition: Incident electromagnetic radiation shining on the material transfers energy to the electrons, allowing them to escape the surface of the metal. Ejected electrons are called photoelectrons

Other methods of electron emission:

- Thermionic emission: Application of heat allows electrons to gain enough energy to escape.
- Secondary emission: The electron gains enough energy by transfer from another high-speed particle that strikes the material from outside.
- Field emission: A strong external electric field pulls the electron out of the material.

Summary of Experimental Observations

- Light intensity does not affect the KE of the photoelectrons
- The max KE of the photoelectrons, for a given emitting material, depends only on the frequency of the light
- The smaller the work function ϕ of the emitter material, the smaller is the threshold frequency of the light that can eject photoelectrons.
- When the photoelectrons are produced, their number is proportional to the intensity of light.
- The photoelectrons are emitted almost instantly following illumination of the photocathode, independent of the intensity of the light. ➔ Totally unexplained by classical physics

Quantum Interpretation – Photoelectric Effect

- KE of the electron depend only on the light frequency and the work function ϕ of the material not the light intensity at all

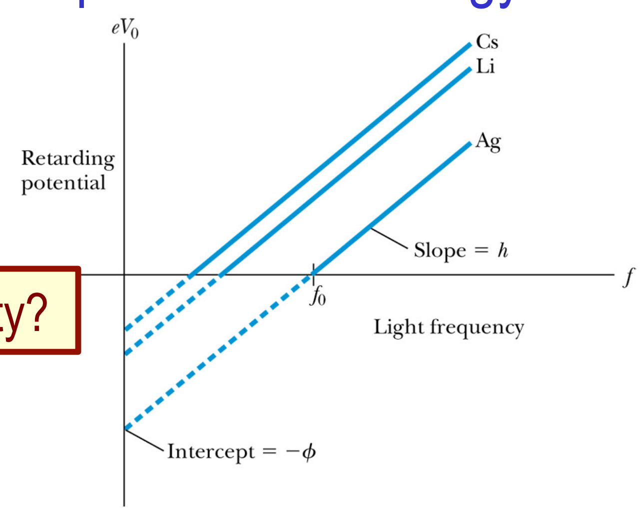
$$\frac{1}{2}mv_{\max}^2 = eV_0 = hf - \phi$$

- Einstein in 1905 predicted that the stopping potential was linearly proportional to the light frequency, with a slope *h*, the same constant found by Planck.

$$eV_0 = \frac{1}{2}mv_{\max}^2 = hf - hf_0 = h\left(f - f_0\right)$$

- From this, Einstein concluded that light is a particle with energy:

$$E = hf = \frac{hc}{\lambda}$$



Was he already thinking about particle/wave duality?

Ex 3.11: Photoelectric Effect

- Light of wavelength 400nm is incident upon lithium (=2.93eV). Calculate (a) the photon energy and (b) the stopping potential V_0.
- Since the wavelength is known, we use plank's formula:

$$E = hf = \frac{hc}{\lambda} = \frac{\left(1.626 \times 10^{-34} J \cdot s\right)\left(3 \times 10^{8}\, m/s\right)}{400 \times 10^{-9} m} = 3.10 eV$$

- The stopping potential can be obtained using Einstein's formula for photoelectron energy

$$eV_0 = hf - \phi = E - \phi$$

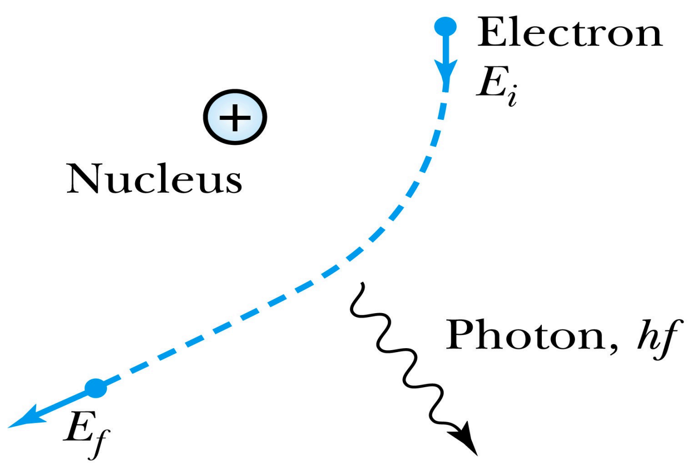
$$V_0 = \frac{E - \phi}{e} = \frac{\left(3.10 - 2.93\right) eV}{e} = 0.17V$$

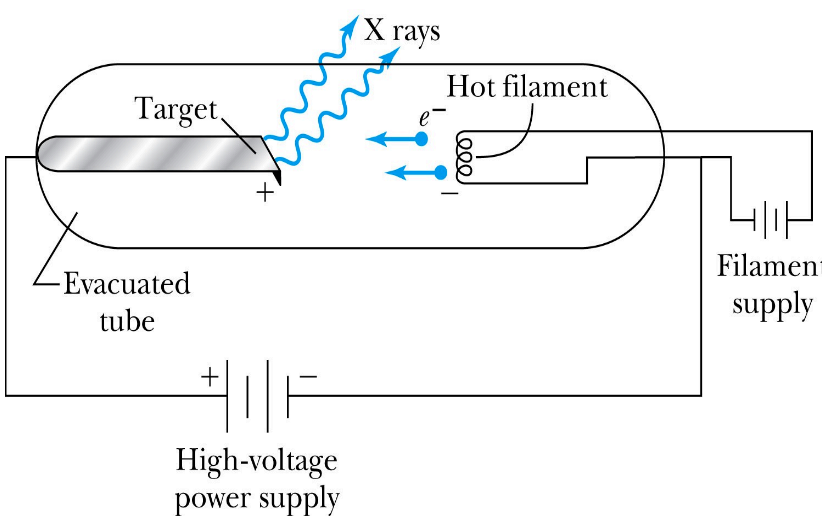
X-Ray Production

- **Bremsstrahlung** (German word for braking radiation): Radiation of a photon from an energetic electron passing through matter due to an acceleration
- Since linear momentum must be conserved, the nucleus absorbs very little energy, and it is ignored. The final energy of the electron is determined from the conservation of energy to be

$$E_f = E_i - hf$$

- An electron that loses a large amount of energy will produce an X-ray photon.
  - Current passing through a filament produces copious numbers of electrons by thermionic emission.
  - These electrons are focused by the cathode structure into a beam and are accelerated by potential differences of thousands of volts until they impinge on a metal anode surface, producing x rays by bremsstrahlung as they stop in the anode material

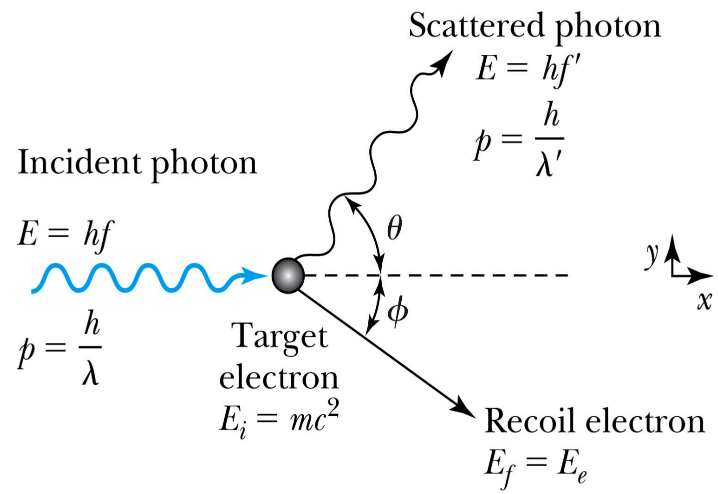




Compton Effect

- When a photon enters matter, it is likely to interact with one of the atomic electrons.
- The photon is scattered from only one electron
- The laws of conservation of energy and momentum apply as in any elastic collision between two particles. The momentum of a particle moving at the speed of light is

$$p = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda}$$



- The electron energy can be written as

$$E_e^2 = \left(mc^2\right)^2 + p_e^2 c^2$$

- Change of the scattered photon wavelength is known as the **Compton effect**:

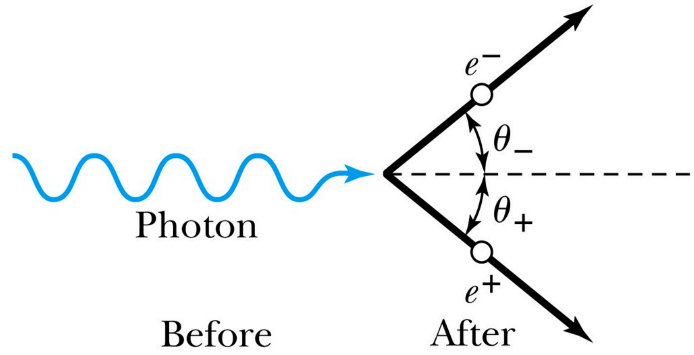
$$\Delta\lambda = \lambda^{'} + \lambda = \frac{h}{mc}\left(1 - \cos\theta\right)$$

Pair Production in Matter

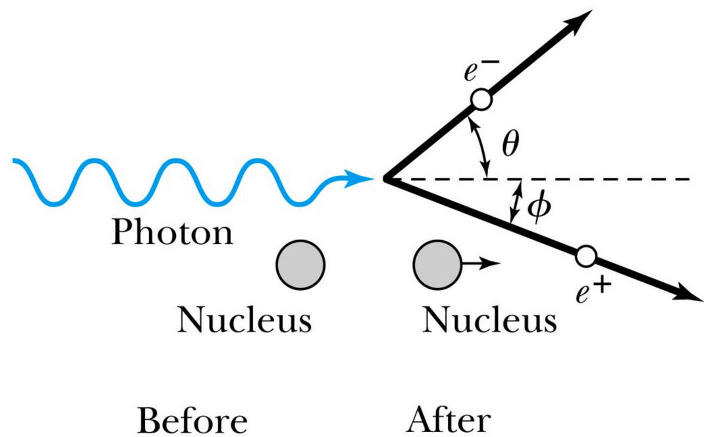
- Since the relations $hf_{\max} = p_- c + p_+ c$ and $hf > p_- c + p_+ c$ contradict each other, a photon can not produce an electron and a positron in empty space.
- In the presence of matter, the nucleus absorbs some energy and momentum.

$$hf = E_+ + E_- + \text{K.E. (nucleus)}$$

- The photon energy required for pair production in the presence of matter is $hf > 2m_e c^2 = 1.022\ \text{MeV}$



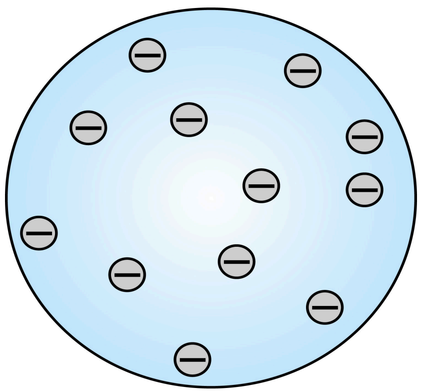
(a) Free space (**cannot occur**)



(b) Beside nucleus

Thomson's Atomic Model

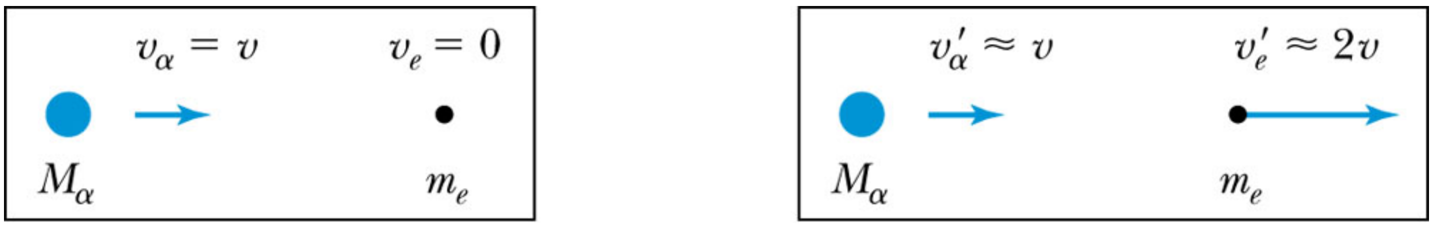
- Thomson's "plum-pudding" model
  - Atoms are electrically neutral and have electrons in them
  - Atoms must have equal amount of positive charges in it to balance electron negative charges
  - So how about positive charges spread uniformly throughout a sphere the size of the atom with, the newly discovered "negative" electrons embedded in the uniform background.



- Thomson's thought when the atom was heated the electrons could vibrate about their equilibrium positions, thus producing electromagnetic radiation.

Ex 4.1: Maximum Scattering Angle

Geiger and Marsden (1909) observed backward-scattered (θ>=90°) α particles when a beam of energetic α particles was directed at a piece of gold foil as thin as 6.0×10^{-7}m. Assuming an α particle scatters from an electron in the foil, what is the maximum scattering angle?



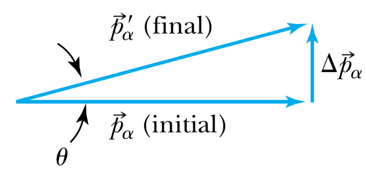
Before　　　　After

- The maximum scattering angle corresponding to the maximum momentum change
- Using the momentum conservation and the KE conservation for an elastic collision, the maximum momentum change of the α particle is

$$M_\alpha \vec{v}_\alpha = M_\alpha \vec{v}_\alpha' + m_e \vec{v}_e'$$
$$\frac{1}{2}M_\alpha v_\alpha^2 = \frac{1}{2}M_\alpha v_\alpha'^2 + \frac{1}{2}m_2 v_e^2$$

$$\Delta\vec{p}_\alpha = M_\alpha \vec{v}_\alpha - M_\alpha \vec{v}_\alpha' = m_e \vec{v}_e' \Rightarrow \Delta p_{\alpha-\max} = 2m_e v_\alpha$$

- Determine θ by letting Δp_{max} be perpendicular to the direction of motion.



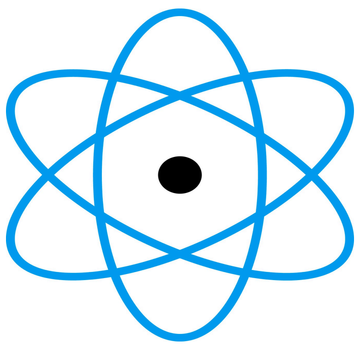
$$\theta_{\max} = \frac{\Delta p_{\alpha-\max}}{p_\alpha} = \frac{2m_e v_\alpha}{m_\alpha v_\alpha} = \frac{2m_e}{m_\alpha} = 2.7\times10^{-4}\,rad = 0.016^\circ$$

Rutherford's Atomic Model

- $<\theta>_{total} \sim 0.8^{o}$ even if the α particle scattered from all 79 electrons in each atom of gold

The experimental results were inconsistent with Thomson's atomic model.

- Rutherford proposed that an atom has a positively charged core (nucleus) surrounded by the negative electrons.

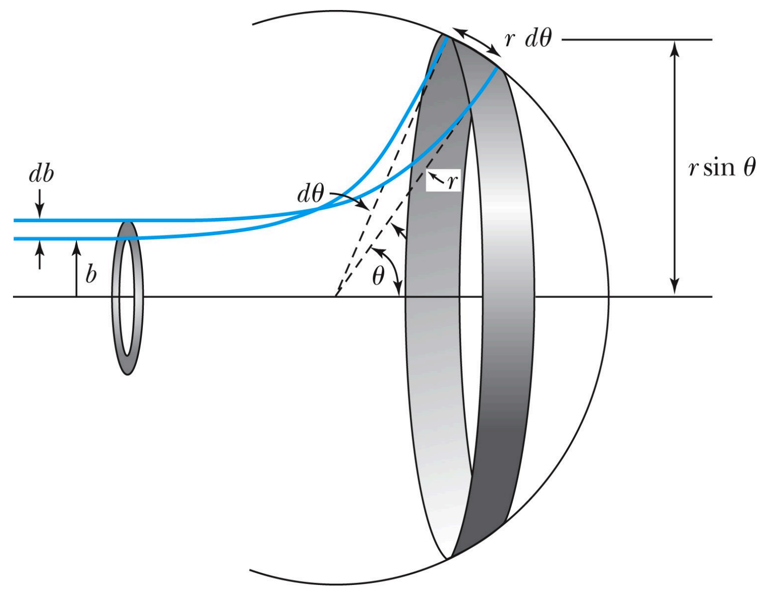


Assumptions of Rutherford Scattering

1. The scatterer is so massive that it does not recoil significantly; therefore the initial and final KE of the α particle are practically equal.
2. The target is so thin that only a single scattering occurs.
3. The bombarding particle and target scatterer are so small that they may be treated as point masses and charges.
4. Only the Coulomb force is effective.

Rutherford Scattering Equation

- In actual experiment a detector is positioned from θ to $\theta + d\theta$ that corresponds to incident particles between b and $b + db$.



- The number of particles scattered into the the angular coverage per unit area is

$$N(\theta) = \frac{N_i nt}{16}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{Z_1^{\,2} Z_2^{\,2}}{r^2 K^2 \sin^4(\theta/2)}$$

The Important Points

1. The scattering is proportional to the square of the atomic number of *both* the incident particle (Z_1) and the target scatterer (Z_2).
2. The number of scattered particles is inversely proportional to the square of the kinetic energy of the incident particle.
3. For the scattering angle θ, the scattering is proportional to 4th power of $\sin(\theta/2)$.
4. The Scattering is proportional to the target thickness for thin targets.

The Classical Atomic Model

As suggested by the Rutherford Model the atom consisted of a small, massive, positively charged nucleus surrounded by moving electrons. This then suggested consideration of a planetary model of the atom.

Let's consider atoms as a planetary model.

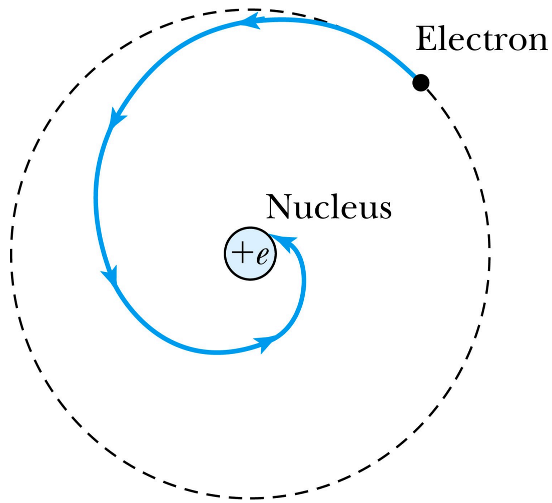
- The force of attraction on the electron by the nucleus and Newton's 2nd law give $$\vec{F}_e = \frac{-1}{4\pi\varepsilon_0}\frac{e^2}{r^2}\hat{e}_r = \frac{mv^2}{r}$$

  where *v* is the tangential velocity of the electron.

- The total energy is $$E = K + V = \frac{e^2}{8\pi\varepsilon_0 r} - \frac{e^2}{4\pi\varepsilon_0 r} = \frac{-e^2}{8\pi\varepsilon_0 r}$$

The Planetary Model is Doomed

- From classical E&M theory, an accelerated electric charge radiates energy (electromagnetic radiation) which means total energy must decrease. → *Radius r must decrease!!*



Electron crashes into the nucleus!?

- Physics had reached a turning point in 1900 with Planck's hypothesis of the quantum behavior of radiation.

The Bohr Model of the Hydrogen Atom – The assumptions

- "Stationary" states or orbits must exist in atoms, i.e., orbiting electrons *do not radiate* energy in these orbits. These orbits or stationary states are of a fixed definite energy E.
- The emission or absorption of electromagnetic radiation can occur only in conjunction with a transition between two stationary states. The frequency, f, of this radiation is proportional to the *difference* in energy of the two stationary states:
- $$E = E_1 - E_2 = hf$$
- *where h is Planck's Constant*
  - *Bohr thought this has to do with fundamental length of order ~10^{-10}m*
- Classical laws of physics do not apply to transitions between stationary states.
- The mean kinetic energy of the electron-nucleus system is quantized as $K = nhf_{orb}/2$, where f_{orb} is the frequency of rotation. This is equivalent to the angular momentum of a stationary state to be an integral multiple of $h/2\pi$

Importance of Bohr's Model

- Demonstrated the need for Plank's constant in understanding atomic structure
- Assumption of quantized angular momentum which led to quantization of other quantities, r, v and E as follows
- Orbital Radius: $$r_n = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}n^2 = a_0 n^2$$
- Orbital Speed: $$v = \frac{n\hbar}{mr_n} = \frac{\hbar}{ma_0}\frac{1}{n}$$
- Energy levels: $$E_n = \frac{e^2}{8\pi\varepsilon_0 a_0 n^2} = \frac{E_0}{n^2}$$

Fine Structure Constant

- The electron's speed on an orbit in the Bohr model:

$$v_e = \frac{n\hbar}{m_e r_n} = \frac{n\hbar}{m_e \dfrac{4\pi\varepsilon_0 n^2\hbar^2}{m_e e^2}} = \frac{1}{n}\frac{e^2}{4\pi\varepsilon_0\hbar}$$

- On the ground state, $v_1 = 2.2 \times 10^6$ m/s ~ less than 1% of the speed of light
- The ratio of v_1 to c is the **fine structure constant, α**.

$$\alpha \equiv \frac{v_1}{c} = \frac{\hbar}{m a_0 c} = \frac{e^2}{4\pi\varepsilon_0\hbar c} =$$

$$\frac{\left(1.6\times10^{-19}C\right)^2}{\left(8.99\times10^9\, N\cdot m^2/C^2\right)\cdot\left(1.055\times10^{-34}\, J\cdot s\right)\cdot\left(3\times10^8\, m/s\right)} \approx \frac{1}{137}$$

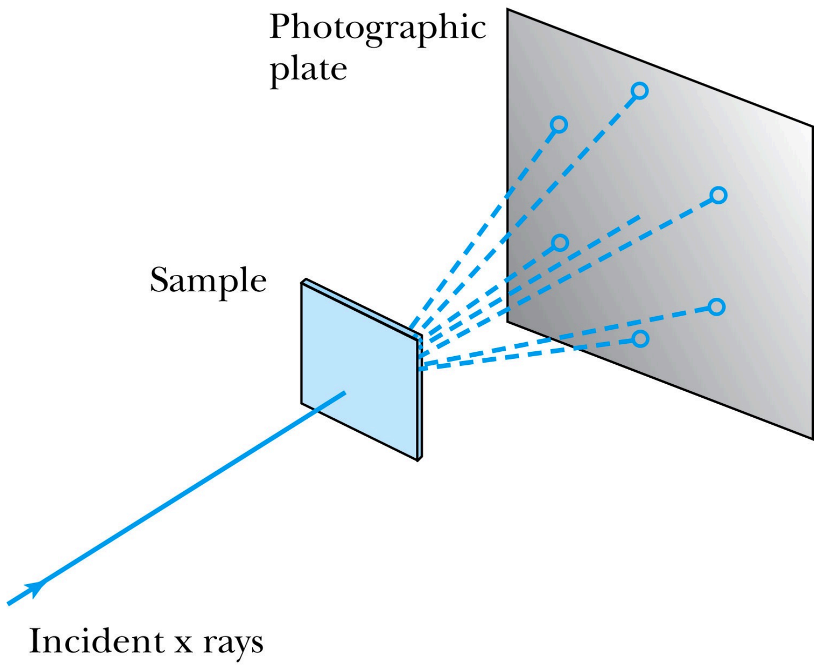
Limitations of the Bohr Model

The Bohr model was a great step of the new quantum theory, but it had its limitations.

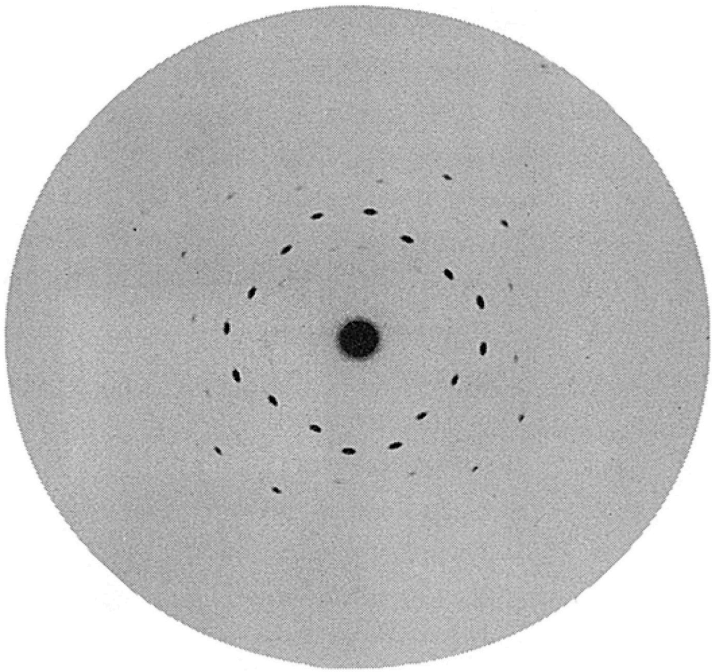
1) Works only to single-electron atoms
   - Even for ions ➔ What would change?
   - The charge of the nucleus $\frac{1}{\lambda} = Z^2 R\left(\frac{1}{n_l^2} - \frac{1}{n_u^2}\right)$
2) Could not account for the intensities or the fine structure of the spectral lines
   - Fine structure is caused by the electron spin
   - When a magnetic field is applied, spectral lines split
3) Could not explain the binding of atoms into molecules

X-Ray Scattering

- Max von Laue suggested that if x rays were a form of electromagnetic radiation, interference effects should be observed. (Wave property!!)
- Crystals act as three-dimensional gratings, scattering the waves and producing observable interference effects.



(a)

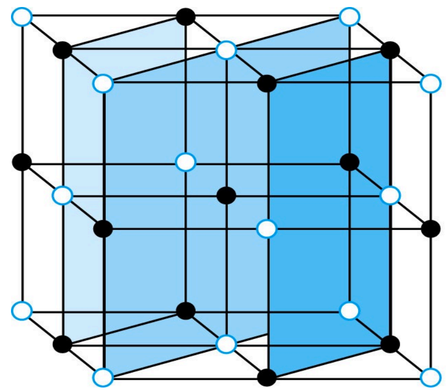
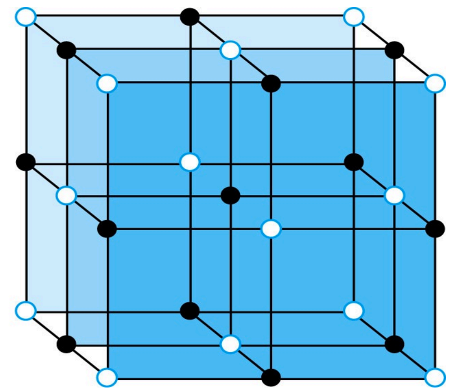


(b)

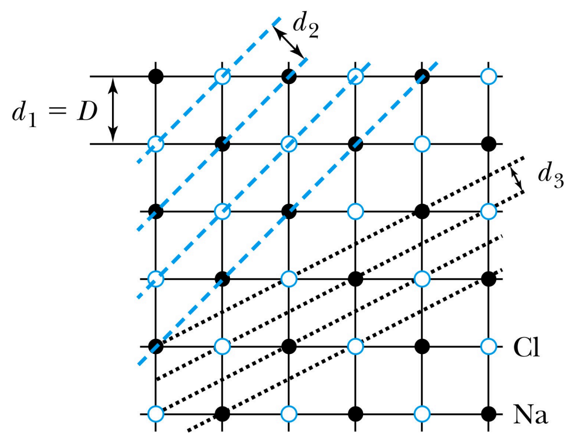
Bragg's Law

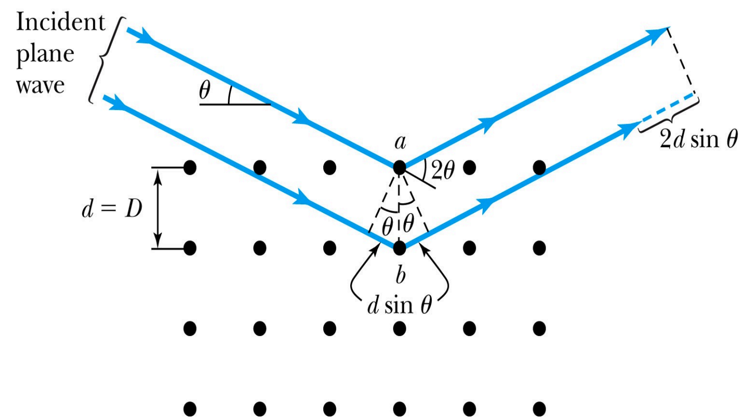
- William Lawrence Bragg interpreted the x-ray scattering as the reflection of the incident x-ray beam from a unique set of planes of atoms within the crystal.
- There are two conditions for constructive interference of the scattered x rays:

1) The angle of incidence must equal the angle of reflection of the outgoing wave. (total reflection)
2) The difference in path lengths between two rays must be an integral number of wavelengths.

- **Bragg's Law:**
- $n\lambda = 2d \sin\theta$
- (n = integer)





Ex 5.1: Bragg's Law

X rays scattered from rock salt (NaCl) are observed to have an intense maximum at an angle of 20^o from the incident direction. Assuming n=1 (from the intensity), what must be the wavelength of the incident radiation?

- Bragg's law: $n\lambda = 2d \sin \theta$
- *What do we need to know to use this? The lattice spacing d!*
- *We know n=1 and 2θ=20^o.*
- *We use the density of NaCl to find out what d is.*

$$\frac{N_{molecules}}{V} = \frac{N_A \rho_{NaCl}}{M} = \frac{\left(6.02\times10^{23}\, molecules/mol\right)\cdot\left(2.16\, g/cm^3\right)}{58.5\, g/mol} =$$

$$= 2.22\times10^{22}\frac{molecules}{cm^3} = 4.45\times10^{22}\frac{atoms}{cm^3} = 4.45\times10^{28}\frac{atoms}{m^3}$$

$$\frac{1}{d^3} = 4.45\times10^{28}\frac{atoms}{m^3} \Rightarrow d = \frac{1}{\sqrt[3]{4.45\times10^{28}}} = 0.282nm$$

$$\lambda = 2d\sin\theta = 2\cdot0.282\cdot\sin10^o = 0.098nm$$

De Broglie Waves

- Prince Louis V. de Broglie suggested that mass particles should have wave properties similar to electromagnetic radiation ➔ many experiments supported this!
- Thus the wavelength of a matter wave is called the de Broglie wavelength:

$$\lambda = \frac{h}{p}$$

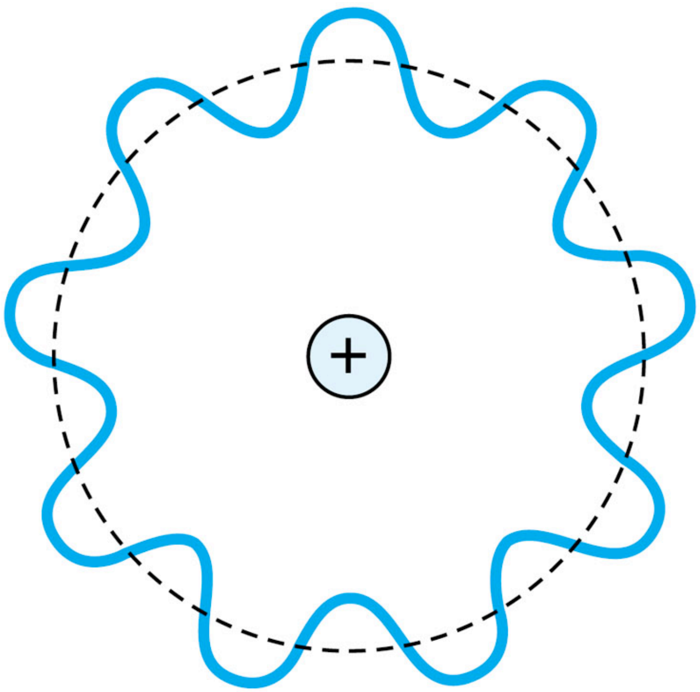
- Since for a photon, $E = pc$ and $E = hf$, the energy can be written as

$$E = hf = pc = p\lambda f$$

Bohr's Quantization Condition

- One of Bohr's assumptions concerning his hydrogen atom model was that the angular momentum of the electron-nucleus system in a stationary state is an integral multiple of $h/2\pi$.
- The electron is a standing wave in an orbit around the proton. This standing wave will have nodes and be an integral number of wavelengths.

$$2\pi r = n\lambda = n\frac{h}{p}$$



- The angular momentum becomes:

$$L = rp = \frac{nh}{2\pi p}p = n\frac{h}{2\pi} = n\hbar$$

Ex 5.2: De Broglie Wavelength

Calculate the De Broglie wavelength of (a) a tennis ball of mass 57g traveling 25m/s (about 56mph) and (b) an electron with kinetic energy 50eV.

- What is the formula for De Broglie Wavelength? $\lambda = \frac{h}{p}$
- (a) for a tennis ball, m=0.057kg.

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}}{0.057 \cdot 25} = 4.7 \times 10^{-34} m$$

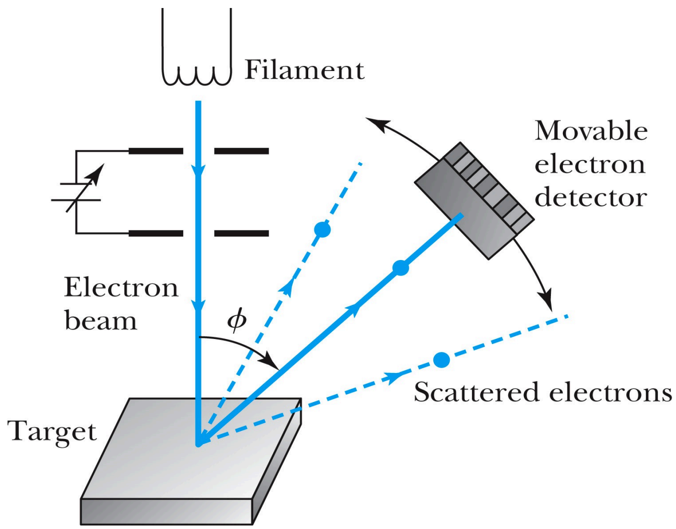
- (b) for electron with 50eV KE, since KE is small, we can use non-relativistic expression of electron momentum!

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m_e K}} = \frac{hc}{\sqrt{2m_e c^2 K}} = \frac{1240 eV \cdot nm}{\sqrt{2 \cdot 0.511 MeV \cdot 50 eV}} = 0.17 nm$$

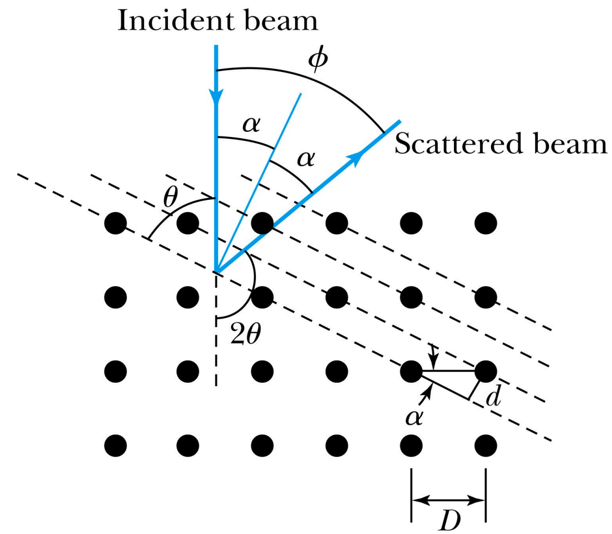
- What are the wavelengths of you running at the speed of 2m/s? What about your car of 2 metric tons at 100mph? How about the proton with 14TeV kinetic energy?
- What is the momentum of the photon from a green laser?

Electron Scattering

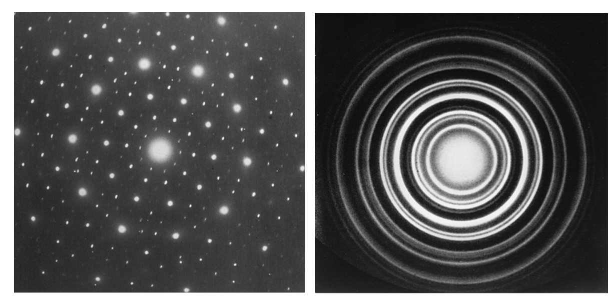
- Davisson and Germer experimentally observed that electrons were diffracted much like x rays in nickel crystals. ➔ direct proof of De Broglie wave!



$$\lambda = \frac{D\sin\phi}{n}$$



- George P. Thomson (1892–1975), son of J. J. Thomson, reported seeing the effects of electron diffraction in transmission experiments. The first target was celluloid, and soon after that gold, aluminum, and platinum were used. The randomly oriented polycrystalline sample of SnO_2 produces rings as shown in the figure at right.



(a) (b)

- Photons, which we thought were waves, act particle like (eg Photoelectric effect or Compton Scattering)
- Electrons, which we thought were particles, act particle like (eg electron scattering)
- De Broglie: All matter has intrinsic wavelength.
  – Wave length inversely proportional to momentum
  – The more massive… the smaller the wavelength… the harder to observe the wavelike properties
  – So while photons appear mostly wavelike, electrons (next lightest particle!) appear mostly particle like.
- How can we reconcile the wave/particle views?

Wave Motion

- De Broglie matter waves suggest a further description. The displacement of a wave is $$\Psi(x,t) = A\sin\left[\frac{2\pi}{\lambda}(x - vt)\right]$$
- This is a solution to the wave equation

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\Psi}{\partial t^2}$$

- Define the wave number *k* and the angular frequency ω as:

$$k \equiv \frac{2\pi}{\lambda} \text{ and } \omega = \frac{2\pi}{T} \qquad \lambda = vT$$

- The wave function is now: $\Psi(x,t) = A\sin[kx - \omega t]$

Wave Properties

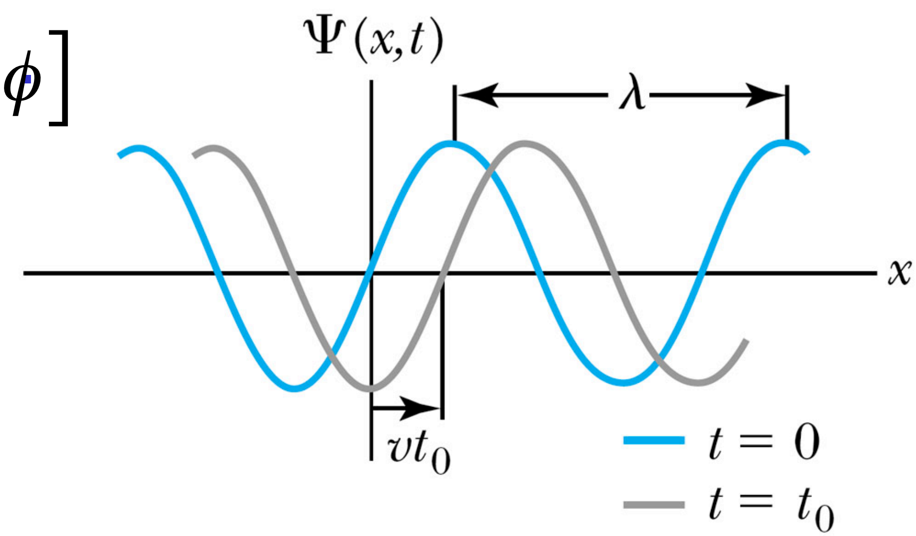
- The phase velocity is the velocity of a point on the wave that has a given phase (for example, the crest) and is given by

$$v_{ph} = \frac{\lambda}{T} = \frac{\lambda}{2\pi}\frac{2\pi}{T} = \frac{\omega}{k}$$

- A phase constant Φ shifts the wave:

$$\Psi(x,t) = A\sin\left[kx - \omega t + \phi\right]$$
$$= A\cos\left[kx - \omega t\right]$$

(When $\phi=\pi/2$)



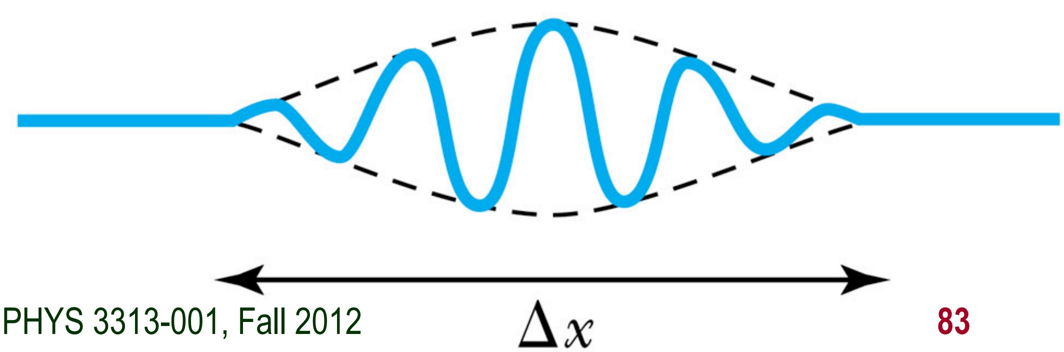
Principle of Superposition

- When two or more waves traverse the same region, they act independently of each other.
- Combining two waves yields:

$$\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t) = 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos\left(k_{\text{av}}x - \omega_{\text{av}}t\right)$$

- The combined wave oscillates within an envelope that denotes the maximum displacement of the combined waves.
- When combining many waves with different amplitudes and frequencies, a pulse, or **wave packet**, can be formed, which can move at a **group velocity**:

$$u_{\text{gr}} = \frac{\Delta\omega}{\Delta k}$$



Wave Packet Envelope

- The superposition of two waves yields a wave number and angular frequency of the wave packet envelope. $$\frac{\Delta k}{2}x - \frac{\Delta \omega}{2}$$
- The range of wave numbers and angular frequencies that produce the wave packet have the following relations:

$$\Delta k \Delta x = 2\pi \qquad \Delta \omega \Delta t = 2\pi$$

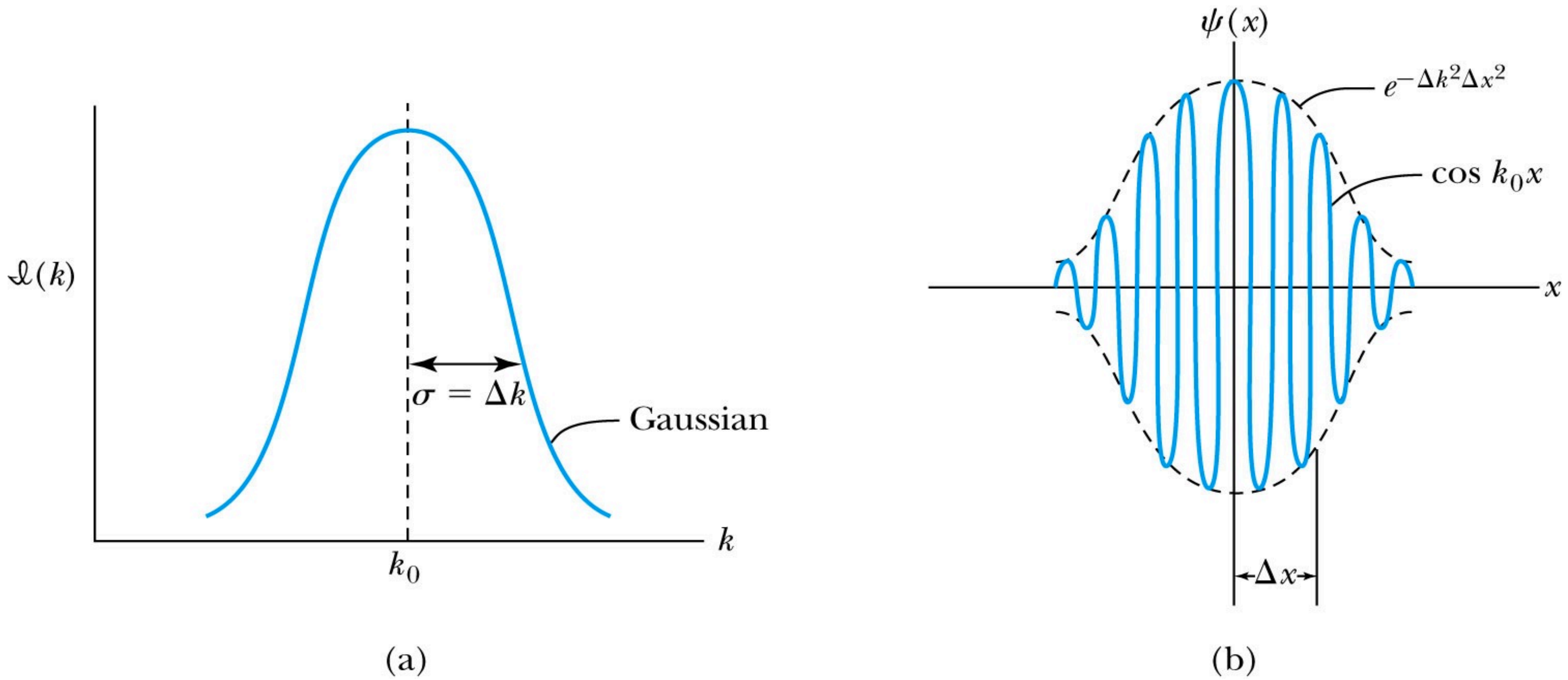
- A **Gaussian wave packet** has similar relations:

$$\Delta k \Delta x = \frac{1}{2} \qquad \Delta \omega \Delta t = \frac{1}{2}$$

- The localization of the wave packet over a small region to describe a particle requires a large range of wave numbers. Conversely, a small range of wave numbers cannot produce a wave packet localized within a small distance.

Gaussian Function

- A Gaussian wave packet describes the envelope of a pulse wave. $\Psi(x,0)=\Psi(x)=Ae^{-\Delta k^2 x^2}\cos(k_0 x)$



- The group velocity is $u_{gr} = \dfrac{d\omega}{dk}$

Wave particle duality solution

- The solution to the wave particle duality of an event is given by the following principle.
- **Bohr's principle of complementarity**: It is not possible to describe physical observables simultaneously in terms of both particles and waves.
- **Physical observables** are the quantities such as position, velocity, momentum, and energy that can be experimentally measured. In any given instance we must use either the particle description or the wave description.

Heisenberg's Uncertainty Principle

- Due to the wave-particle duality of matter, there are limiting factors in precise measurements of closely related physical quantities.
- Momentum – position uncertainty

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

- Energy – time uncertainty

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Probability, Wave Functions, and the Copenhagen Interpretation

- The wave function determines the likelihood (or probability) of finding a particle at a particular position in space at a given time.

$$P(y)dy = \left|\Psi(y,t)^2\right|dy$$

- The total probability of finding the electron is 1. Forcing this condition on the wave function is called normalization.

$$\int_{-\infty}^{+\infty} P(y)dy = \int_{-\infty}^{+\infty} \left|\Psi(y,t)^2\right|dy = 1$$

The Copenhagen Interpretation

- Bohr's interpretation of the wave function consisted of 3 principles:
  1) The uncertainty principle of Heisenberg
  2) The complementarity principle of Bohr
  3) The statistical interpretation of Born, based on probabilities determined by the wave function
- Together these three concepts form a logical interpretation of the physical meaning of quantum theory. According to the Copenhagen interpretation, physics depends on the outcomes of measurement.

Probability of the Particle

- The probability of observing the particle between *x* and *x* + *dx* in each state is

$$P_n\, dx \propto \left|\Psi_n(x)\right|^2 dx$$

- Note that $E_0 = 0$ is not a possible energy level.
- The concept of energy levels, as first discussed in the Bohr model, has surfaced in a natural way by using waves.