# Chemistry 9724y: Materials analysis using synchrotron radiation

**Instructor: T.K. Sham (tsham@uwo.ca)**

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|---|---|---|
| Course outline | see handout | |
| Course evaluation | problem sets | 55% |
| | essay/research proposal | 25% |
| | oral presentation | 20% |

**Essay topics:**

You can select **any topic that is relevant to this course** (e.g. XAFS studies of Hg in the environment etc.) or write a **research proposal** on the analysis of systems of your own research. Send your topic with a couple of key references to me **not later than December 4, 2013**.

The essay/research proposal (5 pages max, single line space, 12 point, 1 page appendix allowed) is due after the new year and the presentation (12 min + 3 min questions) is scheduled for the winter term not later than the end of the reading week.

# Course Objectives

To familiarize students with the principles and the applications of synchrotron techniques for materials analysis.

Emphasis: spectroscopy using X-rays with tunable wavelength (energy)

**References:**

**J. Stöhr**, NEXAFS Spectroscopy (Springer, 1992)

**D. Koningsberger & R. Prins**, (eds), X-ray Absorption Spectroscopy: Principles, Applications and Techniques of EXAFS, SEXAFS and XANES (Wiley, 1988)

**T.K. Sham** (ed) Chemical Applications of Synchrotron Radiation (World Scientific, 2002)

**Frank de Groot and Akio Kotani**, Core Level Spectroscopy of Solids (Taylor & Francis CRC press, 2008)

**Grant Bunker** Introduction to XAFS Cambridge University press, 2012

# Some relevant questions

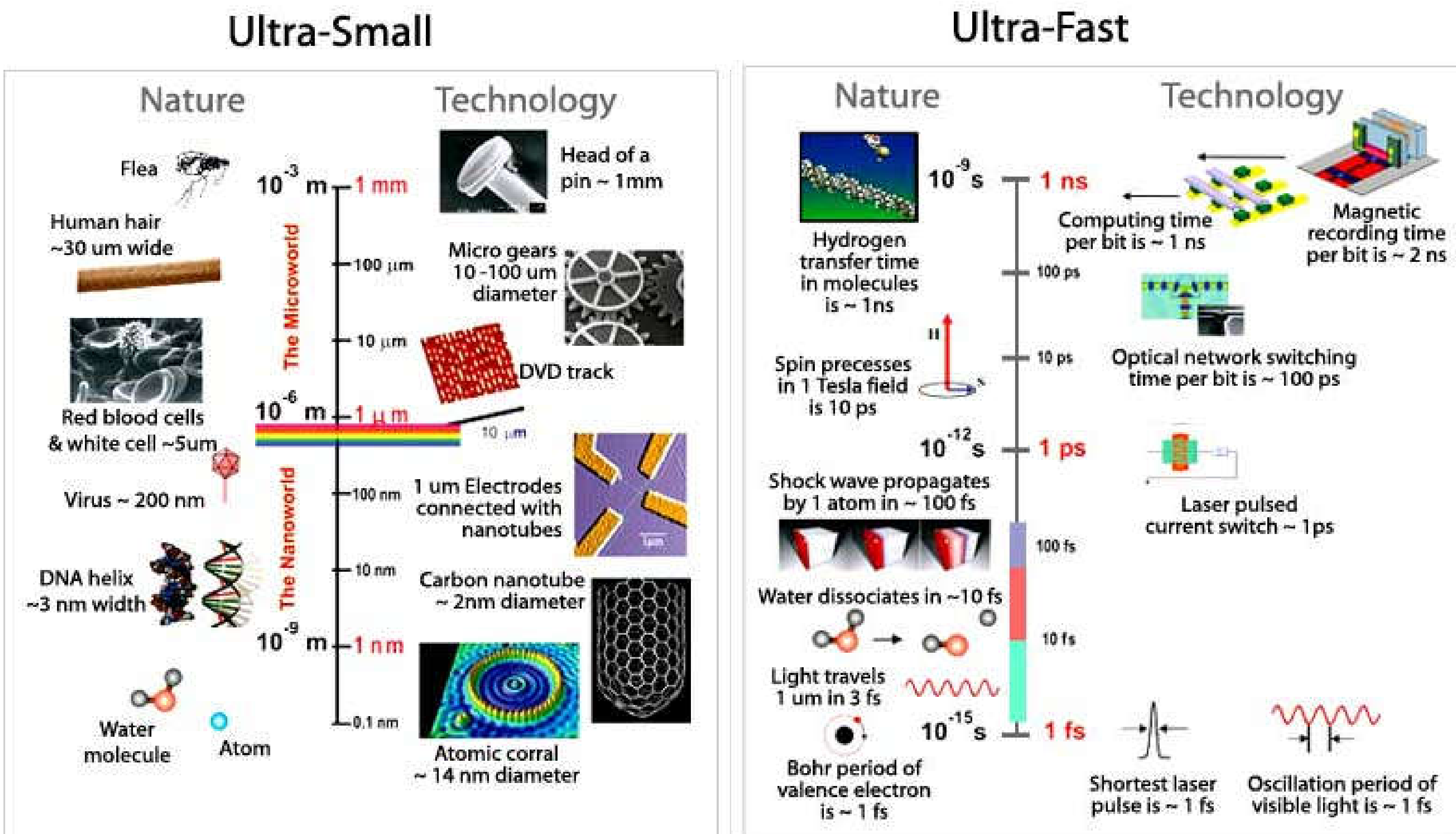
- What is material ?
- Why do we want to analyze materials ?
- What is synchrotron radiation ?
- Why is synchrotron useful in materials analysis ?
- How do we analyze materials using SR?

# Perspective: Science of length scale in size, energy and time

- The **ruler** must have divisions comparable or smaller than the dimension of the object

- The **clock** must have a time response faster than the duration of the event it is measuring

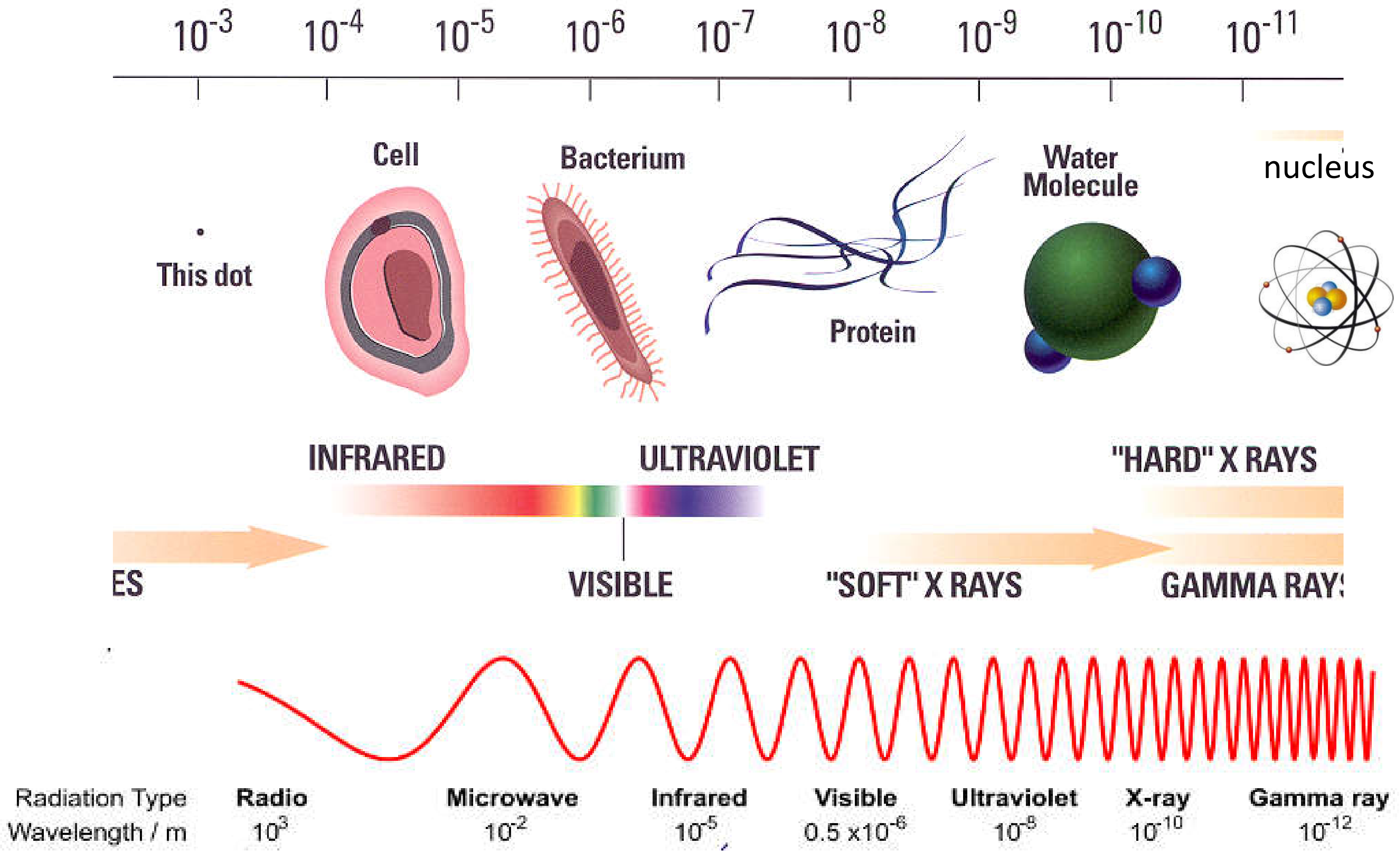
# Scale of things in size and time



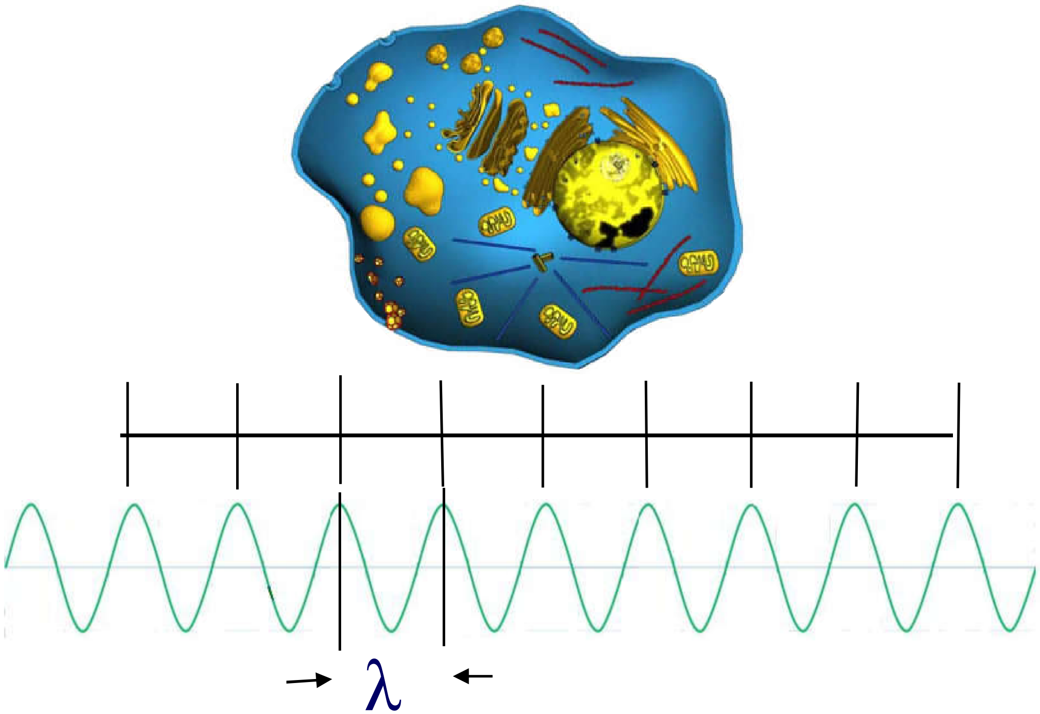

**Synchrotron is a powerful tool for these studies**

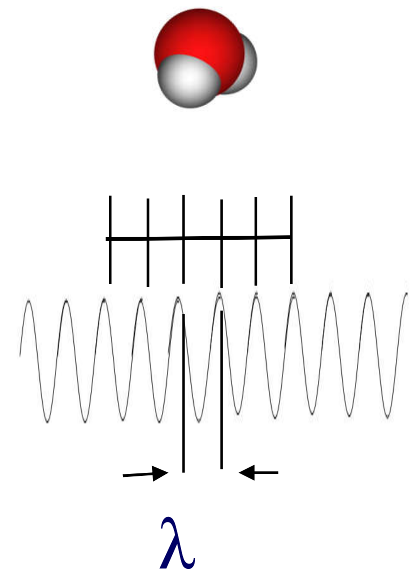
Source: US DOE

# Matching of object dimension and wavelength



# “Rulers” for small length scale: Photons and Electrons




Synchrotron radiation: photons with tunable wavelength, $\lambda$ ($10^4$ nm – $10^{-3}$ nm)

de Broglie wavelength of electrons can also be tuned with its energy 200 kV TEM $\lambda_e = 2.5$ pm = 0.025Å

# Materials: matter with desired functionality

## General considerations

- Materials can be classified by

a) phase: gas, liquid and solid (crystalline, amorphous, polymer)

b) properties: metal, semiconductor, insulator, soft matter, etc.

c) composition: pure substance, composite

d) functionalities: biomaterials, nanomaterials, LED materials, superconductor, energy materials, nuclear materials, soft matter etc.

# Issues in materials analysis

Microscopic:

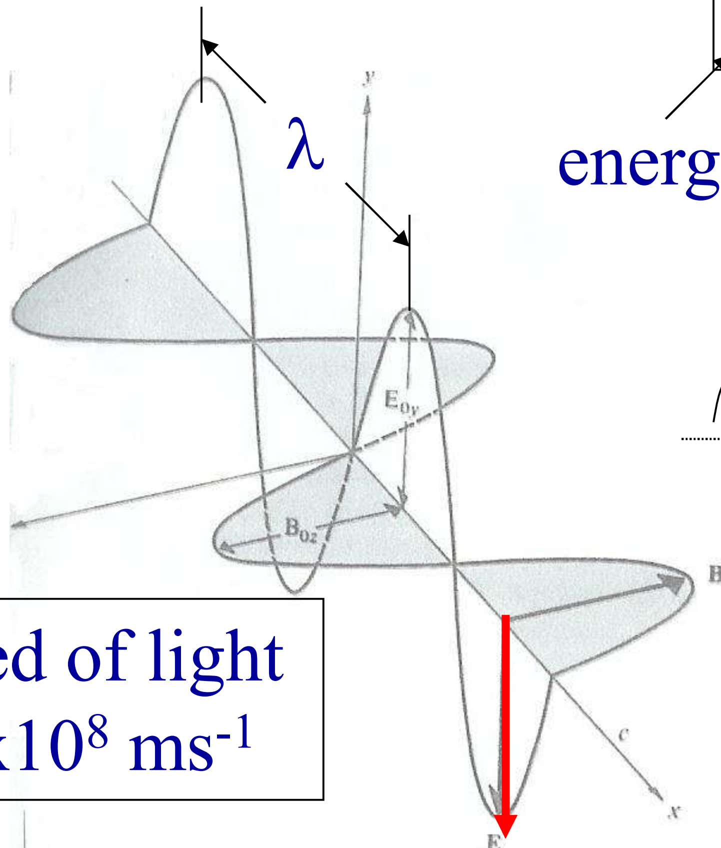
- Structure (arrange of atoms in space)
- Bonding (oxidation state, electronic structure/distribution)

Macroscopic:

- Chemical, mechanical, electrical, magnetic, optical, physiochemical biocompatibility properties, etc.

# Probing matter with SR, a versatile *light source*

## What is *light* ? (wave and particle dual behavior)

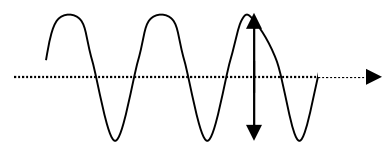



$E = h\nu = hc/\lambda$

energy

frequency($s^{-1}$)

***E*** vector (polarization)



propagation

c: speed of light
$c = 3 \times 10^{8}\ ms^{-1}$

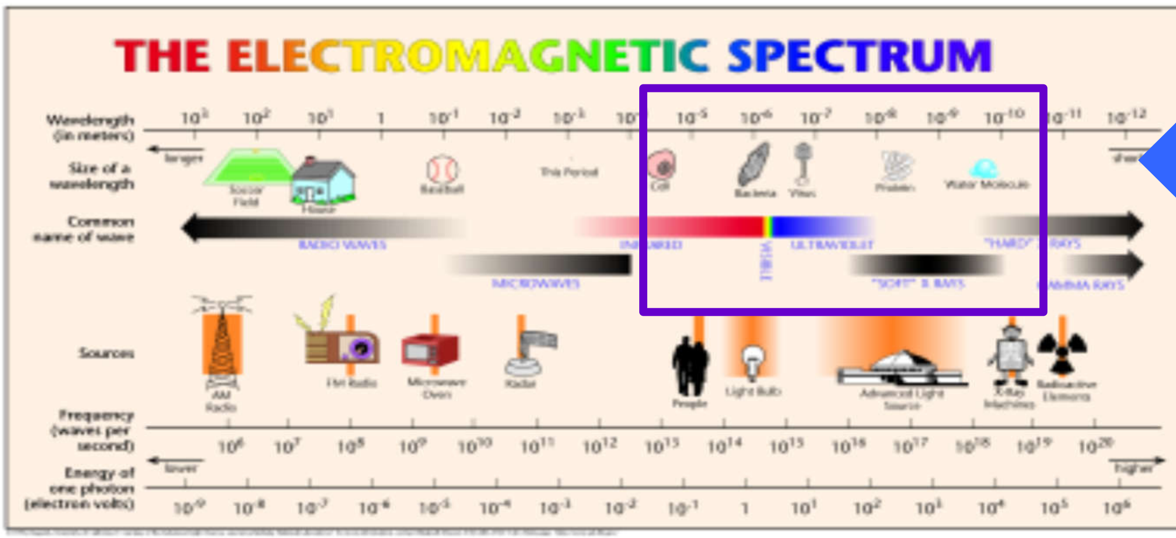
*h*: Planck's constant
$h = 6.626 \times 10^{-34}$ Js

The interaction of ***B*** field with matter is at least 2 orders of magnitude weaker than the ***E*** field

# Electromagnetic wave spectrum

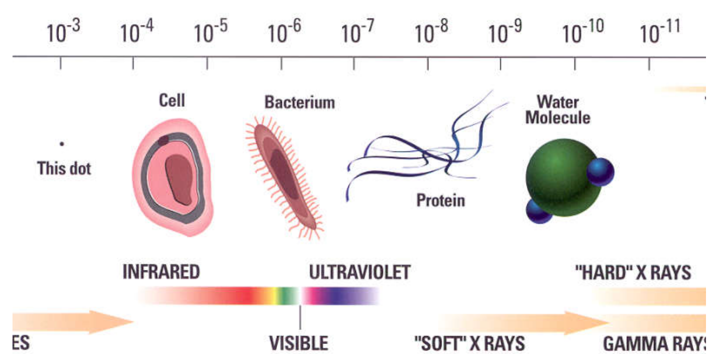
$$\lambda(\text{Å}) = 12398.5/E(\text{eV})$$

$\lambda$



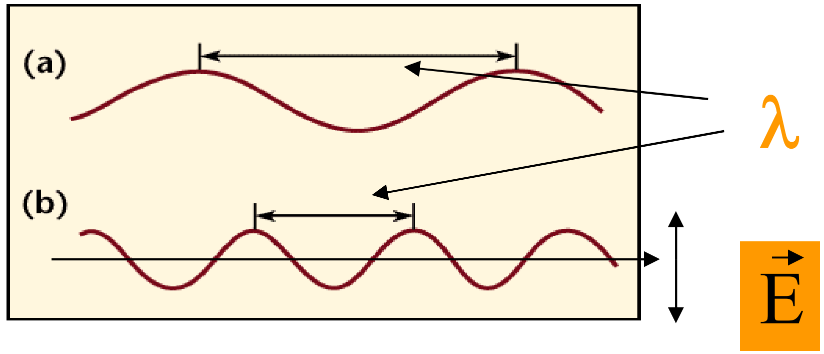

object size

Light sees object with dimension comparable to its wavelength

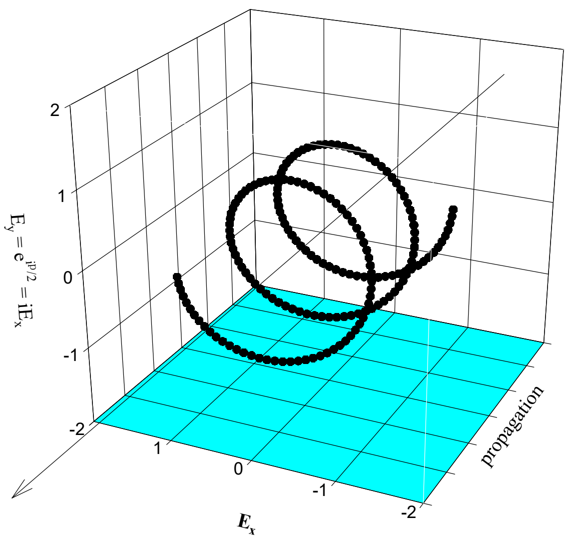


# What is light?

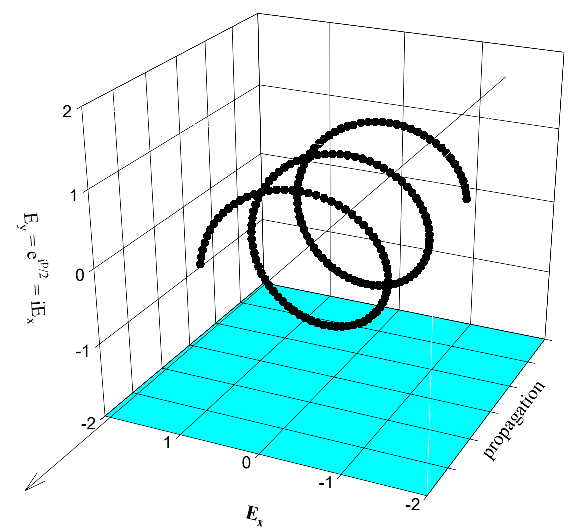
Light is a particle with spin = 1, 0 mass and behaves like a wave




**linear polarized**




**E** precesses to the left or right along the direction of propagation




**circular polarized light**

# How is light produced ?

**“Acceleration of charge particles”**

- Linear acceleration of charge particles
- Electric dipole oscillations
- Synchrotron radiation (centrifugal acceleration)

# How is light produced ?

**“Radiative transitions”**

Line spectrum (single frequency):

- Transition between valence and inner valence/shallow core level yields visible and UV light
- Deep core levels yields X-rays
- Energy levels of the nucleus yields γ rays

**How is light produced ?**

**“Acceleration of charge particles”**

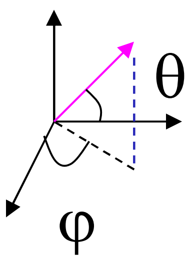
# Linear acceleration of a charge particle

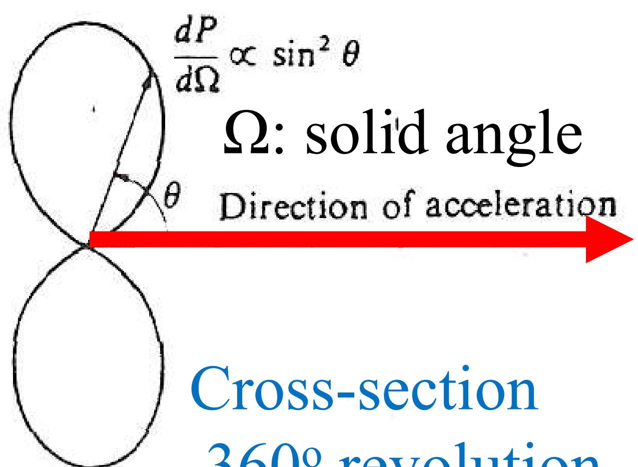
Instantaneous power radiated (energy per unit time)

**Larmor equation** $P = (2/3)\,(e^2/m^2c^3)\,(dp/dt)^2$

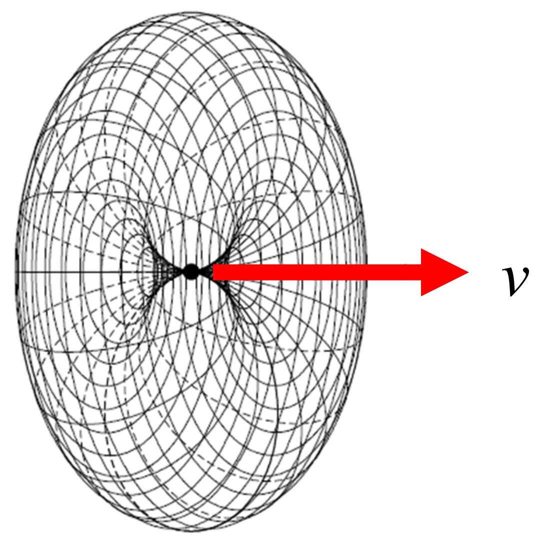
$dp/dt = m(dv/dt) = ma$

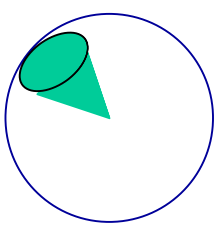
*p*: momentum (mv); m, mass; c, speed of light;
e, electron charge, ***a*: acceleration**



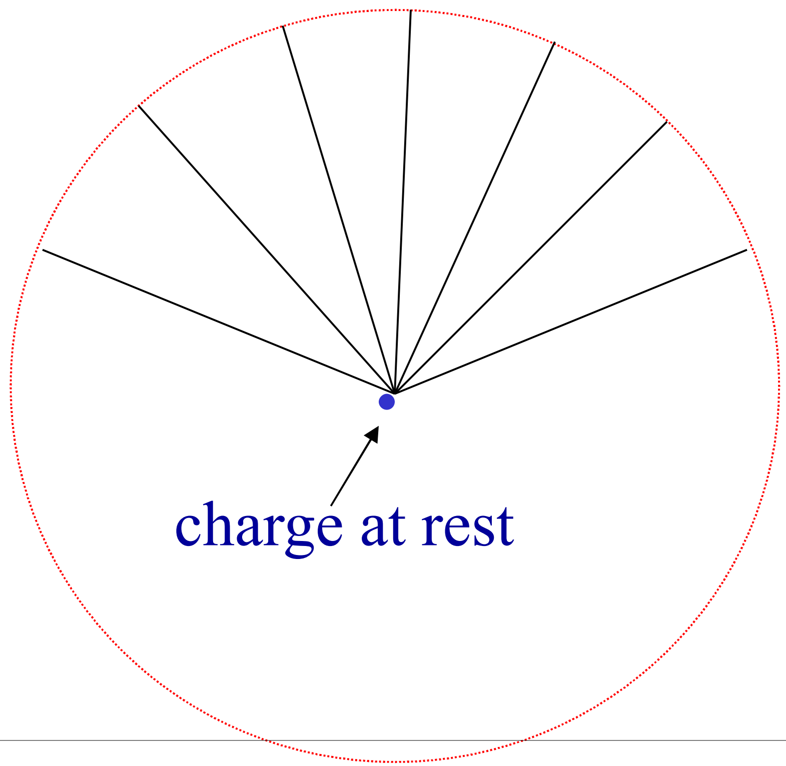

Ω: solid angle  v << c



Cross-section
360° revolution → donut shape

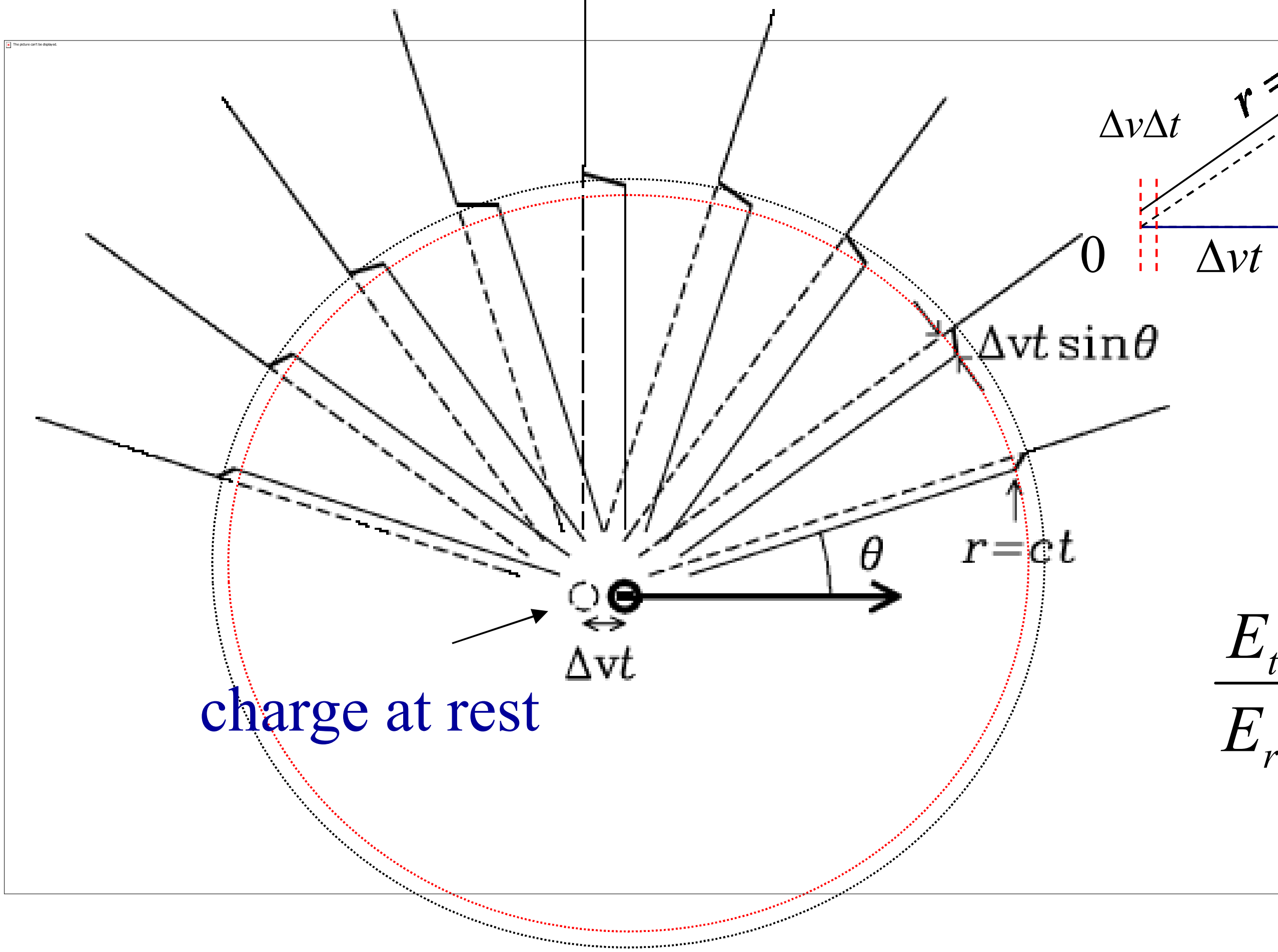
# How does an electron radiate? How does the Larmor equation come about?

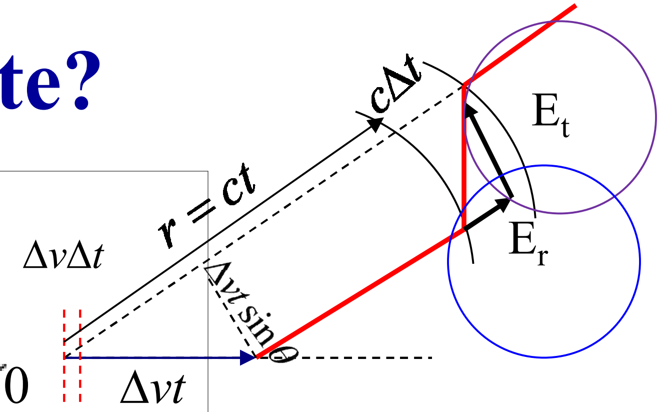



***E*** field lines travels outward at speed of light c; At a given time t, the radius r = ct

charge accelerates to a velocity $\Delta v$ within a very short time interval $\Delta t$, what is the ***E*** field line after a time $t$

# How does an electron radiate?




$$\Delta v \Delta t << \Delta v t$$

$$\theta \sim \theta'$$

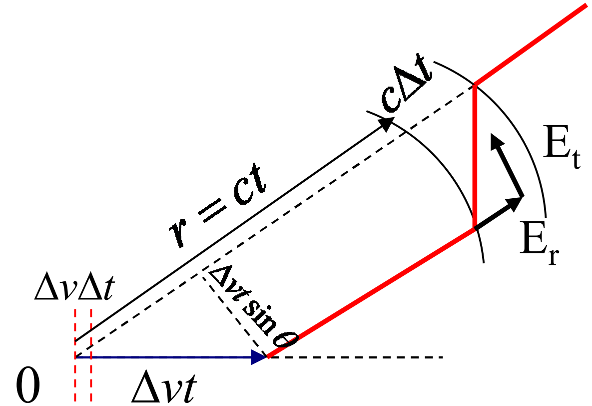
$$\frac{E_t}{E_r} = \frac{\Delta v t \sin\theta}{c\Delta t}$$

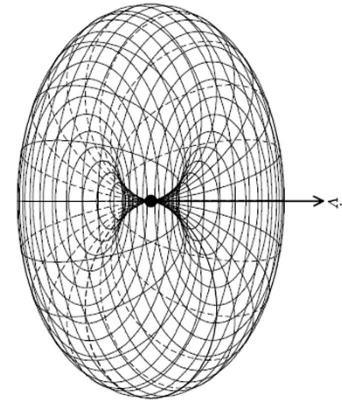
charge at rest is accelerated to a slow velocity $\Delta v$ within a very short time $\Delta t$, ( acceleration $= \dot{v} = \Delta v / \Delta t$ ) the field line E after time $t$

# How does e radiate?

$$\frac{E_t(transverse)}{E_r(radial)} = \frac{\Delta vt \sin\theta}{c\Delta t}$$

$$E_r = \frac{q}{r^2}, \quad E_t = \frac{q}{r^2}\left(\frac{\Delta v}{\Delta t}\right)\frac{r\sin\theta}{c^2},$$



$$E_t \propto \frac{1}{r}; \qquad E_r \propto \frac{1}{r^2}$$

For large r, $E_r$ becomes negligible only $E_t$ remains, thus at large distance, we shall be left with a pulse of a transverse field traveling outward with velocity c

# How much energy per unit time (power) is radiated as light in each direction?

In a vacuum, the Poynting flux, or power per unit area (erg $s^{-1}$ $cm^{-2}$ )

$$\vec{S} = \frac{c\ \vec{E} \times \vec{H}}{4\pi}, \quad in \quad cgs \quad units \quad \left|\vec{E}\right| = \left|\vec{H}\right|, \ \left|\vec{S}\right| = \frac{c}{4\pi} E^2$$

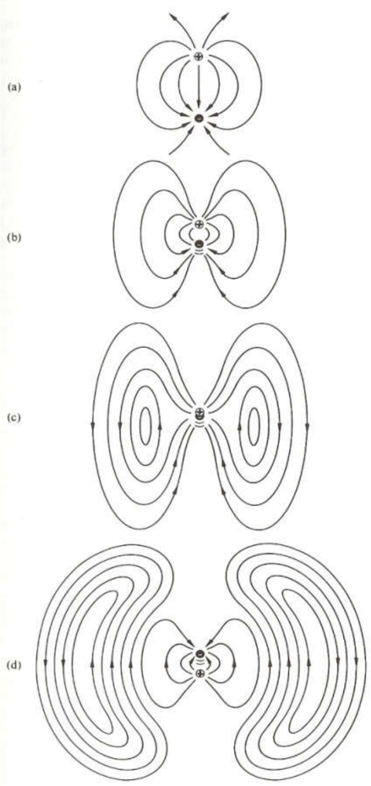
$$\left|\vec{S}\right| = \frac{c}{4\pi} E_t^2 = \frac{q^2}{4\pi}\left(\frac{\Delta v}{\Delta t}\right)^2 \frac{\sin^2\theta}{c^3 r^2}$$

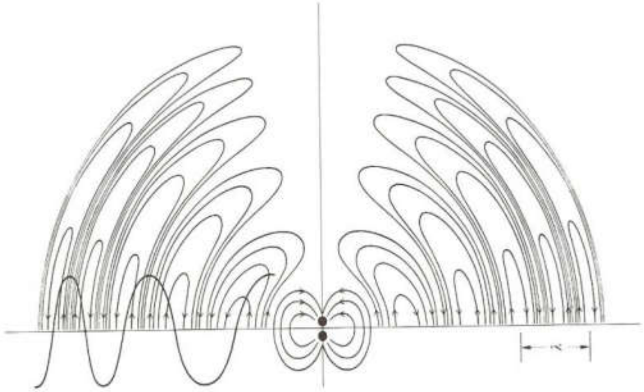
$$P = \int \left|\vec{S}\right| dA = \frac{q^2 \dot{v}^2}{4\pi c^3} \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \frac{\sin^2\theta}{r^2} r \sin\theta d\theta r d\phi$$

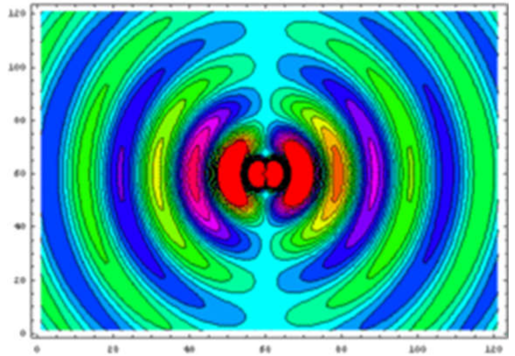
**Larmor equation**

$$P = \frac{2}{3}\frac{q^2\dot{v}^2}{c^3} = \frac{2}{3}\frac{q^2\dot{p}^2}{m^2c^3} = \frac{2}{3}\frac{q^2}{m^2c^3}\left(\frac{dp}{dt}\right)^2$$

# Electric dipole oscillation

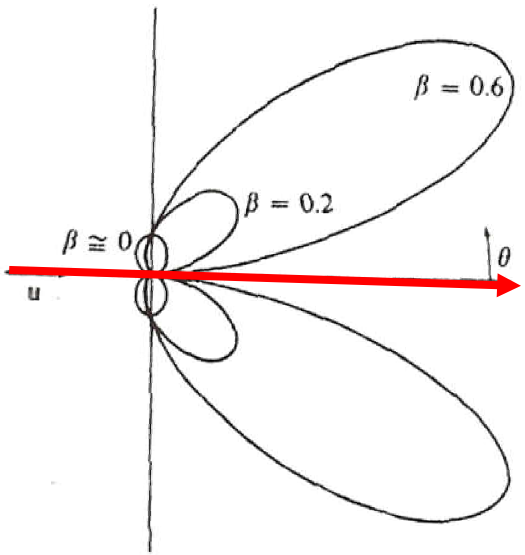





The **E** field of an oscillating dipole

# Linear acceleration of a charge particle traveling at nearly the speed of light (**relativistic**)




$$P = \frac{2}{3}\frac{q^2}{m^2c^3}\left(\frac{dp}{dt}\right)^2,$$

$$p = \frac{mv}{\sqrt{1-\beta^2}}, \quad E = \frac{mc^2}{\sqrt{1-\beta^2}}$$

For **relativistic particles**,

**β** = $v$/c ~1, **γ** = mass (m)/ rest mass ($m_0$)

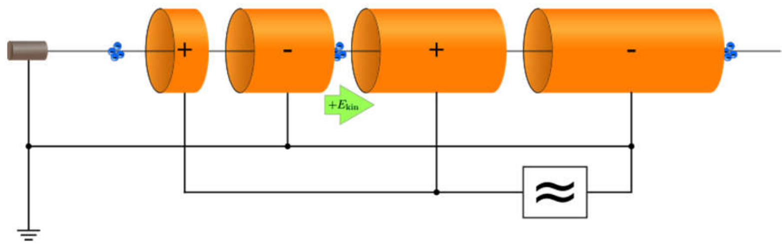
For electrons, the rest mass = 0.511 MeV

For e, γ = $E/m_0c^2 = 1/\sqrt{1-(v/c)^2}$ = 1957 E (GeV)

only true for fast e

# Energy loss to radiation in linear acceleration

$$P = \frac{2}{3}\frac{q^2}{m^2c^3}\left(\frac{dp}{dt}\right)^2 = \frac{2}{3}\frac{q^2}{m^2c^3}\left(\frac{dE}{dx}\right)^2$$



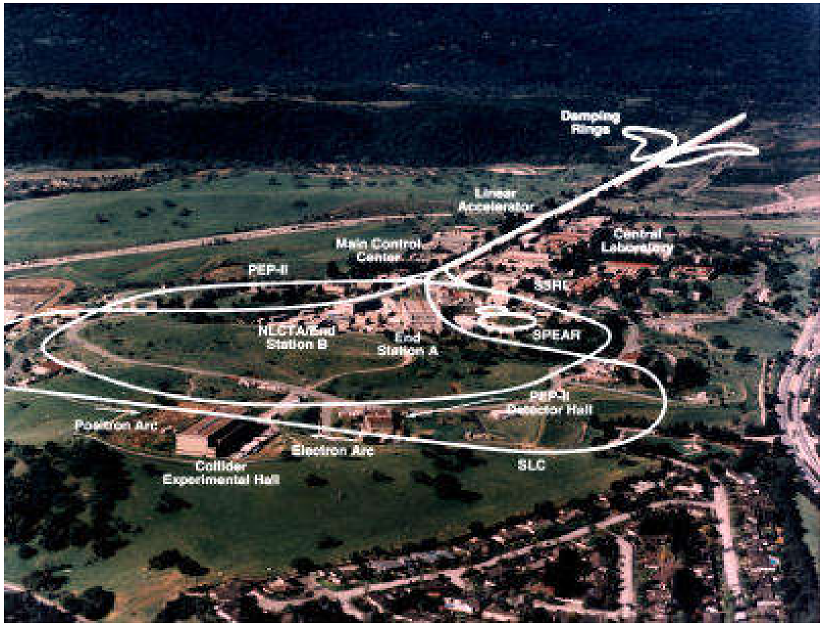
RF cavity

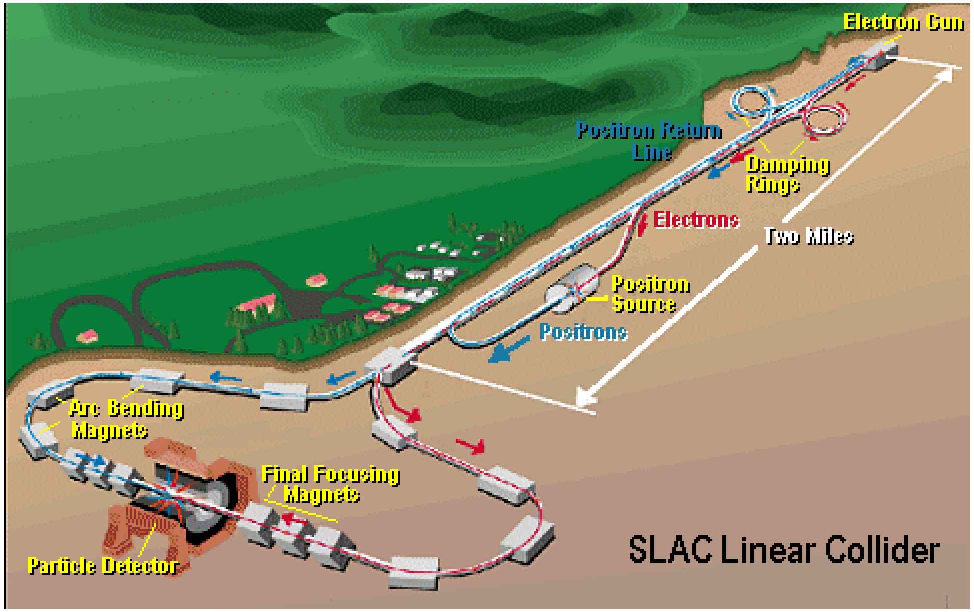
The energy loss via radiation P, compares with the energy gained per unit length *dE/dx* is

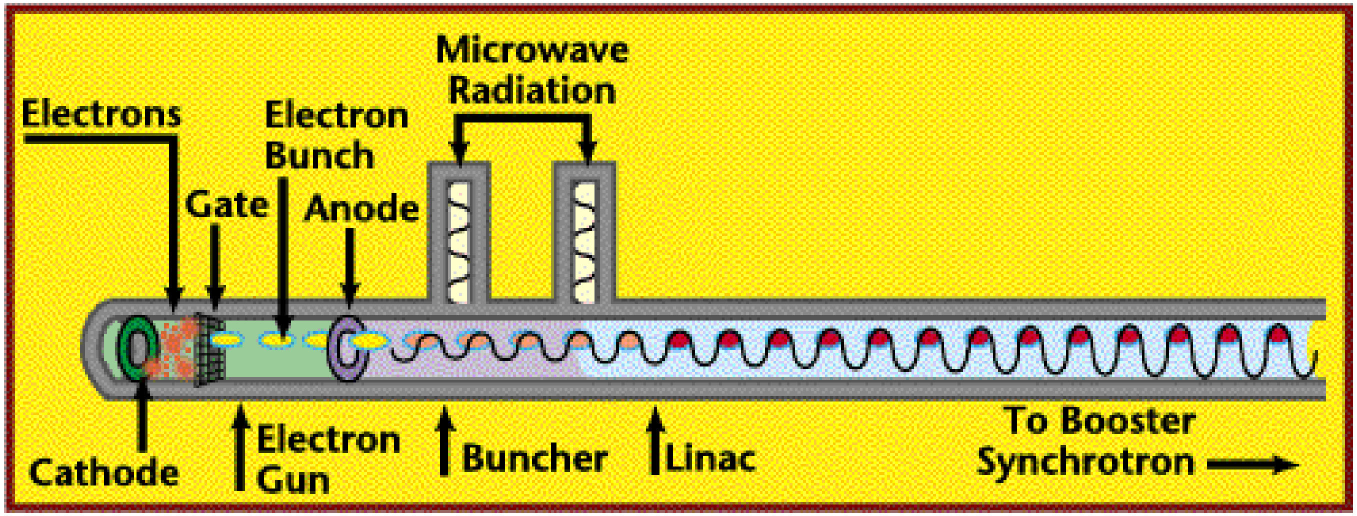
$$\frac{P}{dE/dx} = \frac{2}{3}\frac{e^2}{mc}\frac{dE/mc^2}{dx}$$

The loss for high energy electron is very small, show it!

Further reading, J. Schwinger, Phys. Rev. 75, 1912, (1949)


Damping Rings
Linear Accelerator
Central Laboratory
Main Control Center
PEP-II
SSRL
NLCTA/End Station B
End Station A
SPEAR
PEP-II Detector Hall
Positron Arc
Electron Arc
Collider Experimental Hall
SLC

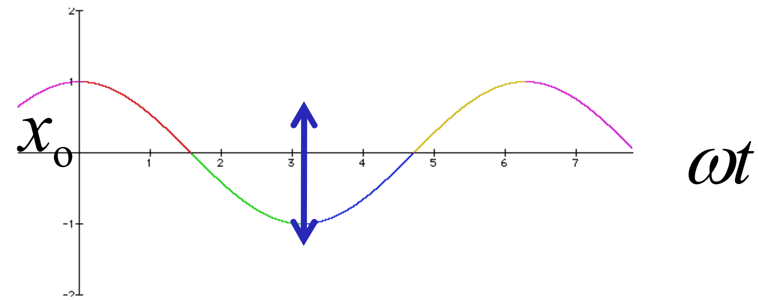

Electron Gun
Positron Return Line
Damping Rings
Electrons
Two Miles
Positron Source
Positrons
Arc Bending Magnets
Final Focusing Magnets
Particle Detector
SLAC Linear Collider


Microwave Radiation
Electrons
Electron Bunch
Gate
Anode
Cathode
Electron Gun
Buncher
Linac
To Booster Synchrotron

# Example

Consider an electron moving in the x direction with the motion described by

$$x = x_o \cos \omega t$$



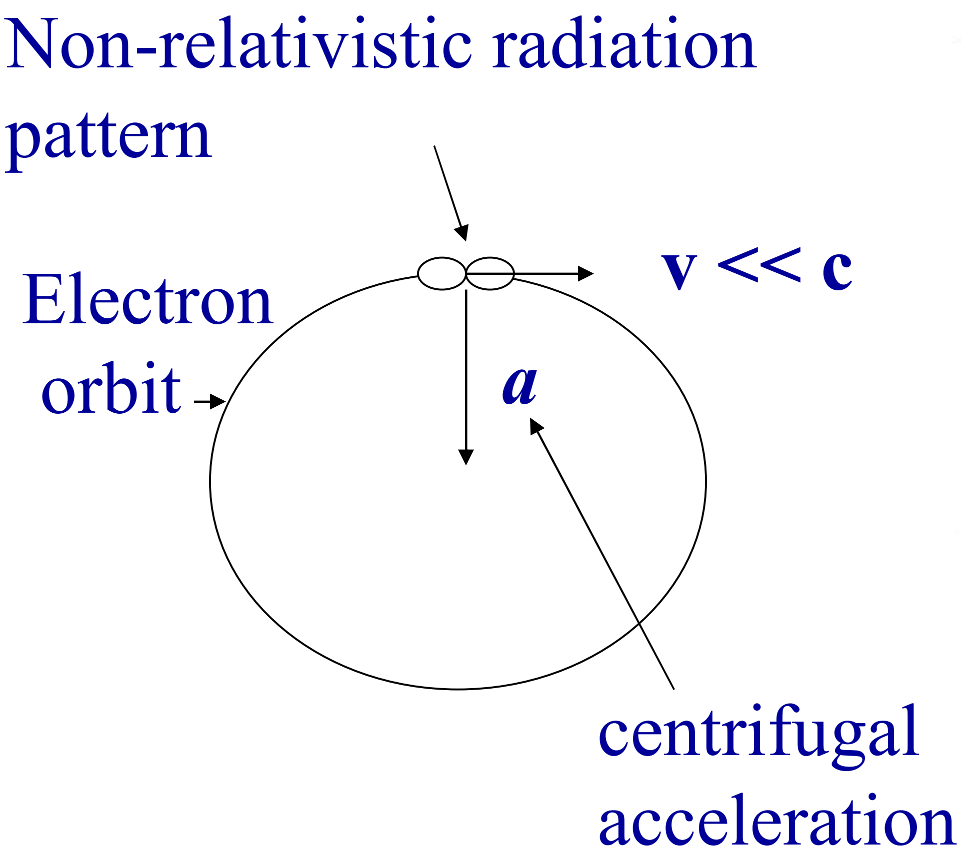

This corresponds to an oscillatory electric dipole with amplitude of $x_o$ and angular frequency $\omega$. If the acceleration $\boldsymbol{a = -\omega^2 x}$, we have

$$P = \frac{2}{3}\frac{q^2}{m^2c^3}\left(\frac{dp}{dt}\right)^2 = \frac{2}{3}\frac{e^2a^2}{c^3} = \frac{2}{3}\frac{e^2x^2\omega^4}{c^3}$$

$$\left\langle x^2 \right\rangle = \tfrac{1}{2}x_o^2$$

$$P_{average} = \frac{2}{3}\frac{e^2x^2\omega^4}{c^3} = \frac{1}{3}\frac{e^2x_o^2\omega^4}{c^3}$$

# Synchrotron Radiation



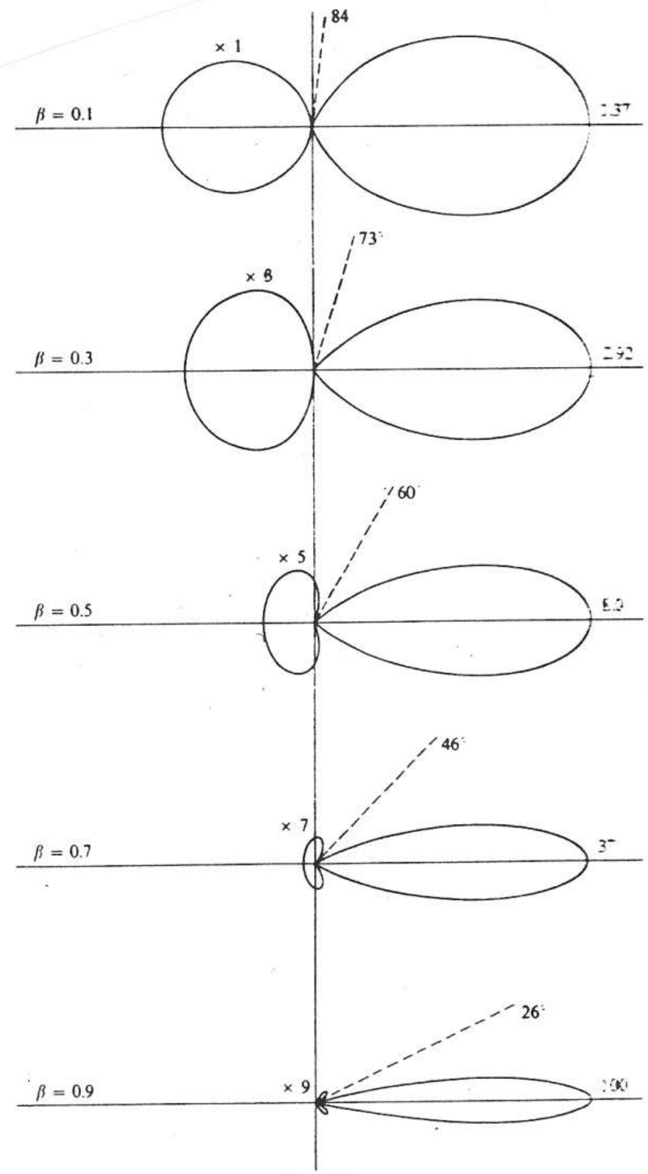
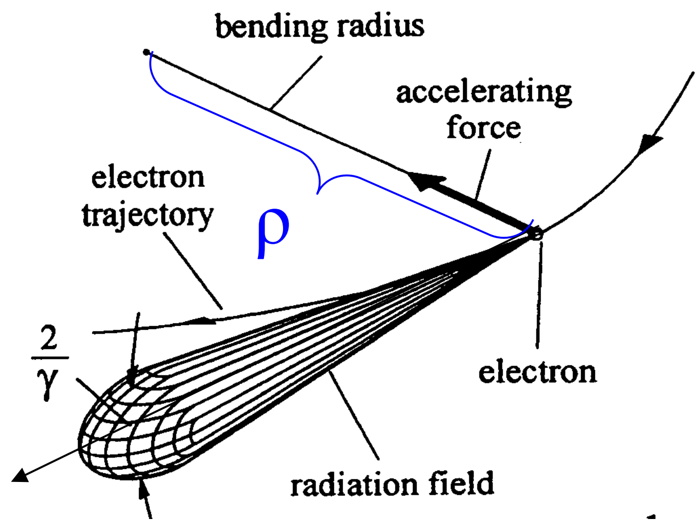




FIG. 7-7

For **relativistic electrons**, $\beta = v/c \sim 1$
$\beta$ = speed (v)/ speed of light (c)
$\gamma$ = mass (m)/ rest mass ($m_0$)
the e rest mass = 0.511 MeV

# Synchrotron radiation

- A relativistic electron with energy **E**, bent by a **magnetic field H**, with a radius of curvature ρ in a circular path will radiate energy ***per turn*** with radiated power, ***P***.
- $P = (2/3)\,(e^2 c/\rho^2)\beta^4\gamma^4$
- ρ is the radius of curvature
- $1/\gamma$ is the opening angle




**Example:** ρ

If the energy of the e is in GeV ($10^9$ eV) and the radius in metre, the power radiated per turn for ring current I in ampere is

$$P = 88.5\ I\ E^4/\rho \qquad \text{(kw)}$$

# Example

- The Synchrotron Radiation Center in Wisconsin has the following parameters

  **E = 0.8 GeV**, **$\rho$ = 2.0833 m**, what is the energy loss of the electron per turn to synchrotron radiation?

  **Solution:**

  From **$P = 88.5\ I\ E^4/\rho$ (kw)**

  we get $P = 17.4\ I$ (kw)

  Energy loss (for a single 0.8 GeV $e^-$): $\delta E = 17.4$ keV/turn

  [show this!]

hint: W= J/s, J = AVs

# How is light produced ?

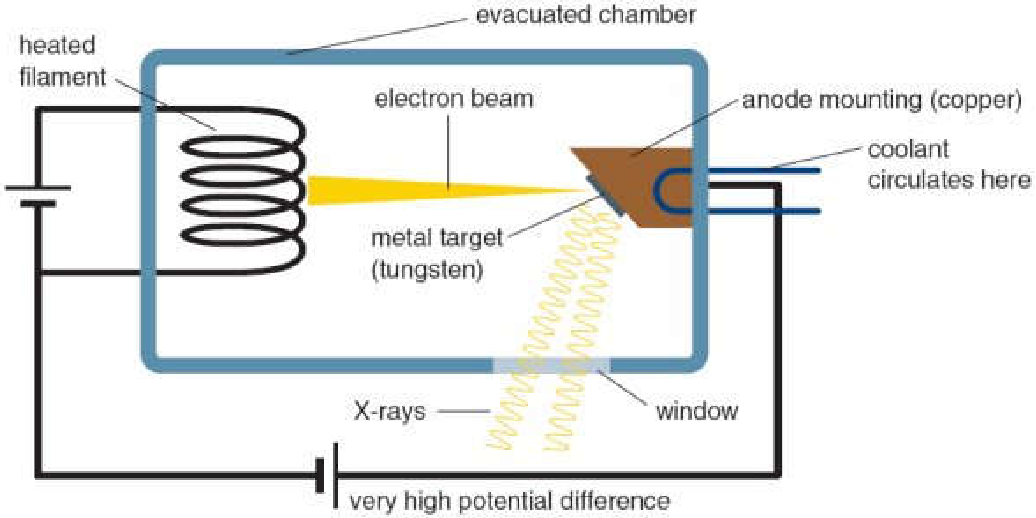
## “Radiative transitions”

**X- ray line spectrum**:
Transition of electrons from shallower levels to fill the core hole in deeper core levels yields X-rays of characteristic energy which is equal to the binding energy of the levels involved.

# X- rays

## November 8, 1895: Roentgen's Discovery of X-Rays

http://www.aps.org/publications/apsnews/200111/history.cfm



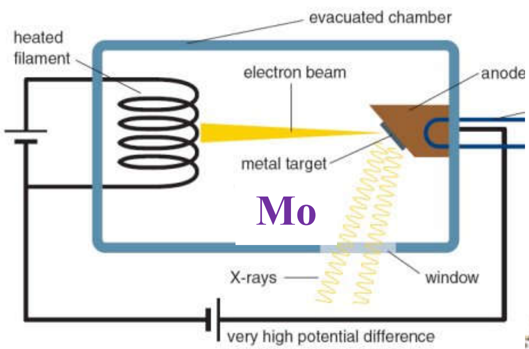

What does the X-ray spectrum look like?

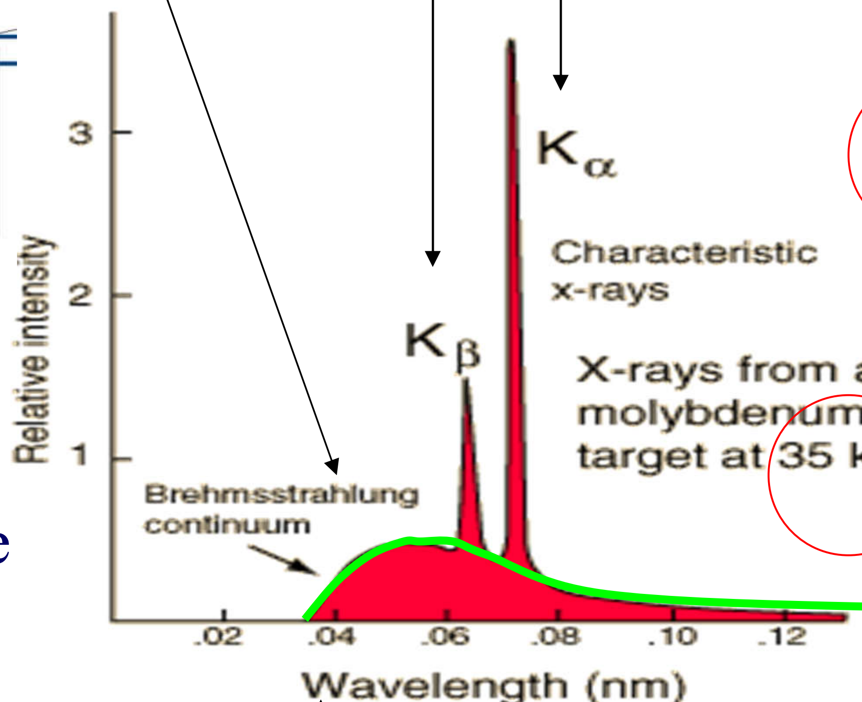
# X-ray spectrum (conventional instrument)

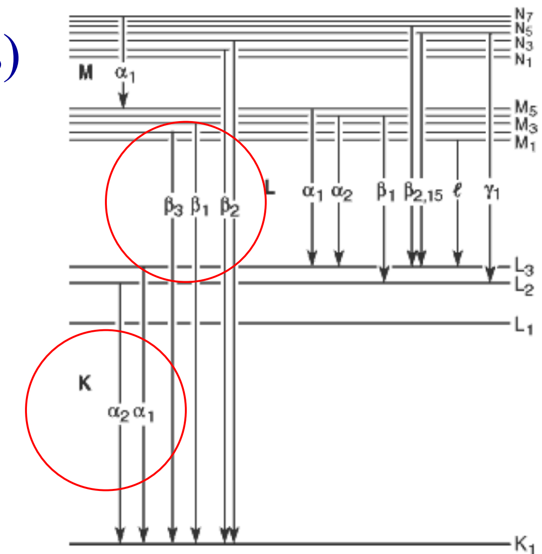
## Continuum and Characteristic Line spectrum

Bremsstrahlung (braking radiation)

Characteristic of element (Mo) and core level (K, 1s)




V must be higher than the energy of the line X-rays

V determines the high energy cut-off of the Bremsstrahlung

$K_{\alpha 1}$ = 17.479 keV (0.071 nm)

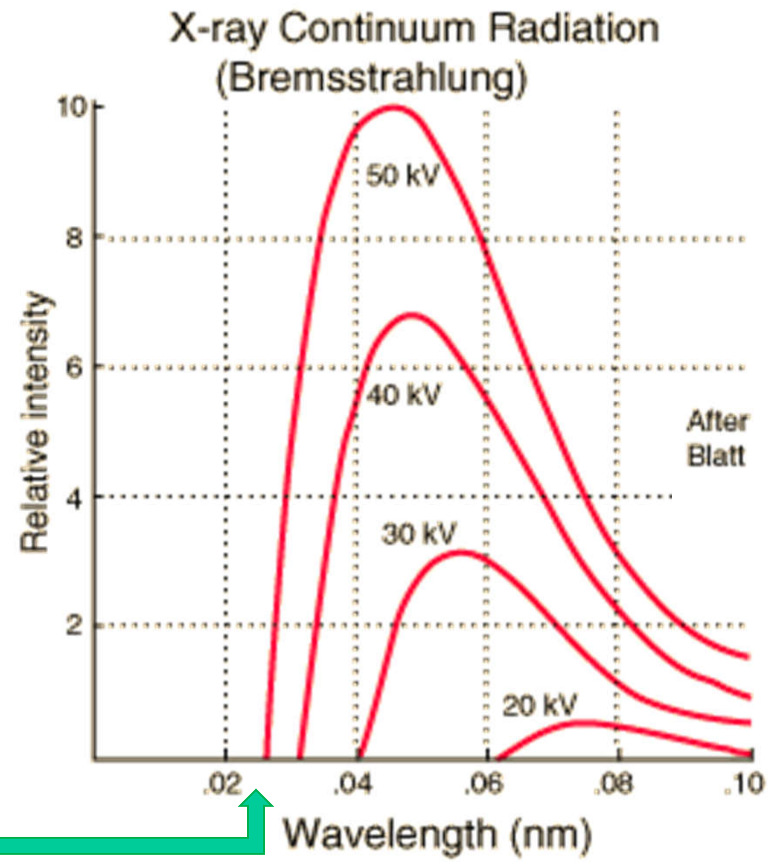
cutoff

How is the measurement made?

# Bremsstrahlung (braking radiation): the continuum

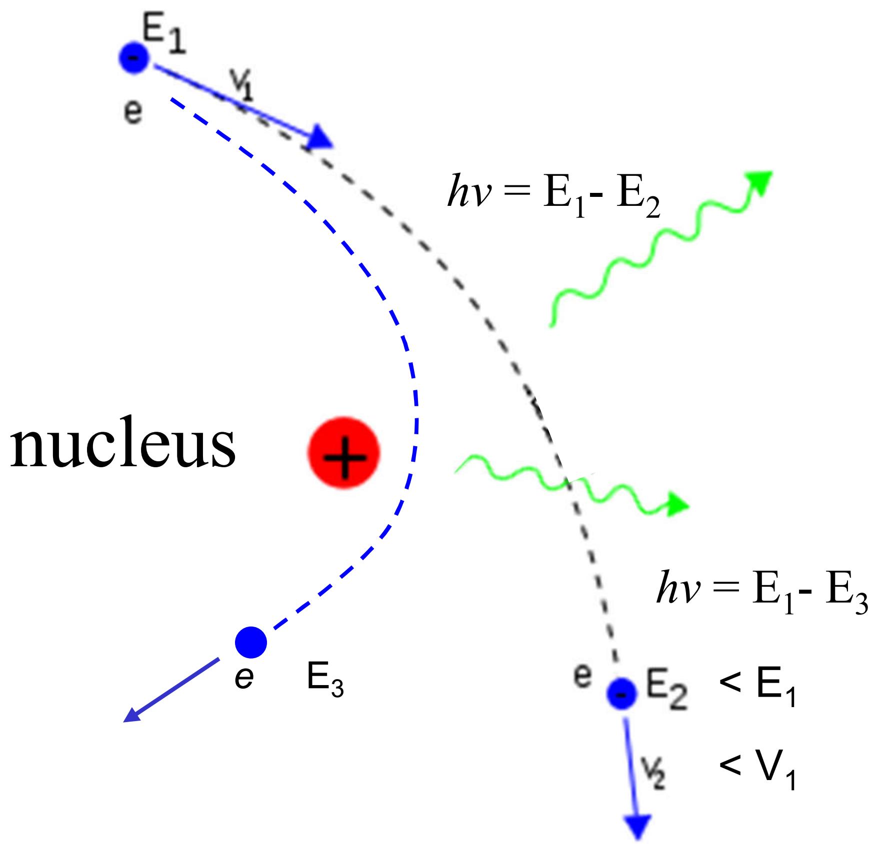
- A broad continuum with a short wavelength cut-off
- The higher the Voltage (energy), the more intense the X-ray and the shorter wavelength the cut-off

$$\lambda_{cut-off}(nm) = \frac{1239.85}{E(eV)}$$




**Before synchrotron radiation, Bremsstrahlung was the only way to produce tunable X-rays**

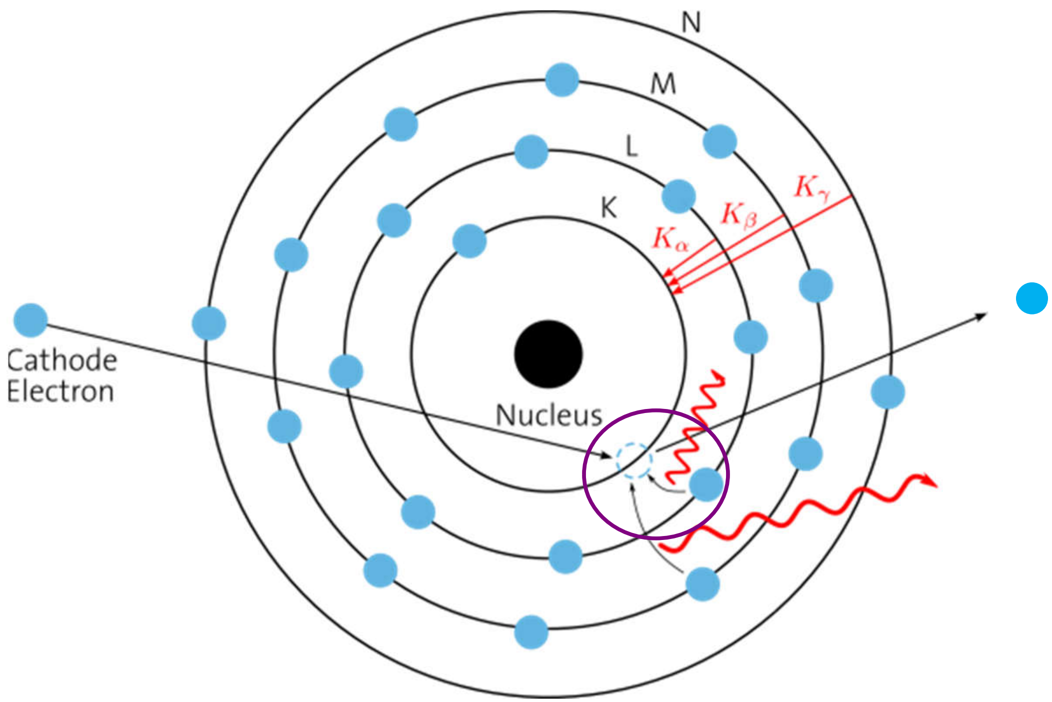
# How does Bremsstrahlung, the continuum come about ?




The closer the electron to the nucleus, the bigger the bent, the bigger the energy loss to radiation

# X-ray: the characteristic line emission

Characteristic X- rays are emitted when outer shell **electron fills** the inner shell **hole** left behind when the inner shell electrons are knocked off by the energetic incoming electron

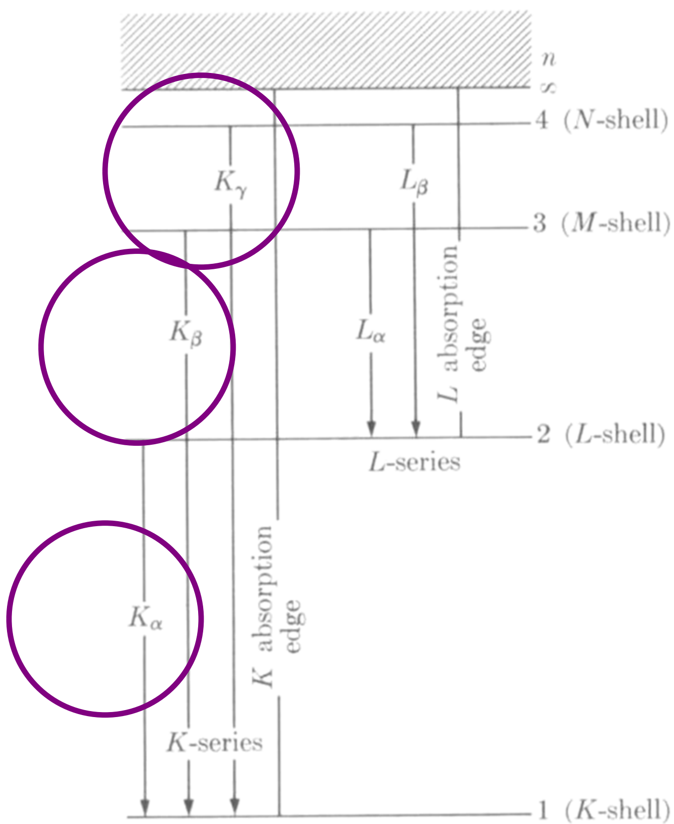


# Nomenclature: characteristic X-ray line emission

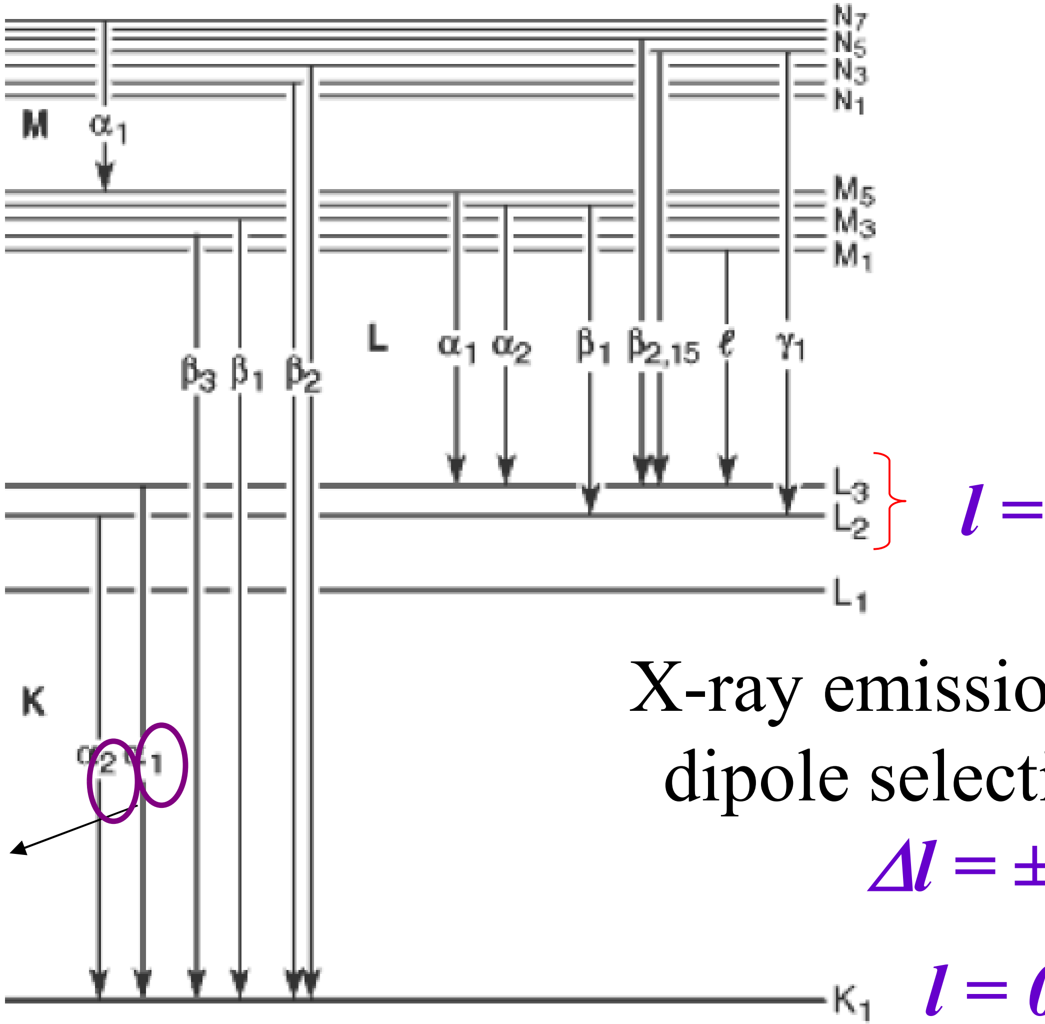
Where the core hole is designated by
The principal quantum #: n
n = 1,  K shell
n = 2,  L shell
n = 3,  M shell
etc.

**$K_{\alpha}$, $K_{\beta}$; $L_{\alpha}$, $L_{\beta}$; etc.**

α, β ,γ  etc., refers to the closest, the second closest *shell* , etc. above the core hole



# Detailed assignment of X-ray lines
## (X-ray data booklet)




*l* = 1 ($2p_{3/2,1/2}$)

higher energy, shorter wavelength

X-ray emission follows dipole selection rules

$\Delta l = \pm 1$

*l* = 0 (1s)

# Some representative X-ray lines

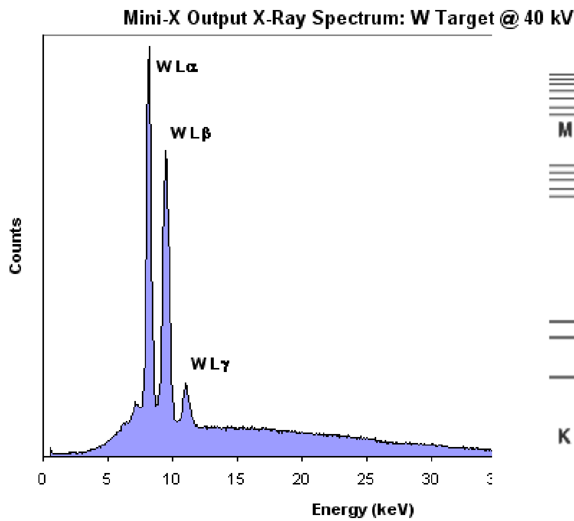
- The nomenclature was developed before the electronic structure of atom was fully understood

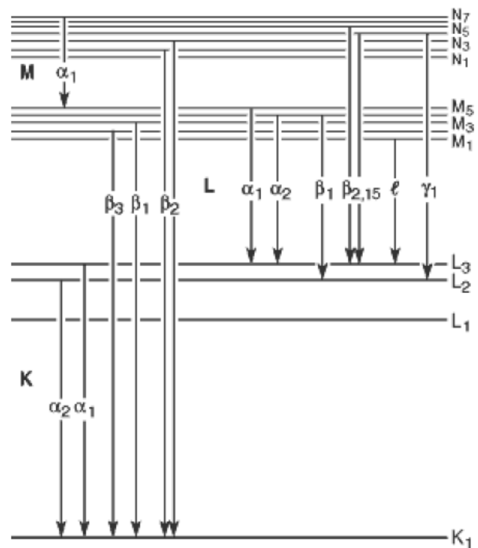
| Source Shell | Shell Filled: K | $L_I$ | $L_{II}$ | $L_{III}$ | $M_{III}$ | $M_{IV}$ | $M_V$ |
|---|---|---|---|---|---|---|---|
| $L_I$ | | | | | | | |
| $L_{II}$ | $K\alpha_2$ (50) | | | | | | |
| $L_{III}$ | $K\alpha_1$ (100) | | | | | | |
| $M_I$ | | | $L\eta$ (1) | $L\ell$ (2) | | | |
| $M_{II}$ | $K\beta_3$ (1) | $L\beta_4$ (5) | | $Lt$ (0.01) | | | |
| $M_{III}$ | $K\beta_1$ (20) | $L\beta_3$ (6) | $L\beta_{17}$ | $Ls$ (0.01) | | | |
| $M_{IV}$ | $K\beta_5'$ | $L\beta_{10}$ | $L\beta_1$ (50) | $L\alpha_2$ (10) | | | |
| $M_V$ | $K\beta_5'$ | $L\beta_9$ | | $L\alpha_1$ (100) | | | |
| $N_I$ | | | $L\gamma_5$ (0.1) | $L\beta_6$ (0.1) | | | |
| $N_{II}$ | $K\beta_2'$ (5) | $L\gamma_2$ (1) | | | | | |
| $N_{III}$ | $K\beta_2'$ | $L\gamma_3$ (2) | | | | | |
| $N_{IV}$ | $K\beta_4$ | | $L\gamma_1$ (10) | $L\beta_{15}$ (1) | $M\gamma_2$ (1) | | |
| $N_V$ | $K\beta_4$ | | | $L\beta_2$ (20) | $M\gamma_1$ (1) | | |
| $N_{VI}$ | | | $Lv$ | | | $M\beta_1$ (50) | $M\alpha_2$ (100) |
| $N_{VII}$ | | | $Lv$ | | | | $M\alpha_1$ (100) |
| $O_I$ | | $L\gamma_4$ | $L\gamma_8$ | $L\beta_7$ | | | |
| $O_{II}$ | $K\delta_2$ (0.1) | $L\gamma_4$ | | | | | |
| $O_{III}$ | $K\delta_1'$ (0.1) | | | | | | |
| $O_{IV}$ | | | $L\gamma_6$ | $L\beta_5$ | | | |
| $O_V$ | | | | $L\beta_5$ | | | |

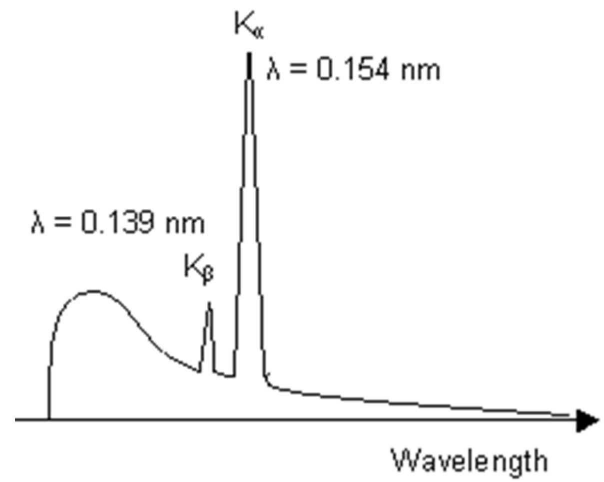
value in parenthesis are intensity, 100 means most intense line (see x-ray data book for more details)

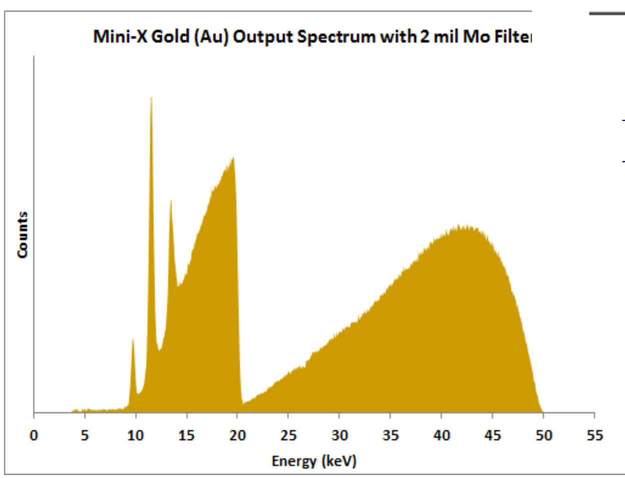
Al $K_\alpha$ used in XPS has $K_{\alpha 1}$ and $K_{\alpha 2}$ line 1486.295 eV & 1486.708eV, respectively; use monochromator to get rid of $K_{\alpha 2}$ to get better energy resolution

# Representative X-ray spectrum

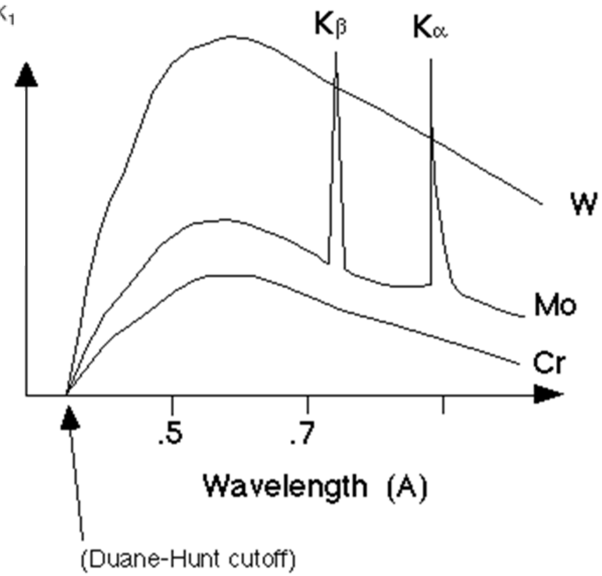



Exercise: assign the sharp peaks

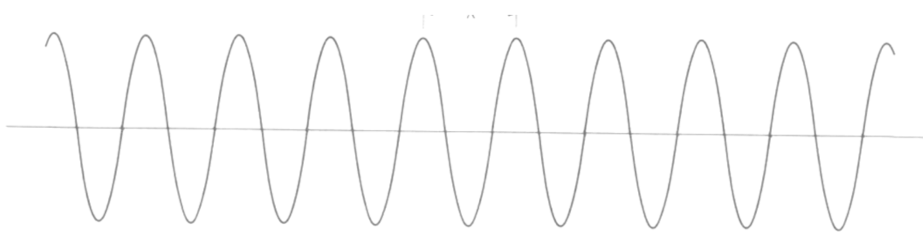


# Materials Properties

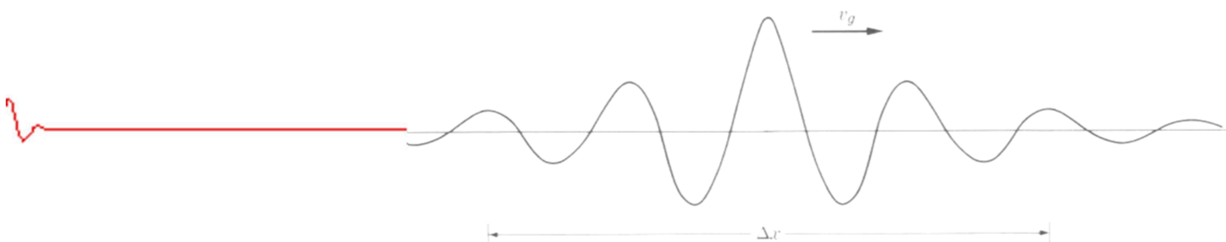
- Material properties are determined by the electronic structure of the materials
- The electronic structure is determined by the behavior of the electron in its environment, technically the *potential* (coulomb and exchange) set up by the nuclei and other electrons (structure and bonding)

# Properties of electrons

- Smallest charge particle that carries a - ve charge
- Exhibits wave behavior $\lambda = h/p$ (de Broglie) where $h$ is the Planck's constant and $p$ the linear momentum
- Posses a spin of ½ (**fermions**, exchange interaction) in contrast to **bosons** which has integral spin
- Absorbs light when it is bound by a potential
- Free electron does not absorb light but scatters light



Plane wave



Wave packet

# Behaviour of electrons in matter

- The time indpendent Schrödinger's equation (1- dimension)

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

Kinetic energy
$p^2/2m = mv^2/2$

Total energy

**Potential energy**

Hamiltonian, $\hat{H}$: $\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)$; $\hat{H}\psi(x)=E\psi(x)$

$\hbar=\frac{h}{2\pi}$ $h$ : planck's constant

# Free particle V($x$) = 0

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

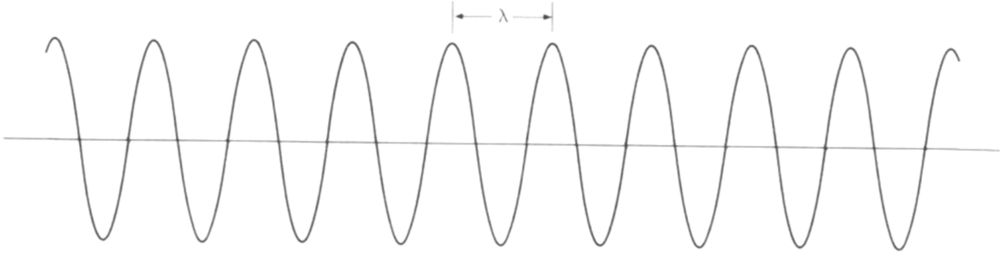
$$E = \frac{p^2}{2m},\ p = k\hbar;\ \frac{d^2\psi}{dx^2} + k^2\psi = 0$$

$k$: wave vector

$$\psi(x) = e^{ikx} \quad and \quad \psi(x) = e^{-ikx}$$

Solution: $\psi(x) = Ae^{ikx} + Be^{-ikx}$

*plane wave*

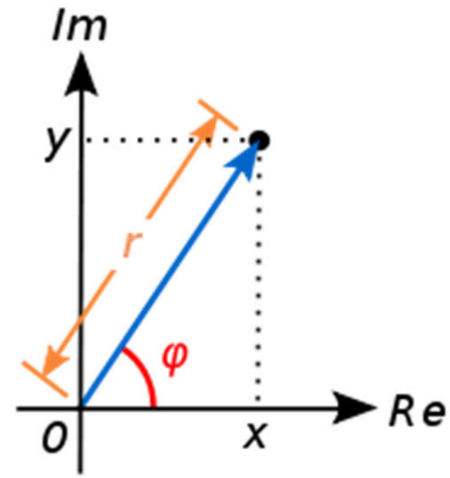



$$k = 2\pi\left(\frac{1}{\lambda}\right)$$

# Math note

$$i=\sqrt{1};\ z=x+iy;\ z^{*}=x-iy$$

**Imaginary #** **Complex number** **Complex conjugate**




**Euler's formula** $$e^{i\varphi}=\cos\varphi+i\sin\varphi$$

$$z=x+iy=|z|(\cos\varphi+i\sin\varphi)=re^{i\varphi}$$

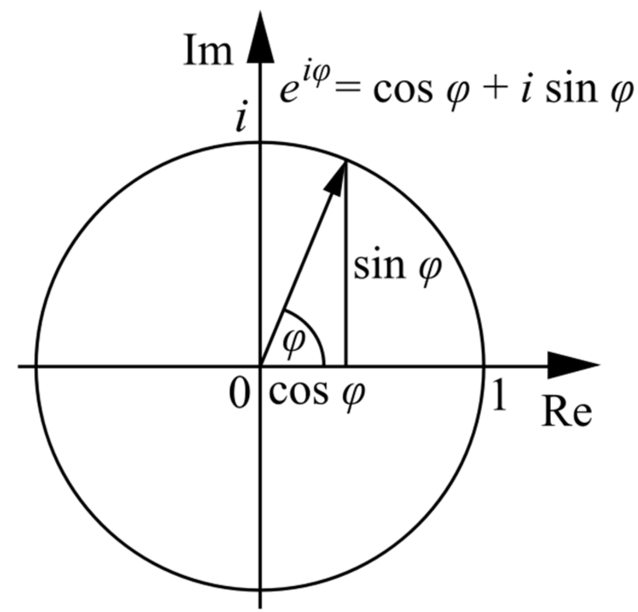
$$z=x-iy=|z|(\cos\varphi-i\sin\varphi)=re^{-i\varphi}$$

$$x=\mathrm{Re}\{z\},\ \ real\ \ part;$$

$$y=\mathrm{Im}\{z\},\ \ imag.\ \ part$$

$$r=|z|=\sqrt{x^{2}+y^{2}}\ \ \ magnitude\ \ of\ \ z$$

$$\varphi=\arg z=\arctan(y/x)$$



# Potentials (a review)

- Particle in a box
- Atomic: coulomb (asymptote) plus centrifugal term (due to no zero angular momentum, $l > 0$)
- Molecule: molecular potential
- Solid: periodic potential (crystals)

- These potentials support discrete energy electronic states (core/valence levels in atoms and small molecules) and closely spaced states (bands in solids, polymers)

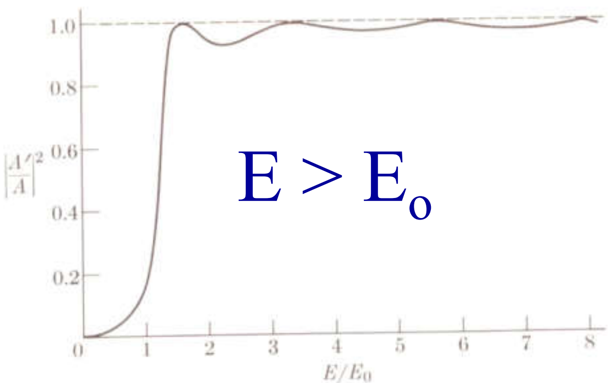
- Synchrotron spectroscopy studies the transitions between these states providing info on structure and bonding

For a brief review of potentials, see Alonso –Finn Fundamental University Physics Vol III Addison-Welsely 1966 or any quantum mechanics text book

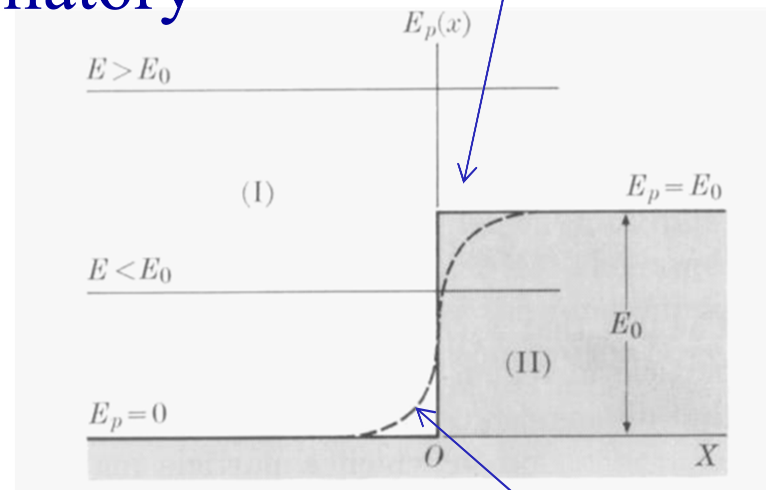
# Potential step

Math: step function

The transmission is oscillatory

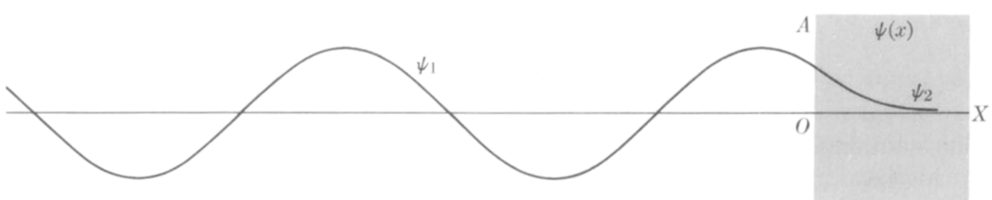



$E > E_o$



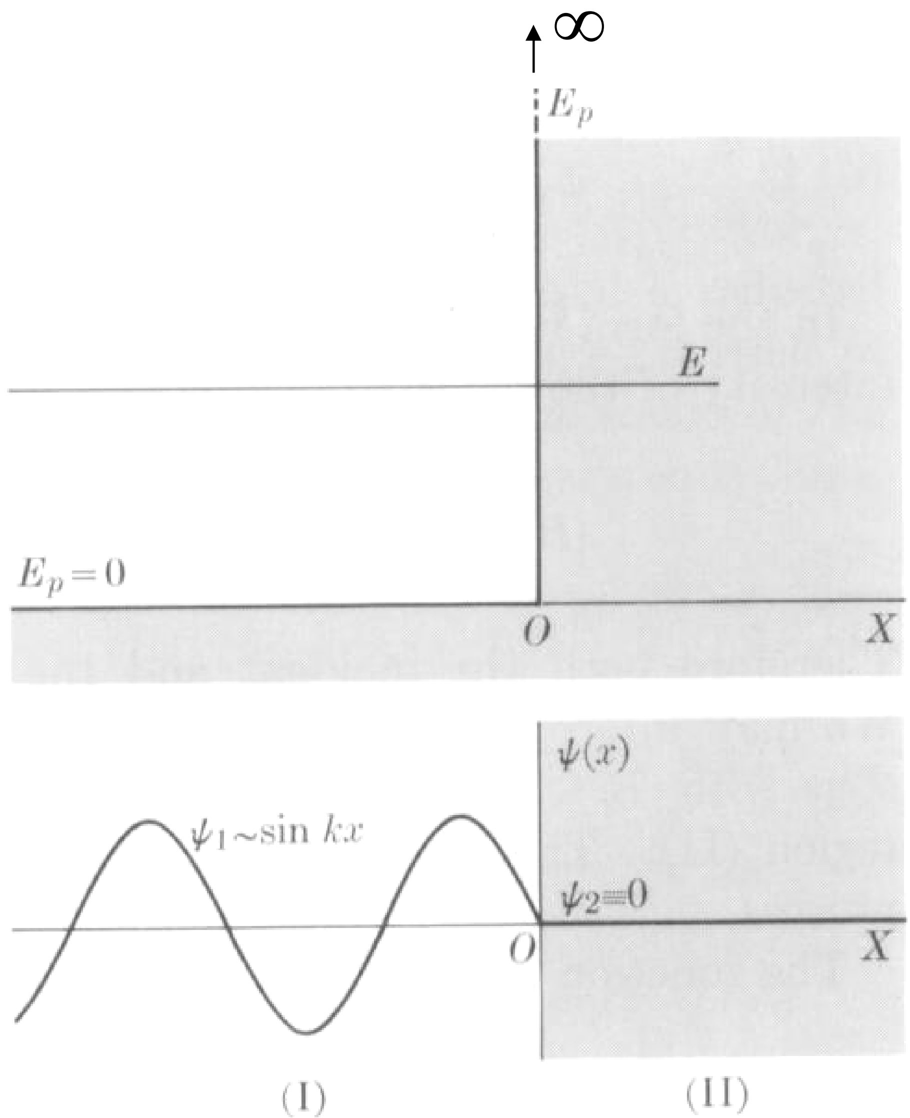

Dashed curve: physically meaningful step (Fermi edge in metals)

**$E < E_o$**




The particle can penetrate the potential wall

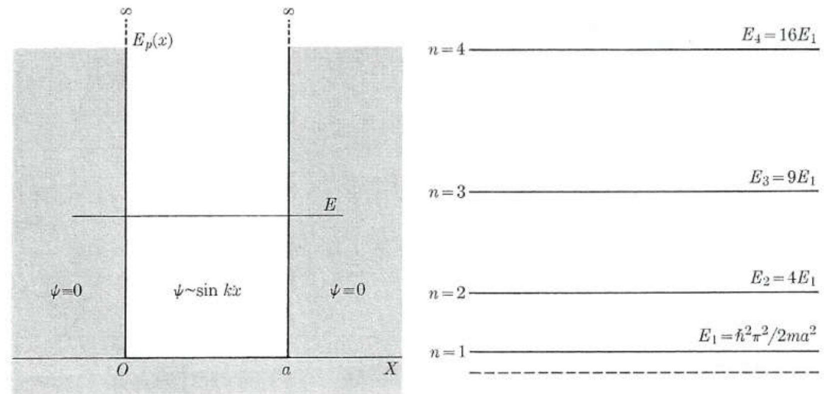
# Potential wall ($E_P \rightarrow \infty$)




The particle can no longer penetrate the wall as in the case of a potential step

# Potentials and electronic states

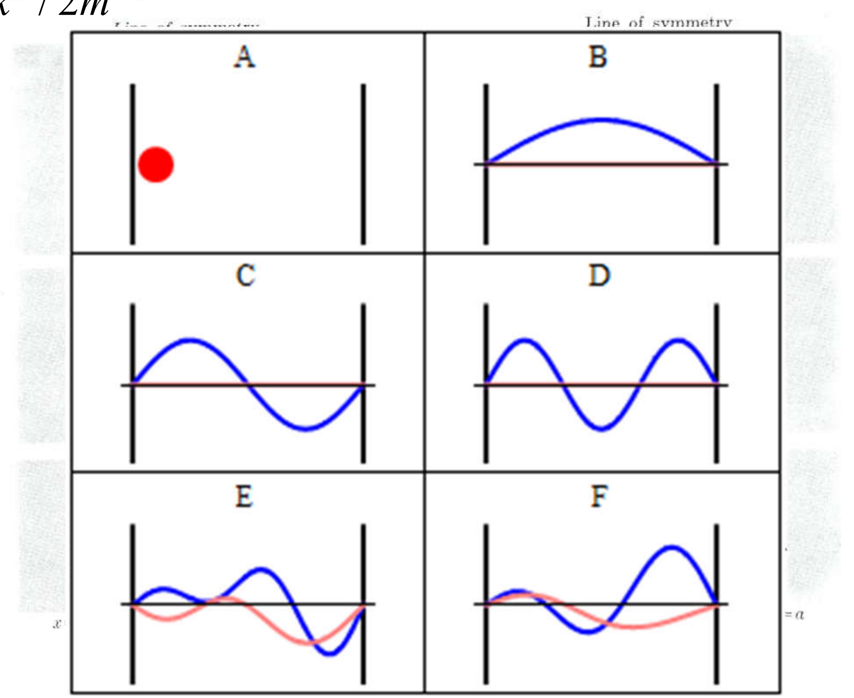
1-D particle in a box;
electronic states are discrete
(quantized), V= 0 inside the box




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

$$k=2\pi/\lambda;\hbar=h/2\pi;E=\hbar^2k^2/2m$$

$$\frac{d^2\psi}{dx^2}+k^2\psi=0$$ *k*: wave vector




$$\psi(x)=Ae^{ikx}+Be^{-ikx}$$

$$\psi(x)=A\sin kx;$$

$$\psi(x)=0 \;\; at \;\; x=0,a$$

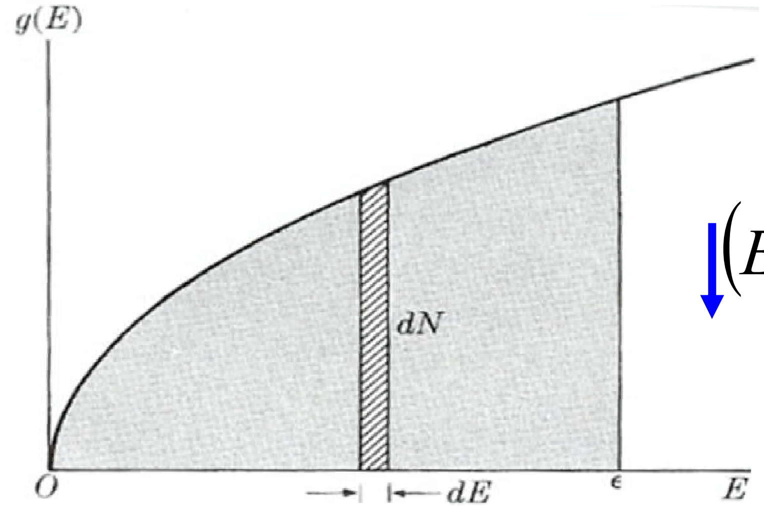
$$E_n=\frac{(n\pi\hbar)^2}{2ma^2};\;\; n=1,2,3$$

# Potentials and electronic states in a large box

As the length of the box increases, the energy separation between states becomes smaller

$$g(E) = \frac{dN}{dE}$$

$$= \frac{4\pi V(2m^3)^{1/2}}{3h^3} E^{1/2}$$

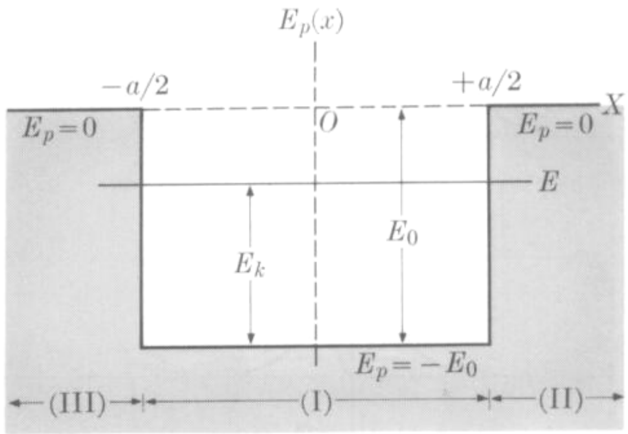


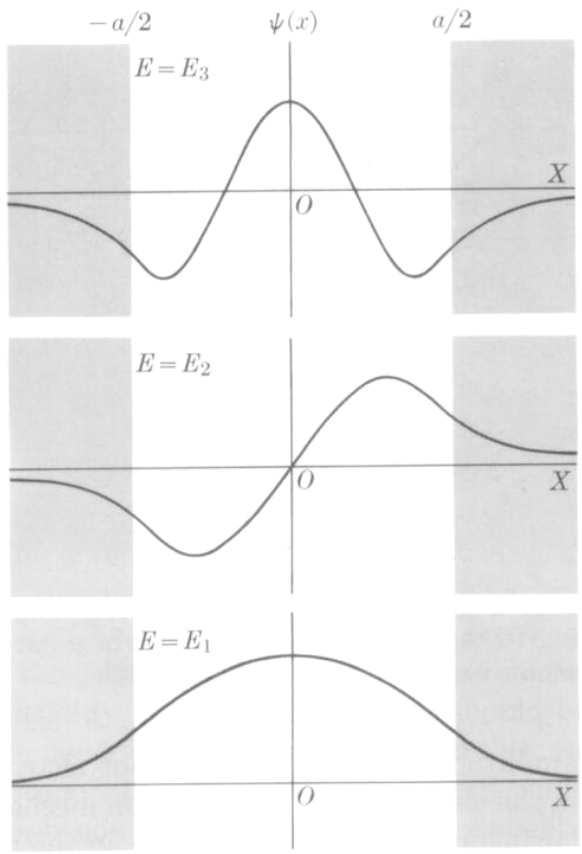

Density of energy states in a large cubic box (3D) e.g. atoms forming solids, polymers, etc.

$$\downarrow \left(E_{n+1} - E_n\right) = \frac{(\pi\hbar)^2}{2ma^2}$$

As ***a*** gets larger, the separation between state becomes smaller

# Potential well

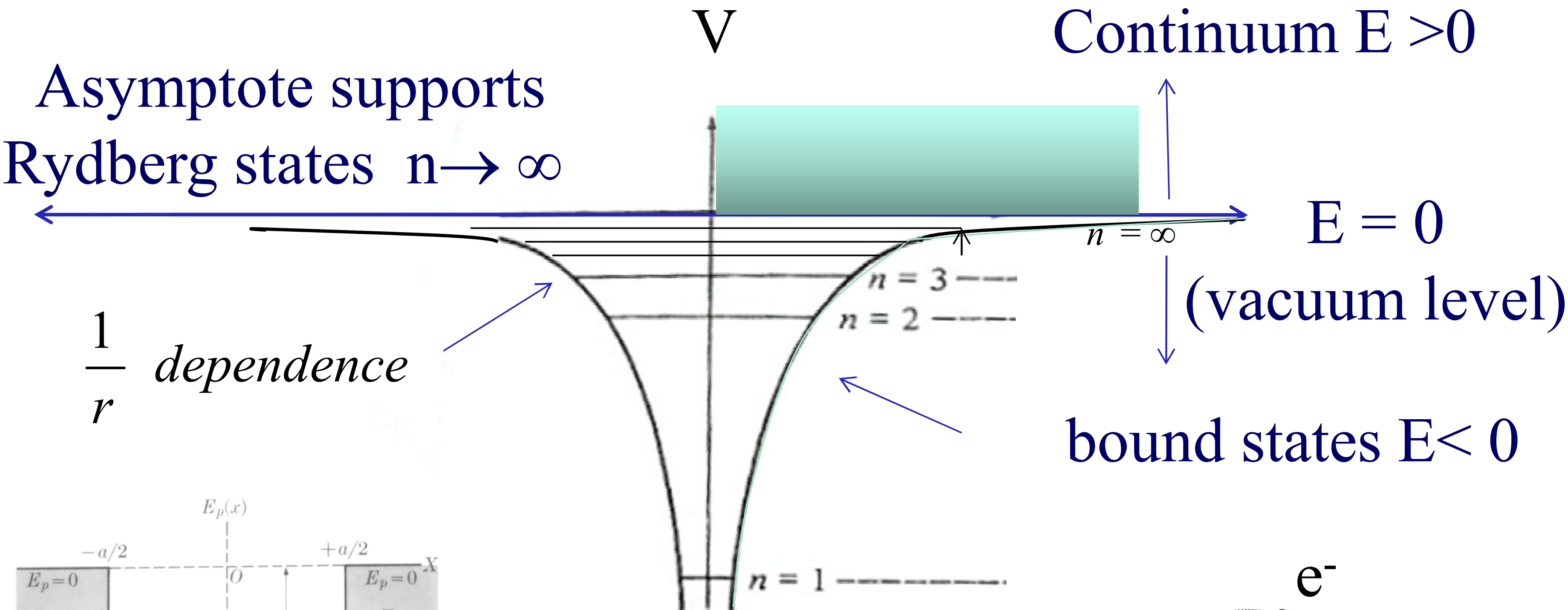


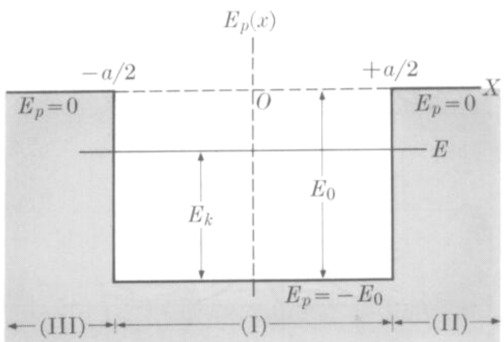




One dimensional well with width ***a*** and depth $\boldsymbol{E_o}$ (2 opposing steps)

Potential wells can support discrete energy states

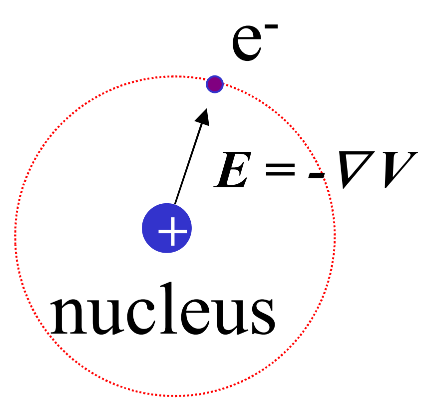
# Atomic potential



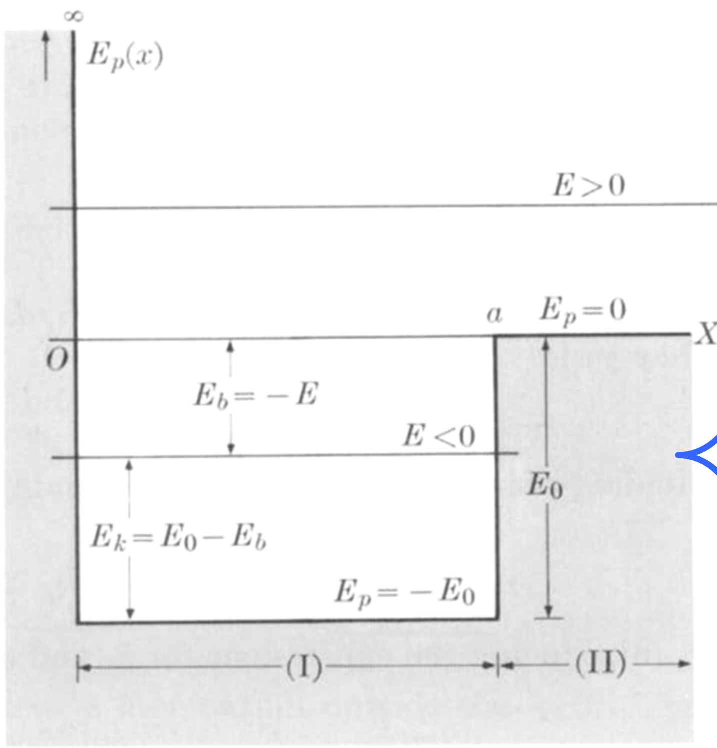




Coulomb potential

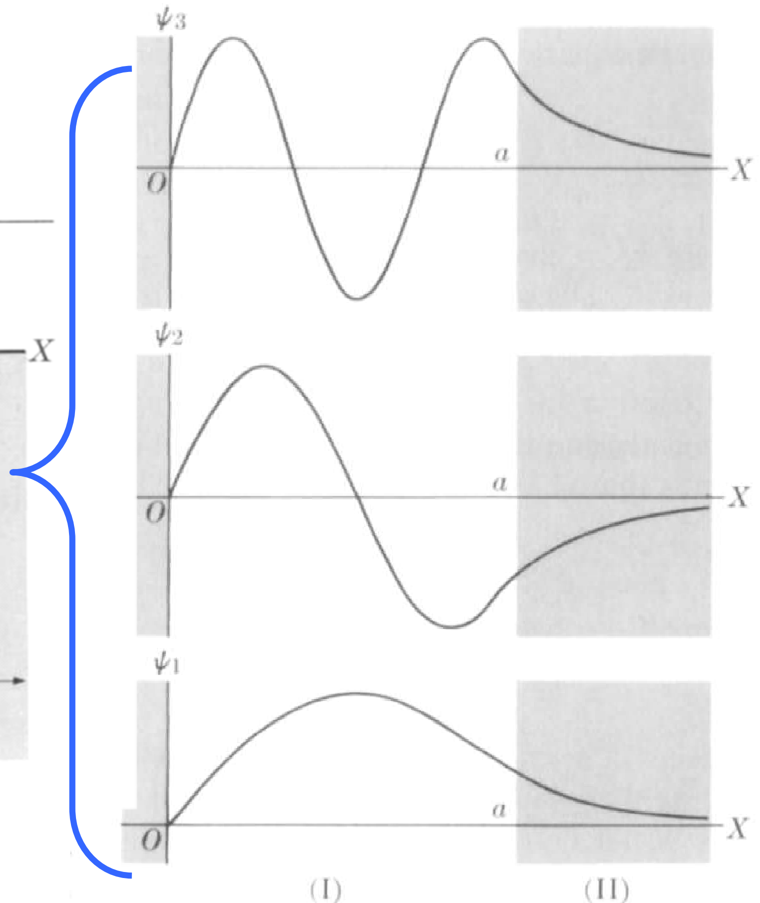
$$V = \frac{1}{4\pi\varepsilon}\frac{q}{r} \propto \frac{1}{r}$$



# Rectangular potential well

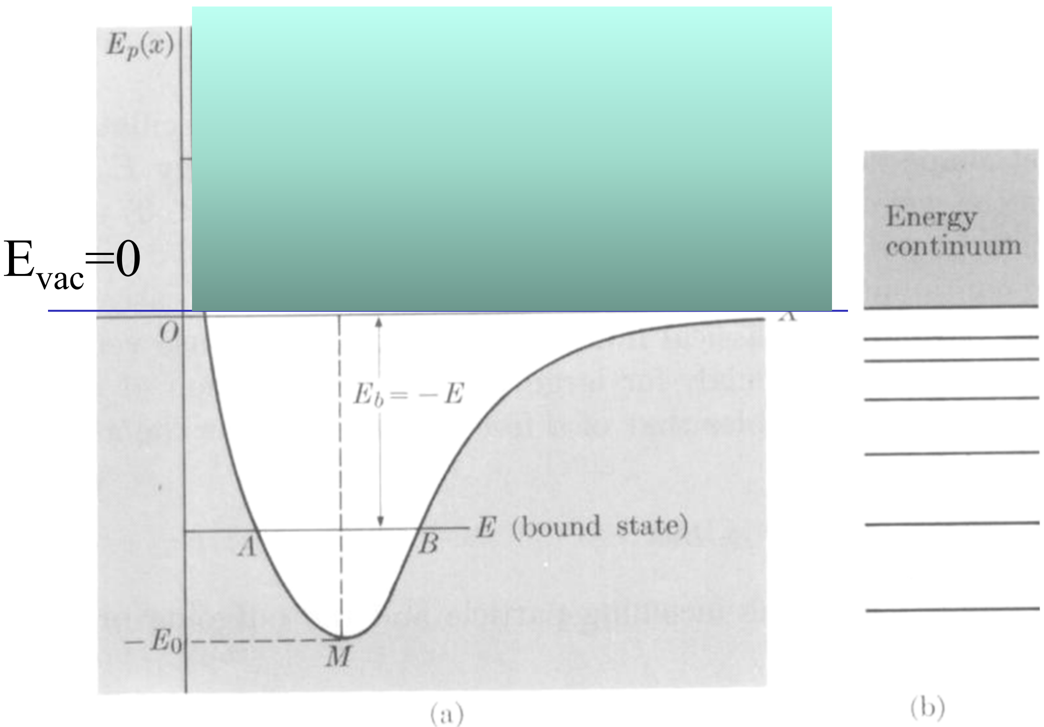



Rectangular potential well states

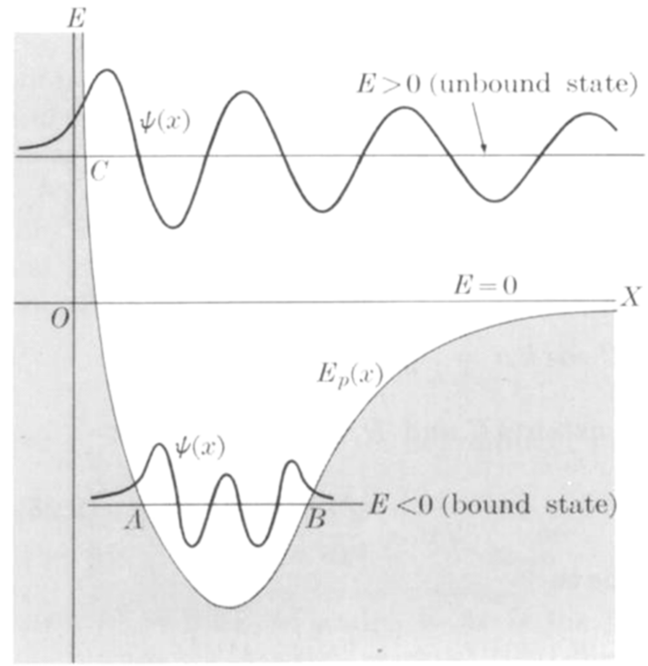



First 3 bound state wave function

# General potentials




Continuum state wave function

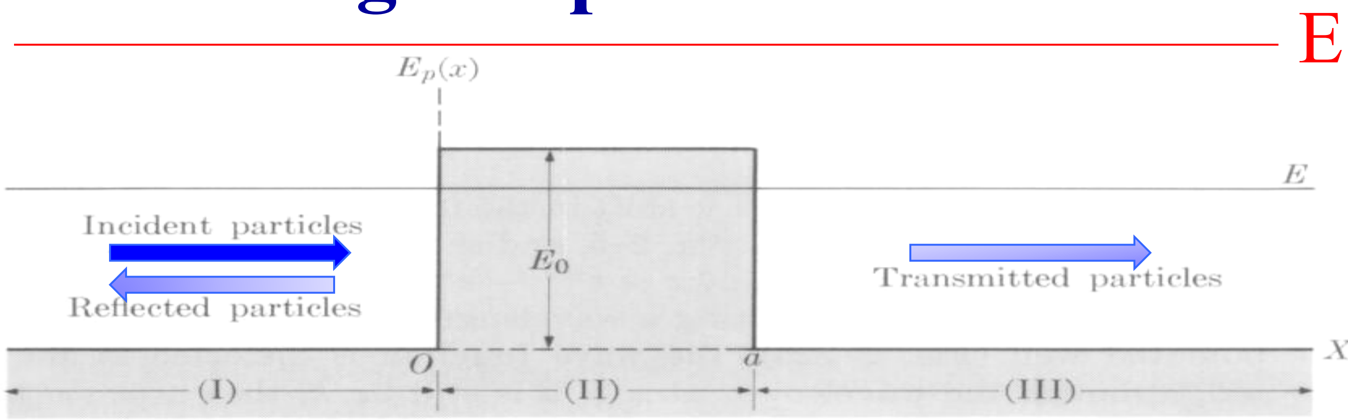



(a) Potential curve for strong repulsion at small *x* and negligible interaction at large *x* (e.g. diatomic molecule)

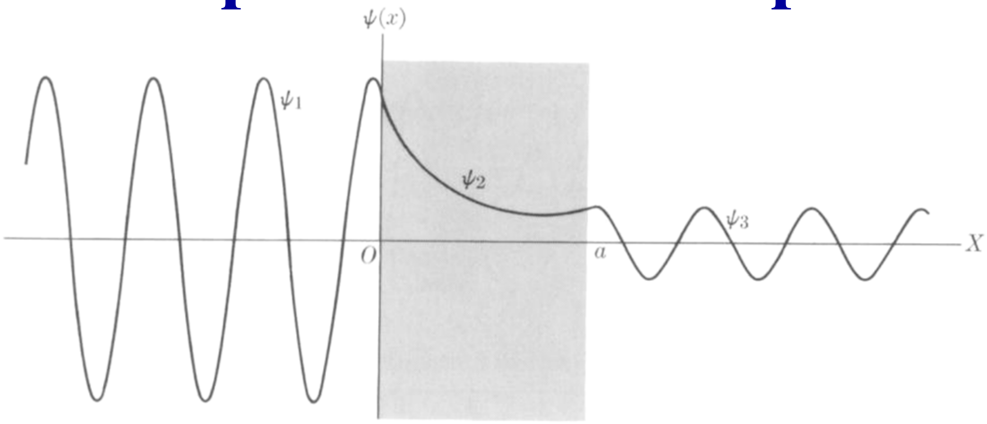
(b) Discrete energy levels and continuum

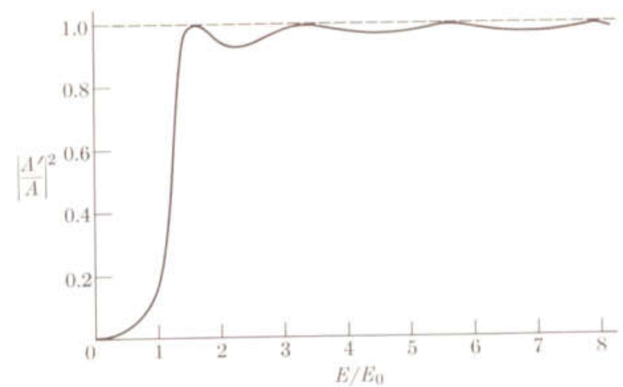
Wave function of bound and continuum states

# Rectangular potential barrier




## potential barrier penetration - tunneling

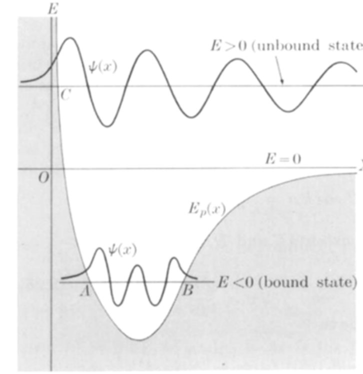


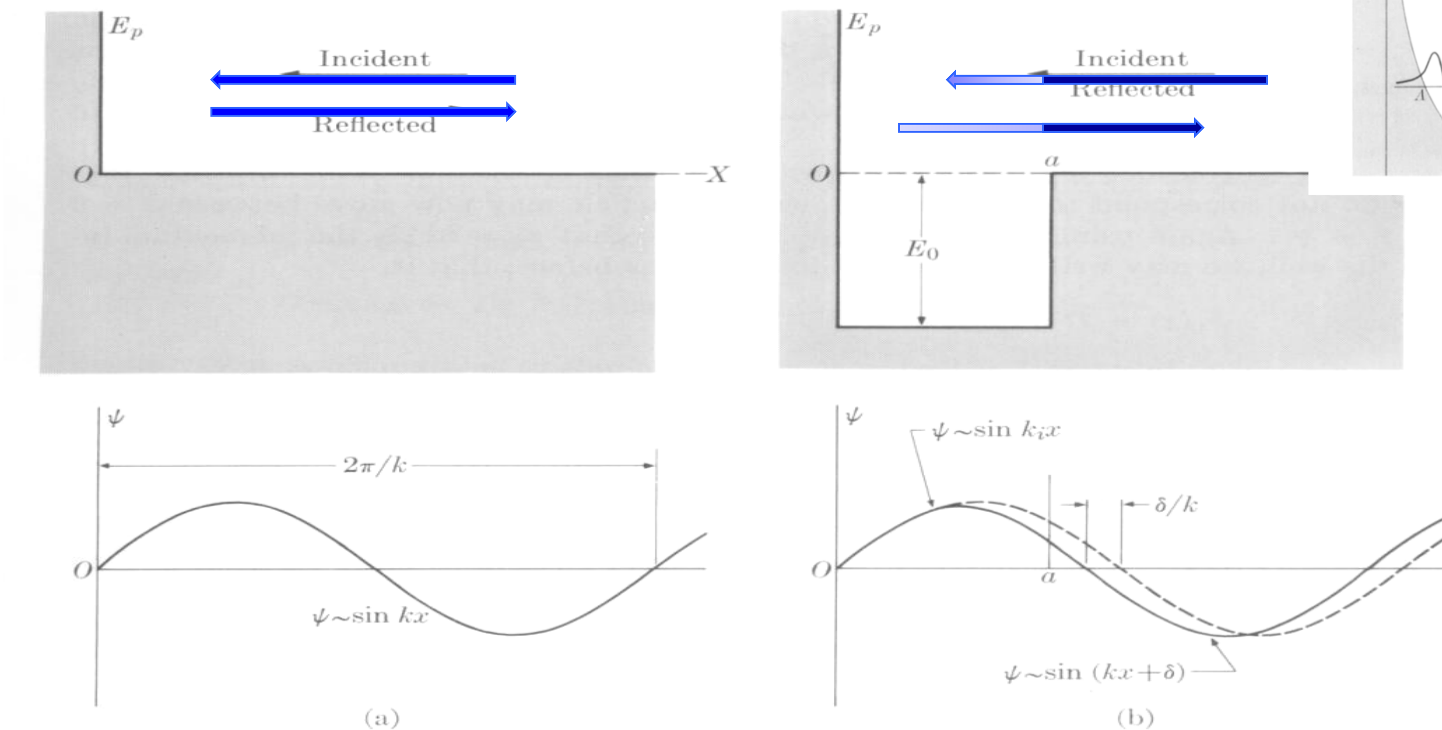




Wavefunction of an energy less than the height of the barrier, $E < E_o$

Transmission of a particle with $E > E_o$

# Phase shifts

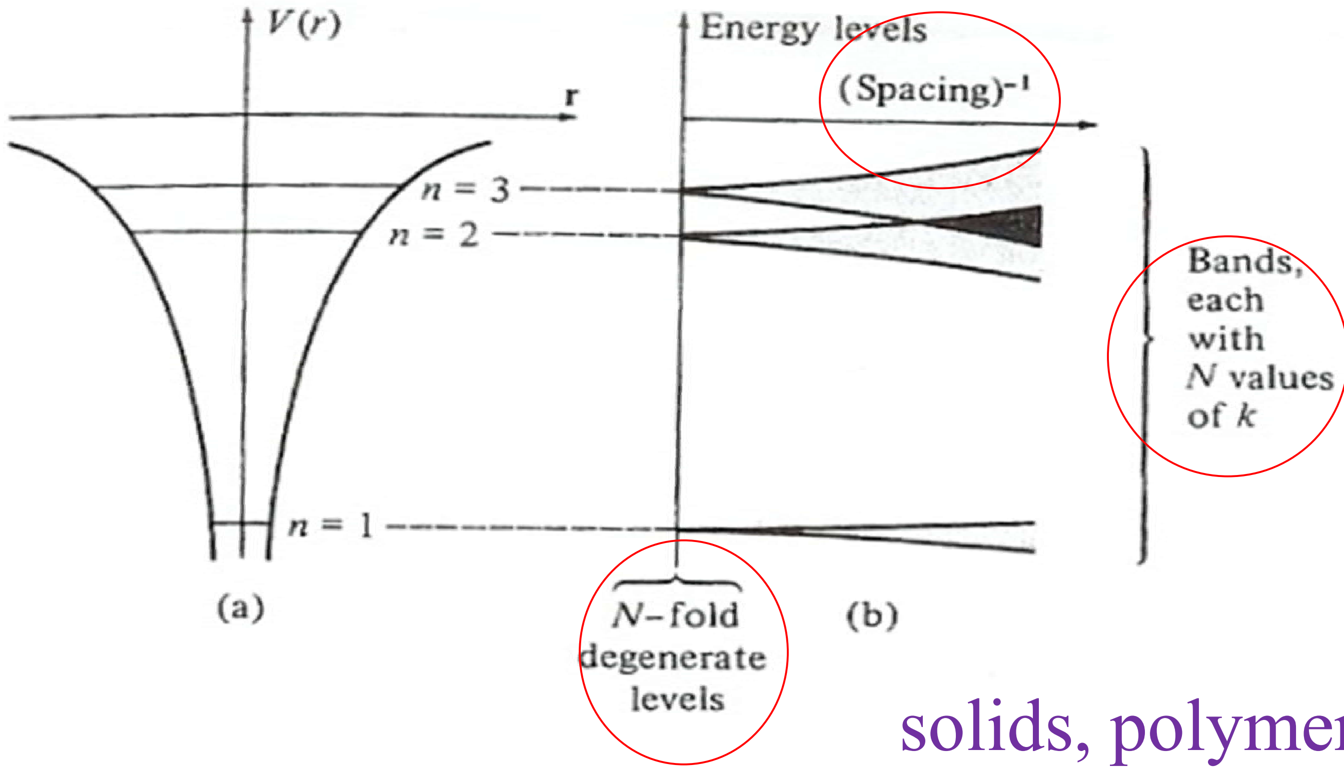



When $e^-$ is scattered by a **potential,** its wavefunction is distorted (experiences a phase shift, *δ)*

the wave function outside the area of $x$ = ***a*** is modified by *δ/k so that it smoothly joins the wavefunction at x =* ***a*** *inside the potential well; a local modification of the potential x= 0 to x= a affects the wavefunction at x>a, expresses in* phase shift, *δ*

# Potentials and electronic states:
## from atom to condensed matter



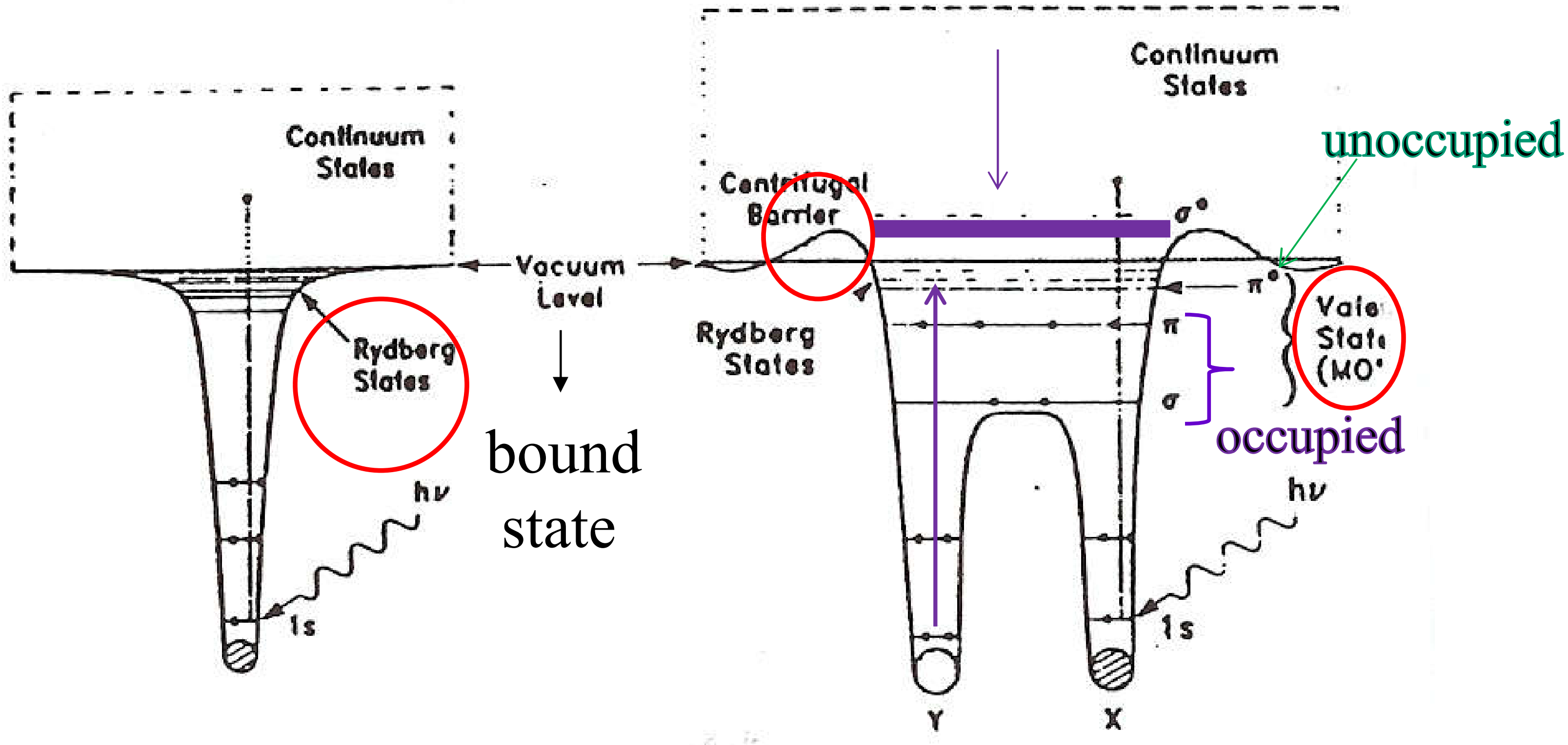

solids, polymers

1 atom

N atoms

# Potential in diatomic molecule

**Quasi bound states**, potential barrier states, electron in these states will eventually tunnels out into the continuum (short lifetime)




free atom diatomic molecule

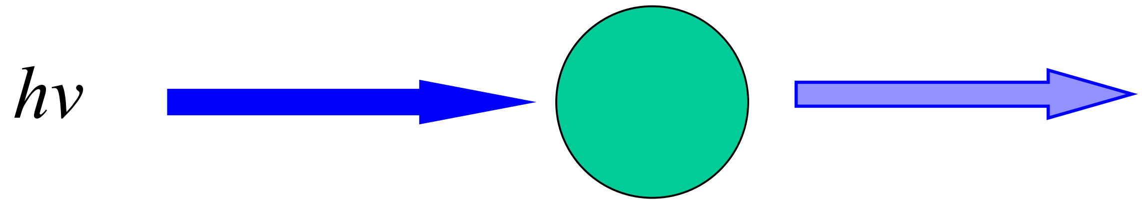
## Atomic to valence (MO) transitions

# Interaction of light with matter

- Scattering (elastic and inelastic)
- Absorption (annihilation of the photon)
- Scattering and absorption are taking place simultaneously
- Scattering amplitude /Absorption cross-sections (coefficient) of atoms

# Atomic scattering factors

- The interaction of light and atom for photons in the energy range of VUV to hard x-rays (> 30 eV) can be expressed in terms of their scattering factor **in the forward scattering position (θ = 0)**




$$f(0) = f_1 + if_2$$

related

Refractive index

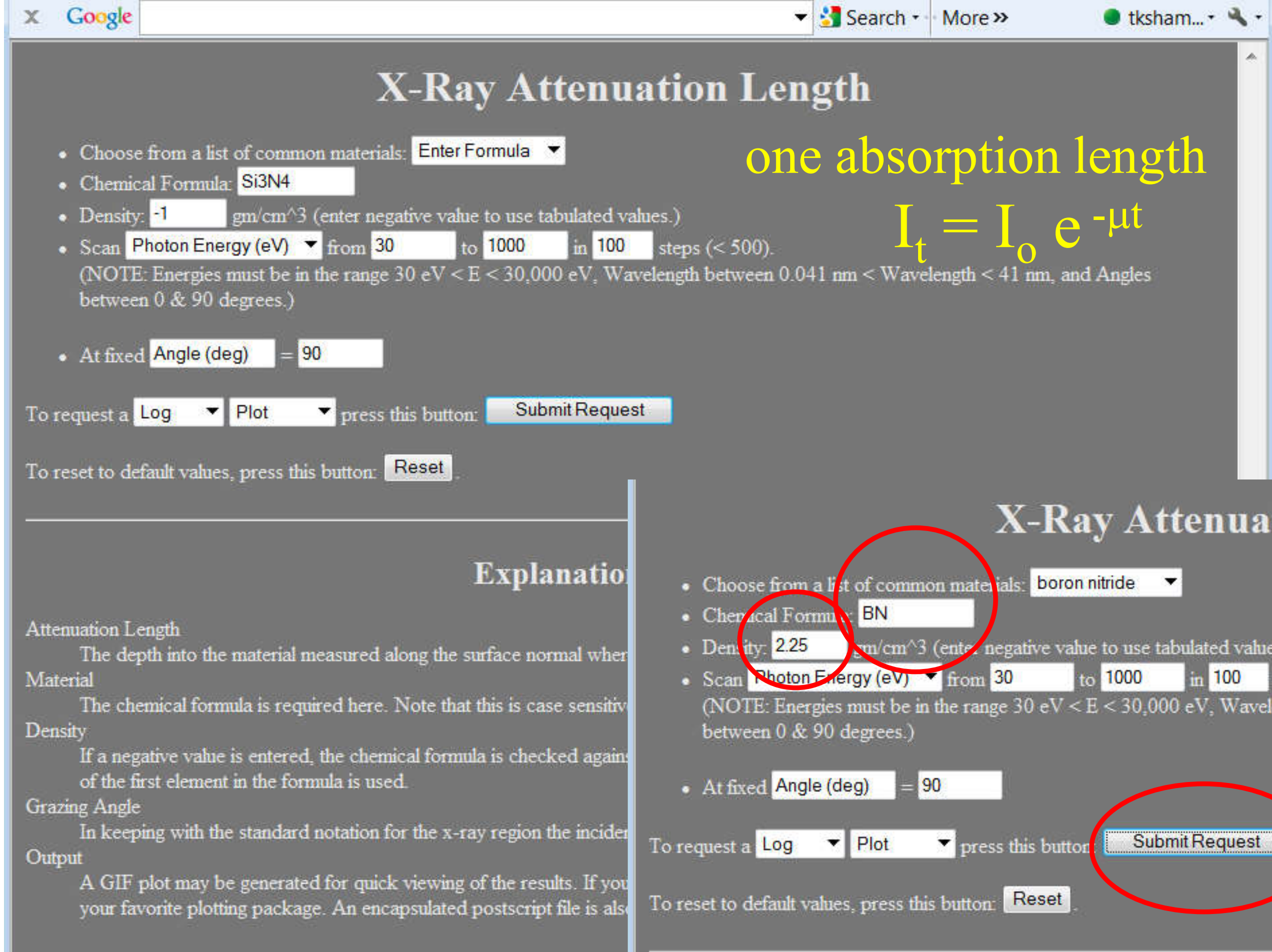
Scattering

Absorption coefficient

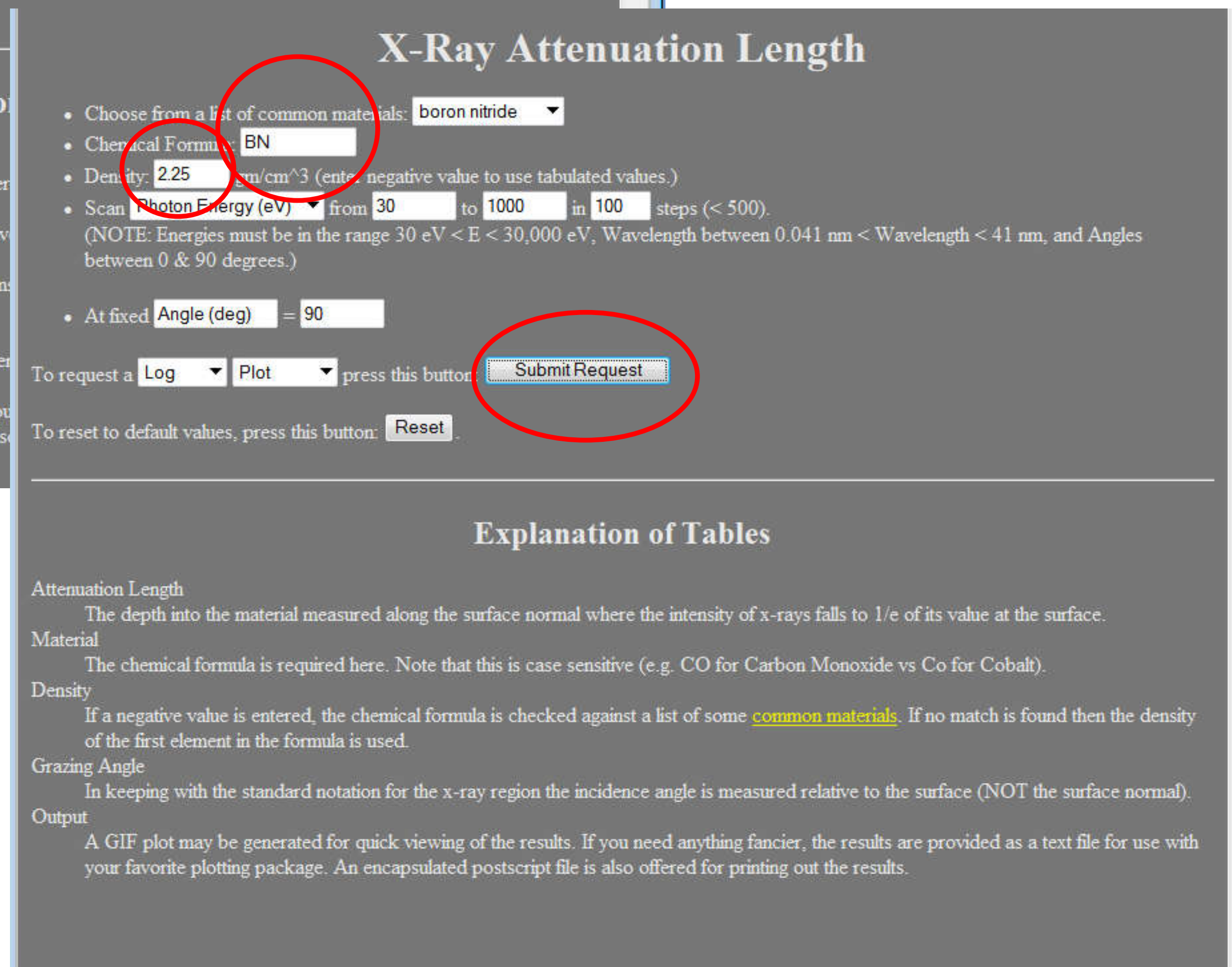
# the X-ray calculator

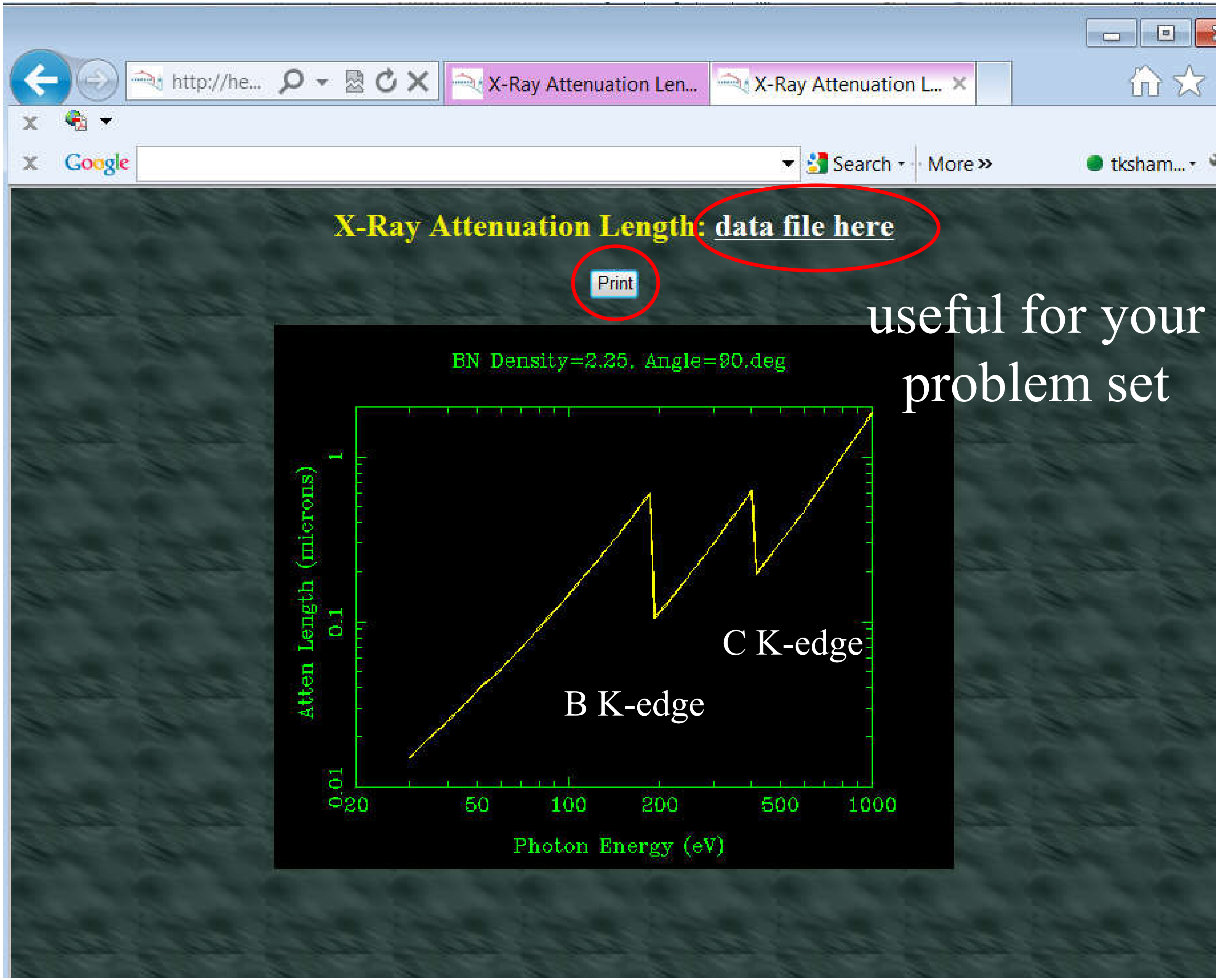
1. Go to the web: http://www-cxro.lbl.gov/
2. Click "X-ray Database" on the left panel
3. You will find " X-ray interaction with matter " from which you can calculate X-ray properties of elements, attenuation length, transmission of gas and solid, etc. that are most relevant to X-ray spectroscopy.

***Exercise:*** Use the calculator to calculate the x-ray properties of the materials relevant to your research




The value of $t$ when $\mu t = 1$, $I_t/I_o = 1/e \sim 34\%$ transmission 63% absorption

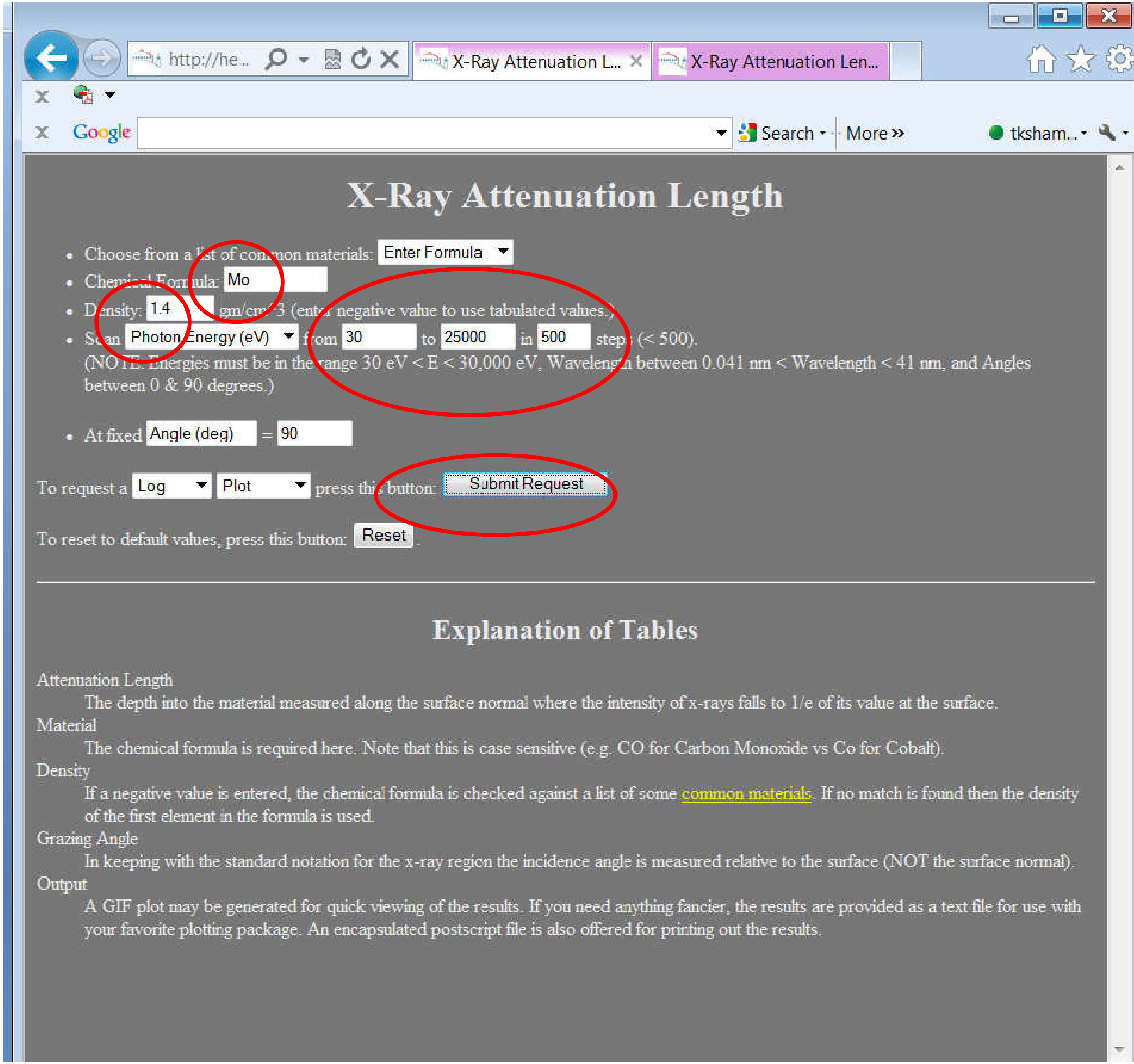





useful for your problem set

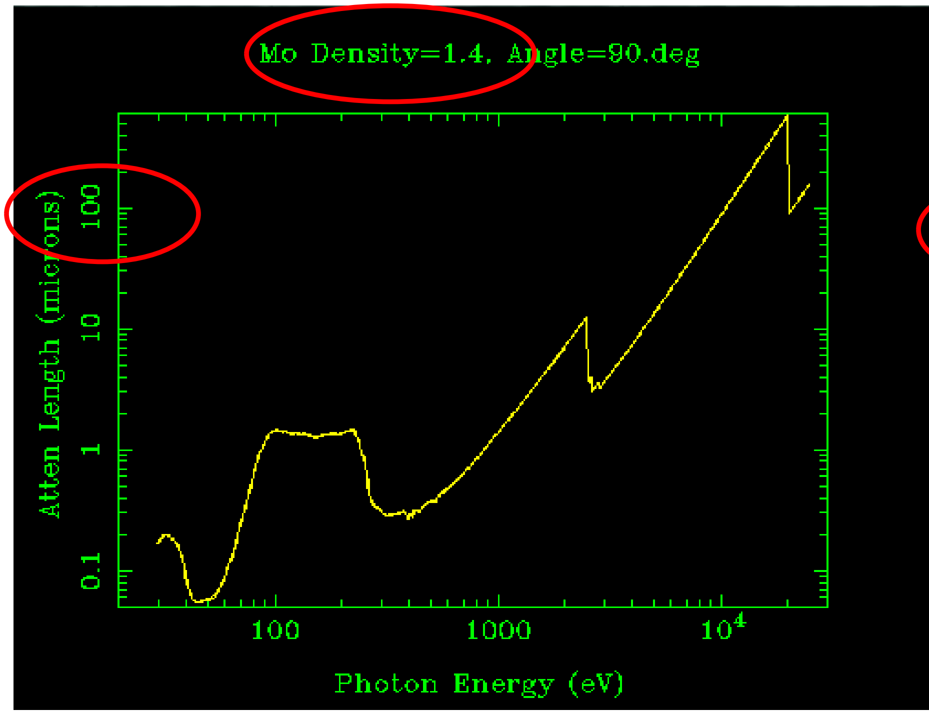
# Attenuation length of Mo

this value is incorrect; correct value is 10.22

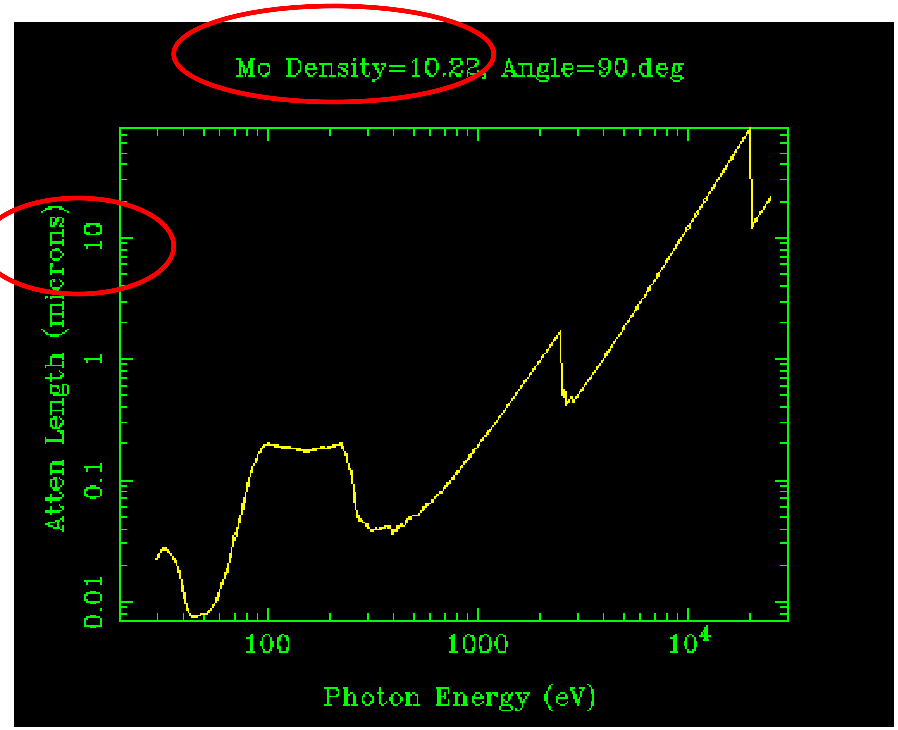


# Attenuation length of Mo

incorrect density




correct density




Use this to explain the Au X-ray spectrum with a Mo filter (slide 33)