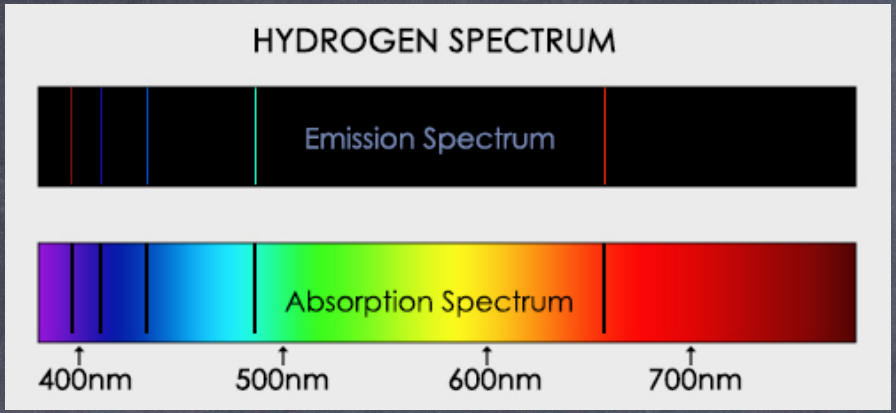
PHY127 FS 2022

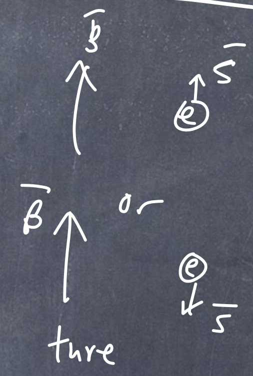
Prof. Ben Kilminster
Lecture April 28^{th}, 2023

Last week:

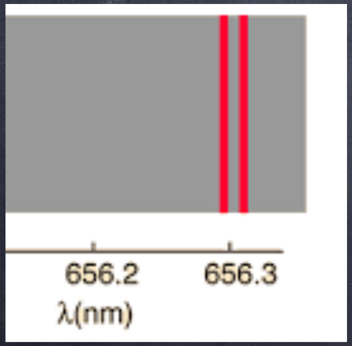
Fine structure is 4th quantum number, m_s



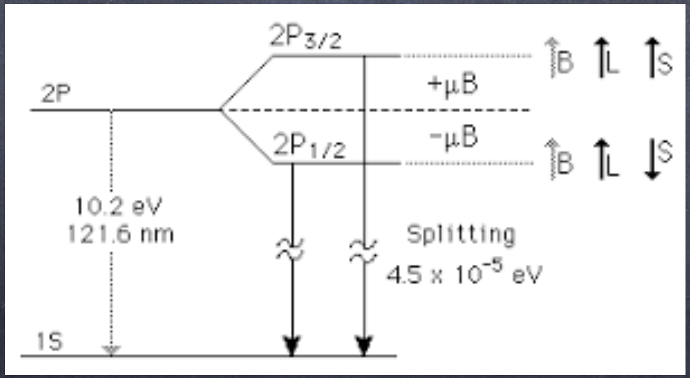
from spin of electron when atom is in a magnetic field.



correspond to either $m_s = +\frac{1}{2}$ or $-\frac{1}{2}$



2p line is actually split into two energy levels



"Fine" structure = detailed structure

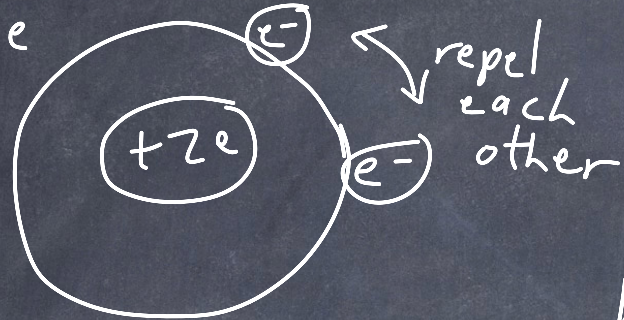
"hyperfine"

Note: there are other effects that split spectral lines into more than one line.
The Zeeman effect and Stark effect add more possibilities. (Not covered in this class)

Atoms with many electrons

(cannot be solved exactly with the Schroedinger equation)

He



Pauli exclusion principle:
no two electrons in an atom may have the same set of quantum numbers.
(n, l, m, m_s)

This rule applies to all "fermions", particles with a spin of ½.

Fundamental fermions (like electrons) have a spin of ½. Can have spin as $+\frac{1}{2}$ or $-\frac{1}{2}$

Fermions are the particles that compose matter.

Fermions: electrons, muons, protons, neutrons, ...

Applied to the hydrogen atom (with one electron)

ground state (n, ℓ, m, m_s) : $(1, 0, 0, +\frac{1}{2})$ allowed

$(1, 0, 0, -\frac{1}{2})$ states

In the absense of a magnetic field, both have the same energy.

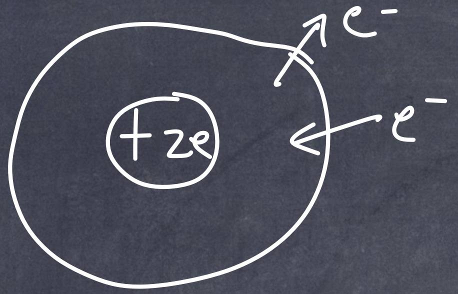
So the rules for atomic electron structure:

1) Electrons tend to occupy the lowest available energy levels.

2) Electrons must have a unique set of quantum numbers.

Consider Helium: According to our principles, the first and second electrons occupy: $(1, 0, 0, +\frac{1}{2})$

$(1, 0, 0, -\frac{1}{2})$



Experimental evidence confirms this.
The electrons have spins that anti-align.
This state with 2 electrons anti-aligned forms a rather strong bond, with total spin of Ø.

Sometimes, we refer to shells

$n =$	1	2	3	4	...
shell $=$	K	L	M	N	...

And sub-shells

$\ell =$	0	1	2	3	...
sub-shells $=$	s	p	d	f	...

Hydrogen description : $1s^1$ or $1s$

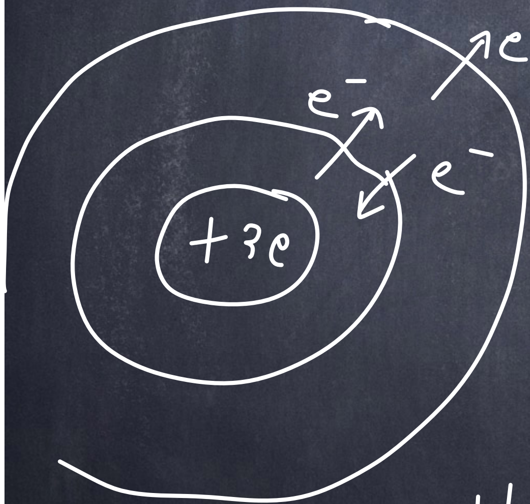
Helium description : $1s^2$

After H, He, next is lithium, with $3e^-$

But since only 2 electrons are allowed in the $n=1$ (K-shell), the third electron must be in $n=2$ (L-shell). So Li is described as $1s^2 2s^1$

It's third electron can occupy $(2, 0, 0, \pm\frac{1}{2})$

Screening: Electrons in higher energy levels see (or feel) a smaller positive charge.



The outer electron is screened by the two K-shell electrons. It feels a positive nuclear charge, $Z_{effective} = Z_{eff} = +1e$

How many electrons can be in each sub-shell? (And not violate the Pauli exclusion principle)

		total
For each m:	two values of m_s	2
For each ℓ:	$(2\ell+1)$ values of m	$2(2\ell+1)$

$\vdots$
$4p$
$3d$
$\boxed{4s}$
$3p$
$\uparrow$ energy $3s$
$2s$
$1s$

Note: $4s$ is bound with less energy than the $3d$.

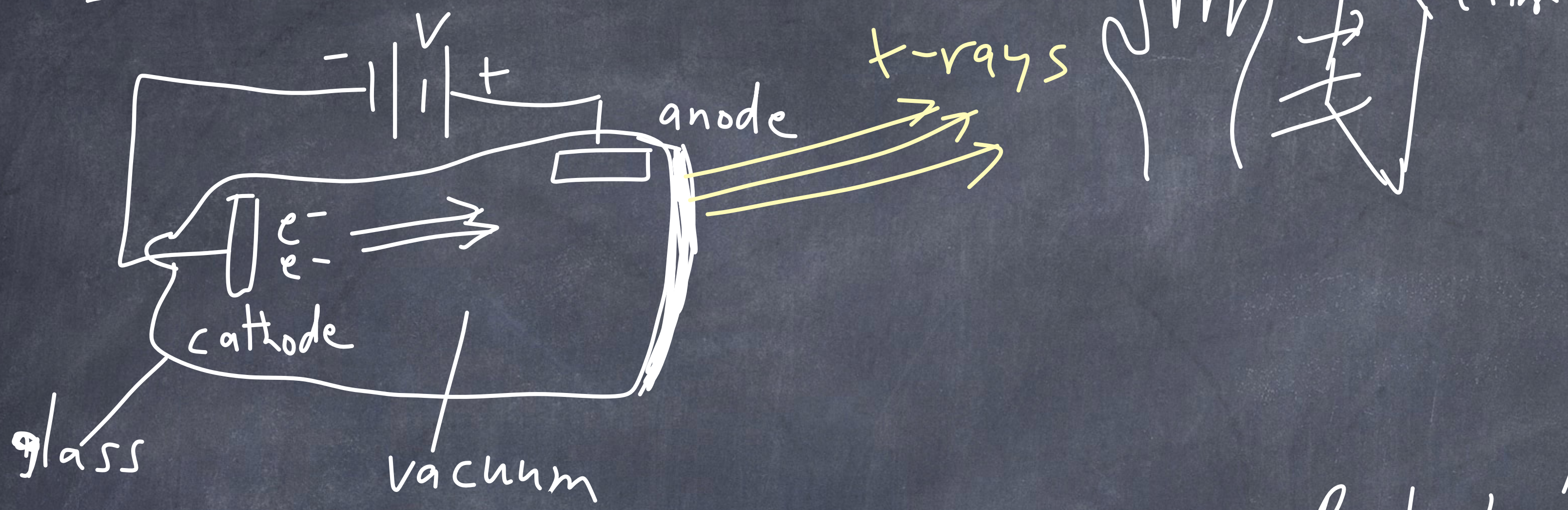
This is because of the shape of the electron orbit, which changes the amount of screening that happens.

Electrons with higher ℓ are more screened.
Lower ℓ orbits are less screened because the orbits are more eliptical.

n	ℓ	sub-shell	sub-shell capacity	total electrons in
1	0	1s	2	2
2	0	2s	2	4
2	1	2p	6	10
3	0	3s	2	12
3	1	3p	6	18
4	0	4s	2	20
3	2	3d	10	30
...	...	...	...	...

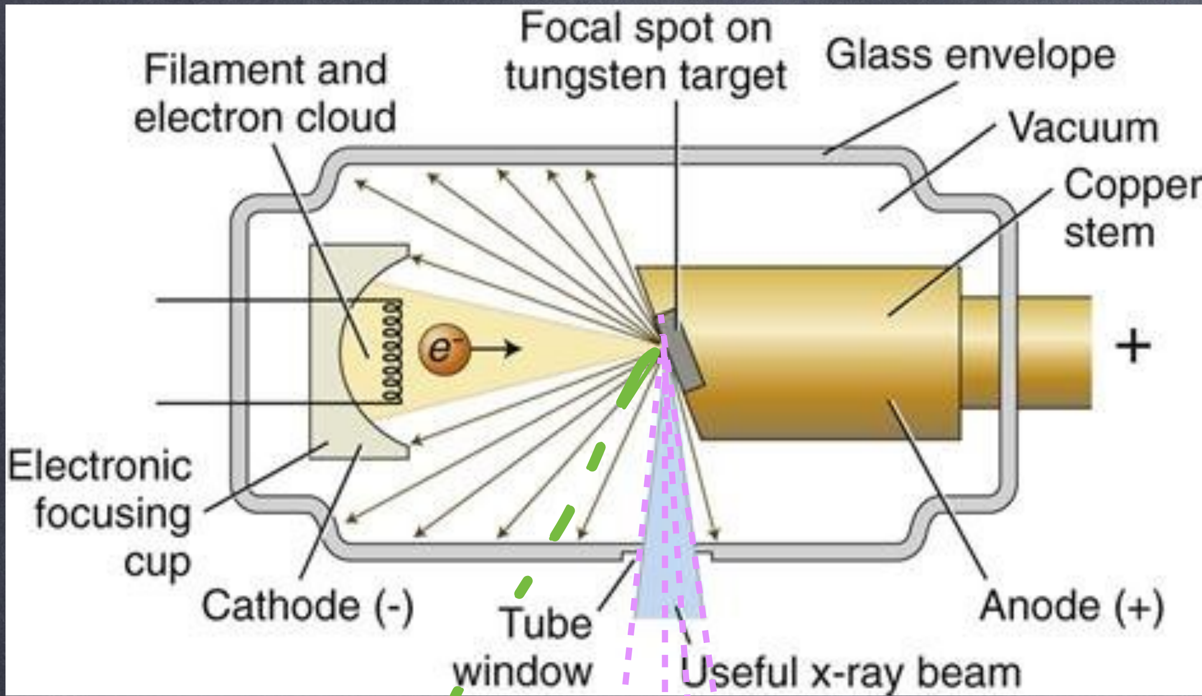
Discovery of the x-ray

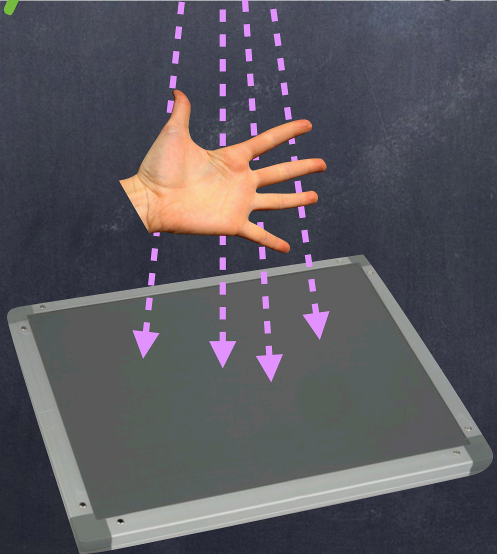
Roentgen, 1895



First "medical" x-ray
1895

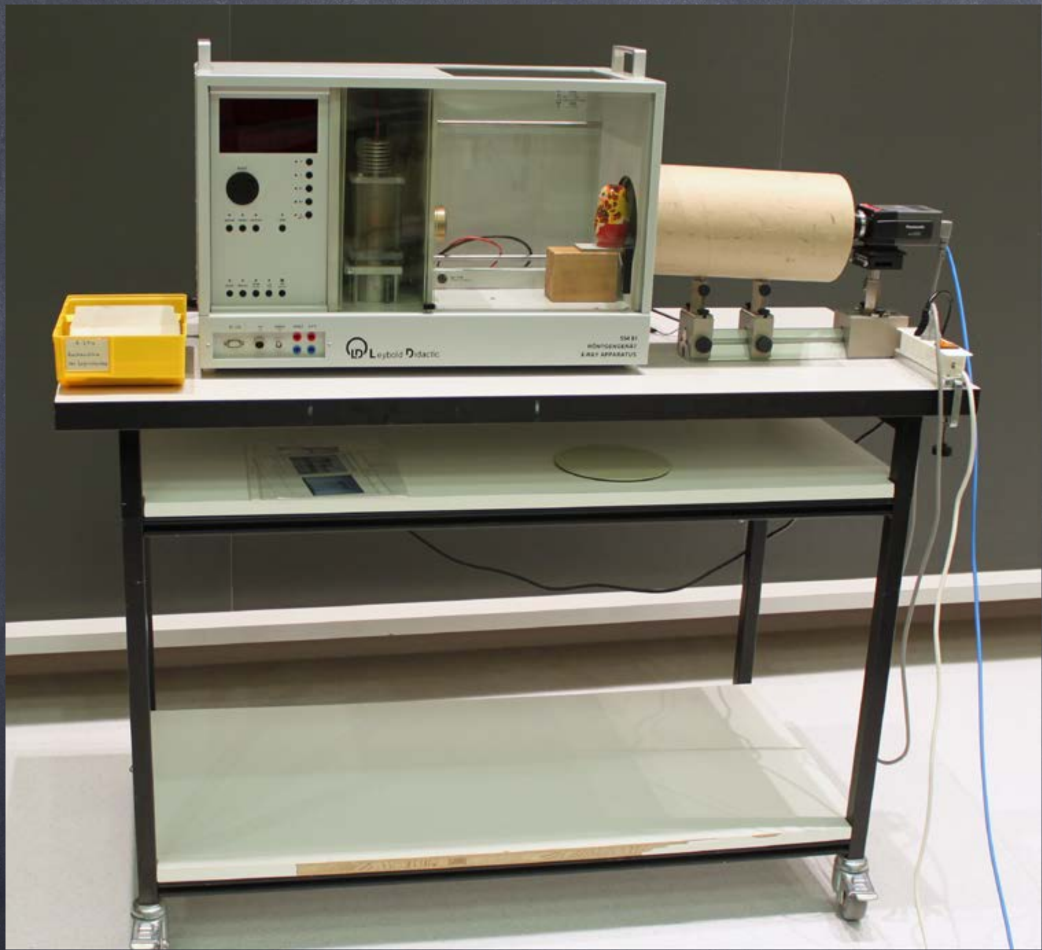
Roentgen's wife:
"I have seen my death."





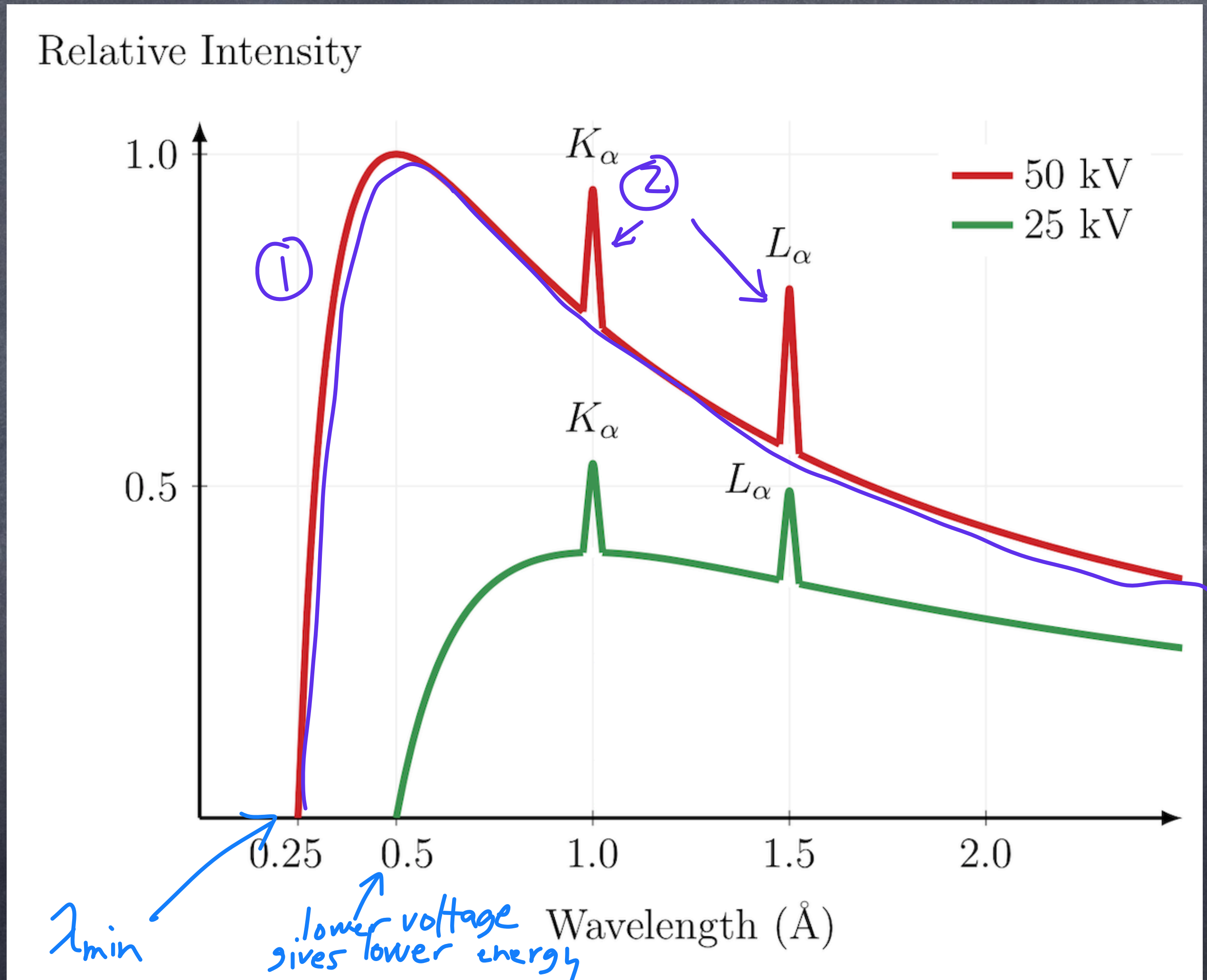
x-ray
production
here
in 2 ways

Fun with x-rays in class :



X-ray production: 2 components
1) Bremmstrahlung
2) characteristic X-rays (atomic excitations)

X-ray wavelength spectrum

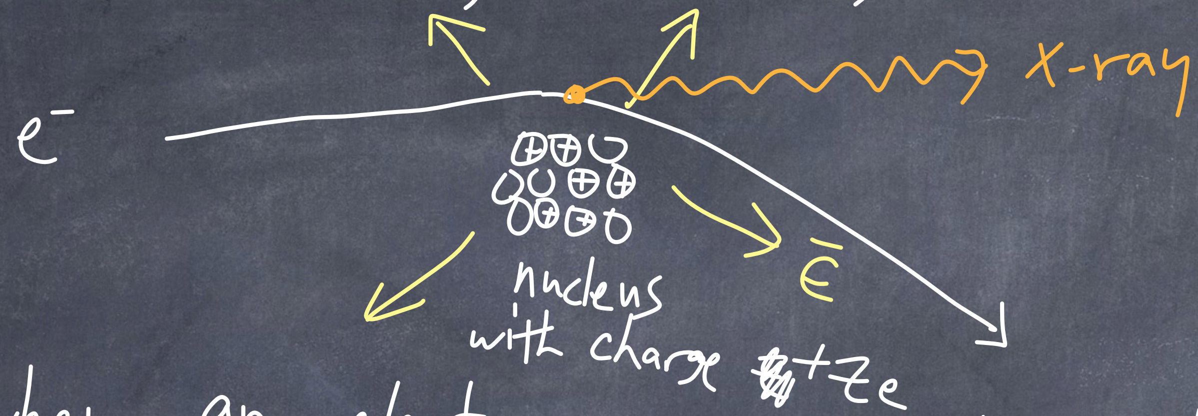


voltage of the electrons that are accelerated to produce the X-rays

Å = 1E-10 m (Angstrom)

← higher energy is lower wavelength

1) Bremmstrahlung "braking radiation"



when an electron passes closely to a nucleus, it has a large deflection angle and a photon (or more) is radiated.

Feynman diagram

an electron and a positron anhhilate into a photon and then the photon decays into a electron and positron

Maximum energy from Bremmstrahlung is if all of the initial electron energy $(U = eV)$ is converted to an x-ray.

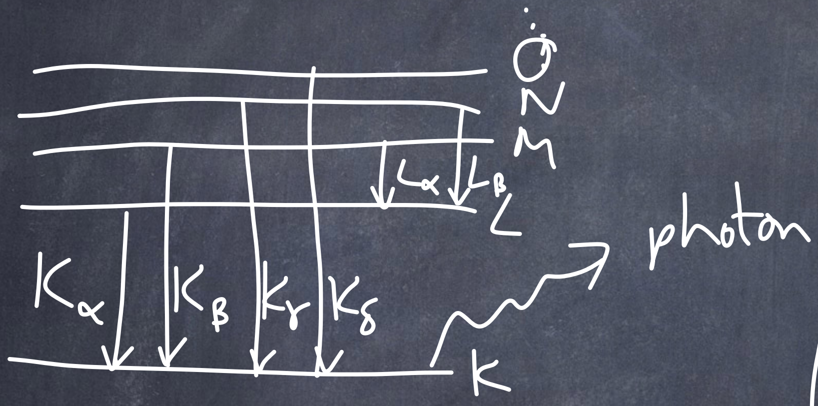
Then $\epsilon = h\nu = \frac{hc}{\lambda} = U = eV$

So for a voltage V, the minimum wavelength of the x-ray is $\lambda_{min} = \frac{hc}{eV}$.

This is the cutoff wavelength.

2) Characteristic x-rays

1) accelerated electrons hit inner orbital electrons.
2) once the inner electron is removed (knocked out), electrons from hiher energy levels fill the vacancy. This energy difference becomes the x-ray.



To estimate the photon energy of characteristic x-rays, we cannot simply use $\Delta E = \frac{hc}{\lambda}$ where $\frac{1}{\lambda} = RZ^2\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$

Because of screening, we need to use a Z_{eff}.

Principle is to take Z, then subtract the number of electrons at lower energies than the electron in the transition.

In the K-shell, $E_K = (Z-1)^2 \cdot E_1$

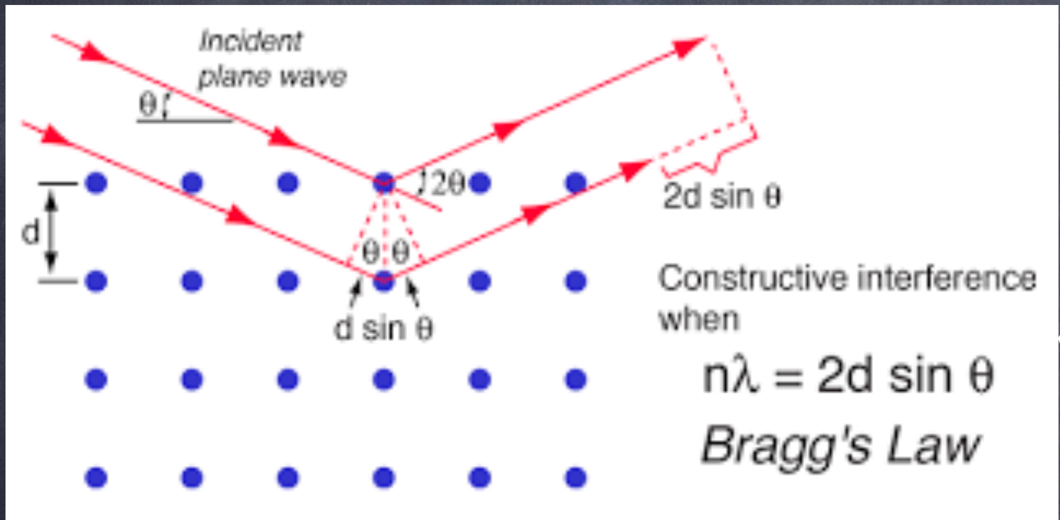
M-shell, $E_M = (Z-9)^2 \cdot E_3$

$\left.\begin{matrix} Z-1 \\ Z-9 \end{matrix}\right\} Z_{eff}$

There are 8 electrons in the L-shell and only one left in the K-shell (other removed) so $9 = 8+1$

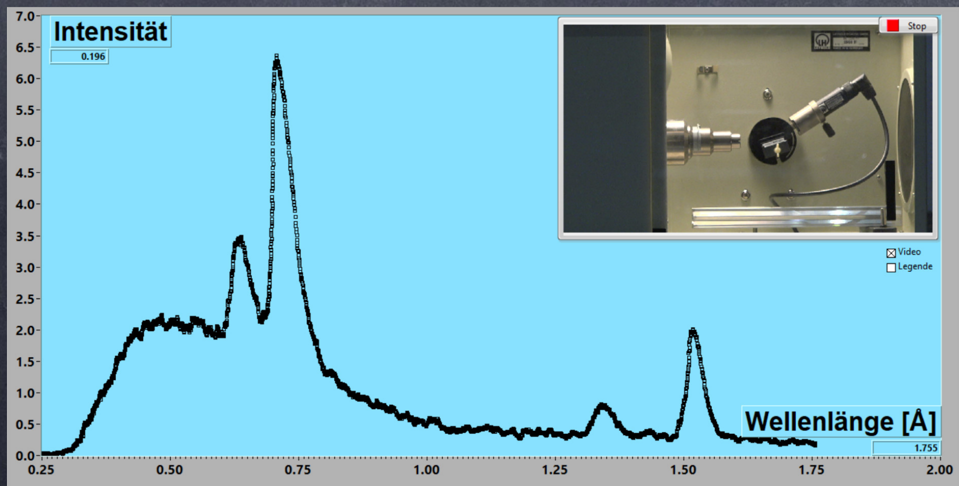
Bragg's Law: we use this to measure the intensity of x-rays at different wavelengths by moving the ~~det~~ detector at different angles.

crystal



λ depends on θ

d is the lattice spacing of the crystal



detector rotates in θ

$$\lambda = \frac{2d\sin\theta}{n}$$

($n=1$ here)

x-rays

energy for medical applications
lies between 30 keV − 150 keV

30 keV: mammography
150 keV: high-kilovoltage radiology

These correspond to 10^{-10} m and 10^{-12} m

x-ray scattering and energy loss. (in any tissue or material)

1) Thomson scattering - doesn't change the photon energy.
2) Compton scattering
3) Photoelectric effect

Thomson scattering:

① photon, frequency ν | electron

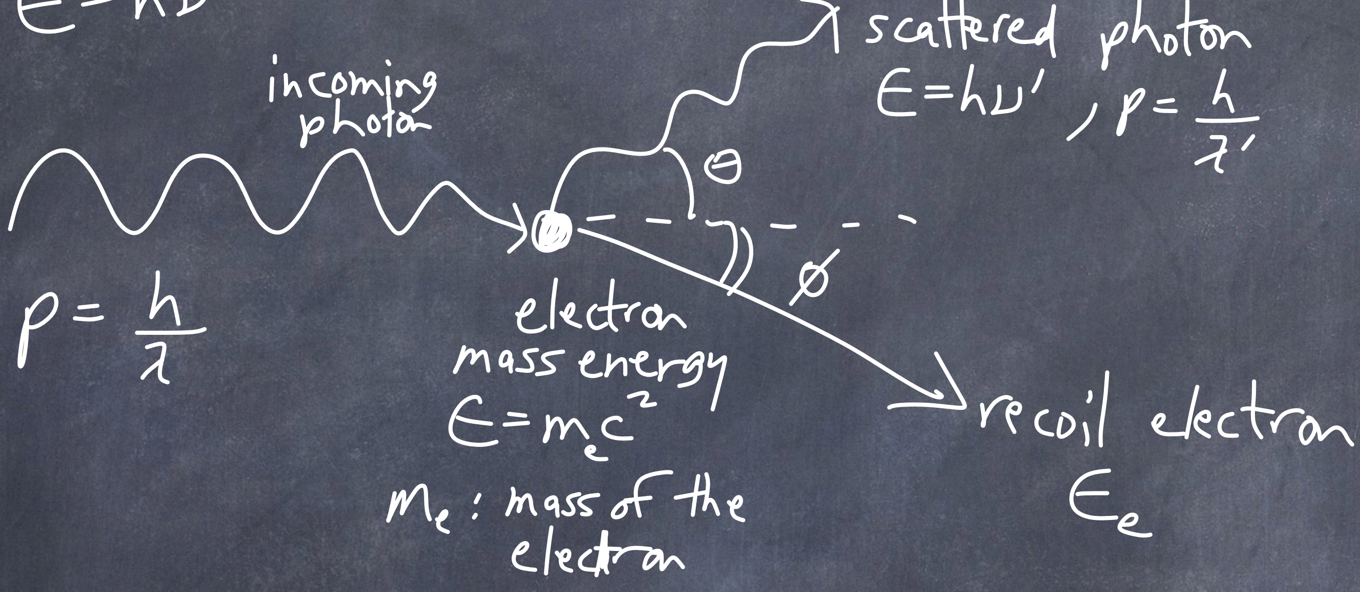
② electron oscillates at ν

③ electron emits a photon at the same frequency ν

Compton scattering - process that makes the γ-ray wavelength larger (reduces the energy & frequency of γ-ray)

$E = h\nu$

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



$\nu' < \nu$, $\lambda' > \lambda$

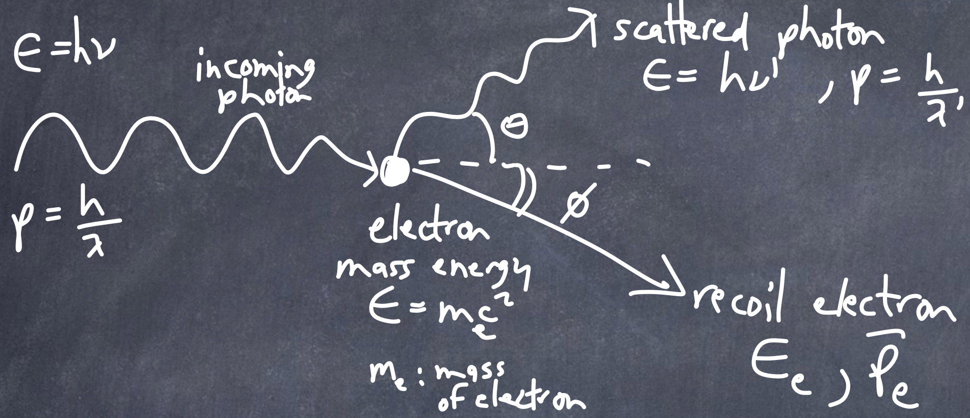
$$\boxed{\Delta\lambda = \lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)}$$

Compton effect

(In the notes, I'll add a derivation)

start:

Supplementary: how to derive the Compton effect formula:



we do it using momentum + energy conservation.

	Initial state	Final state
photon energy	$h\nu$	$h\nu'$
photon momentum in x-direction	$\frac{h}{\lambda}$	$\frac{h}{\lambda'}\cos\theta$
photon momentum in y-direction	0	$\frac{h}{\lambda'}\sin\theta$
Electron energy	mc^2	$E_e = m_e c^2 + K$ ← Kinetic energy
Electron momentum in x-direction	0	$p_e \cos\phi$
Electron momentum in y-direction	0	$p_e \sin\phi$

Relativistically, the energy of a massive particle is $\boxed{E^2 = (mc^2)^2 + (cp)^2}$ ⓪ True in general!

from rest mass — from momentum

For our problem:

Energy conservation means $E_{initial} = E_{final}$

$$\boxed{h\nu + m_e c^2 = h\nu' + E_e} \quad ①$$

Momentum conservation in x direction:

$$\boxed{\frac{h}{\lambda} = \frac{h}{\lambda'}\cos\theta + p_e \cos\phi} \quad ②$$

in y direction:

$$0 = \frac{h}{\lambda'}\sin\theta - \underbrace{p_e \sin\phi}_{-y \text{ direction}}$$

$$\boxed{\frac{h}{\lambda'}\sin\theta = p_e \sin\phi} \quad ③$$

Now we solve this. First, square ② + ③ and add. This removes ϕ:

$$p_e^2(\cancelto{1}{\sin^2\phi+\cos^2\phi}) = \left(\frac{h}{\lambda}\right)^2 + \left(\frac{h}{\lambda'}\right)^2(\cancelto{1}{\cos^2\phi+\sin^2\phi}) - 2\frac{h}{\lambda}\frac{h}{\lambda'}\cos\theta \qquad ④$$

Now substitute E_e from ① & p_e from ④ into ⓪:
(Setting $\lambda = \frac{c}{\nu}$)

$$\left[h(\nu-\nu') + (mc^2)\right]^2 = m_e^2c^4 + (h\nu)^2 + (h\nu')^2 - 2h\nu(h\nu')\cos\theta$$

Do the squaring of the left side & cancel terms to get:

$$m_ec^2(\nu-\nu') = h\nu\nu'(1-\cos\theta)$$

rearranging: $\frac{h}{m_ec^2}(1-\cos\theta) = \frac{\nu-\nu'}{\nu\nu'} = \frac{\frac{c}{\lambda}-\frac{c}{\lambda'}}{\frac{c^2}{\lambda\lambda'}} = \frac{1}{c}(\lambda'-\lambda)$

end: or $\boxed{\Delta\lambda = \lambda'-\lambda = \frac{h}{m_ec}(1-\cos\theta)}$

Done!

Back to notes ...

The quantity $\frac{h}{m_e c^2}$ is called the Compton wavelength of the electron, $\lambda_c = \frac{h}{m_e c^2} = 2.43\,E{-3}$ nm

Only for wavelengths λ_c or smaller, is Compton scattering observed.

For example, visible light has $\lambda \sim 500$ nm

The maximum change is $\frac{\Delta\lambda}{\lambda} \sim 10^{-5}$

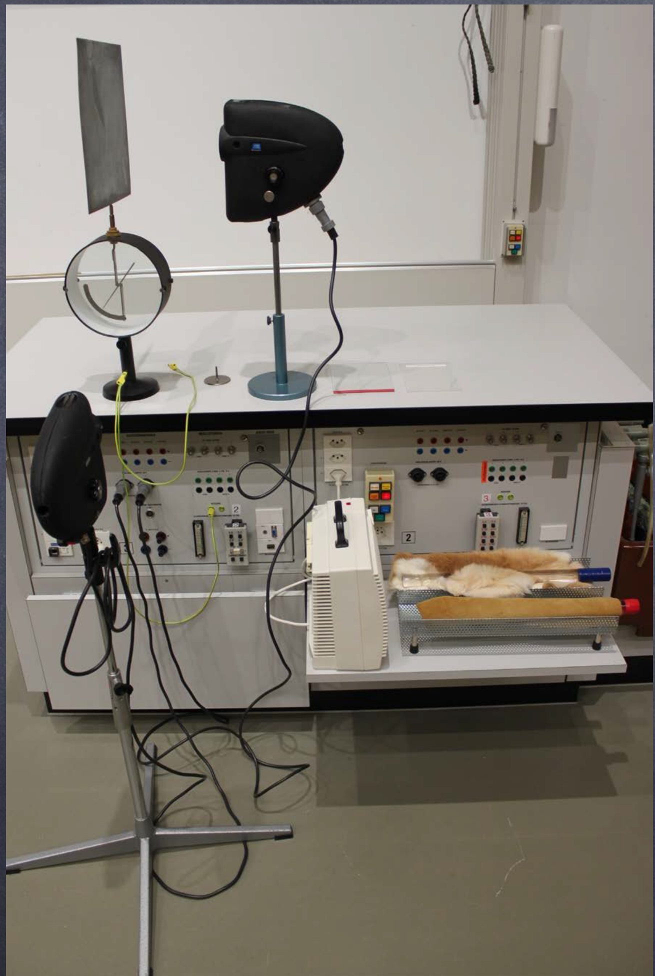
For an x-ray, $\lambda \cong 0.07$ nm,

$$\frac{\Delta\lambda}{\lambda} \sim 0.03$$

So Compton effect is only important for x-rays or gamma rays.

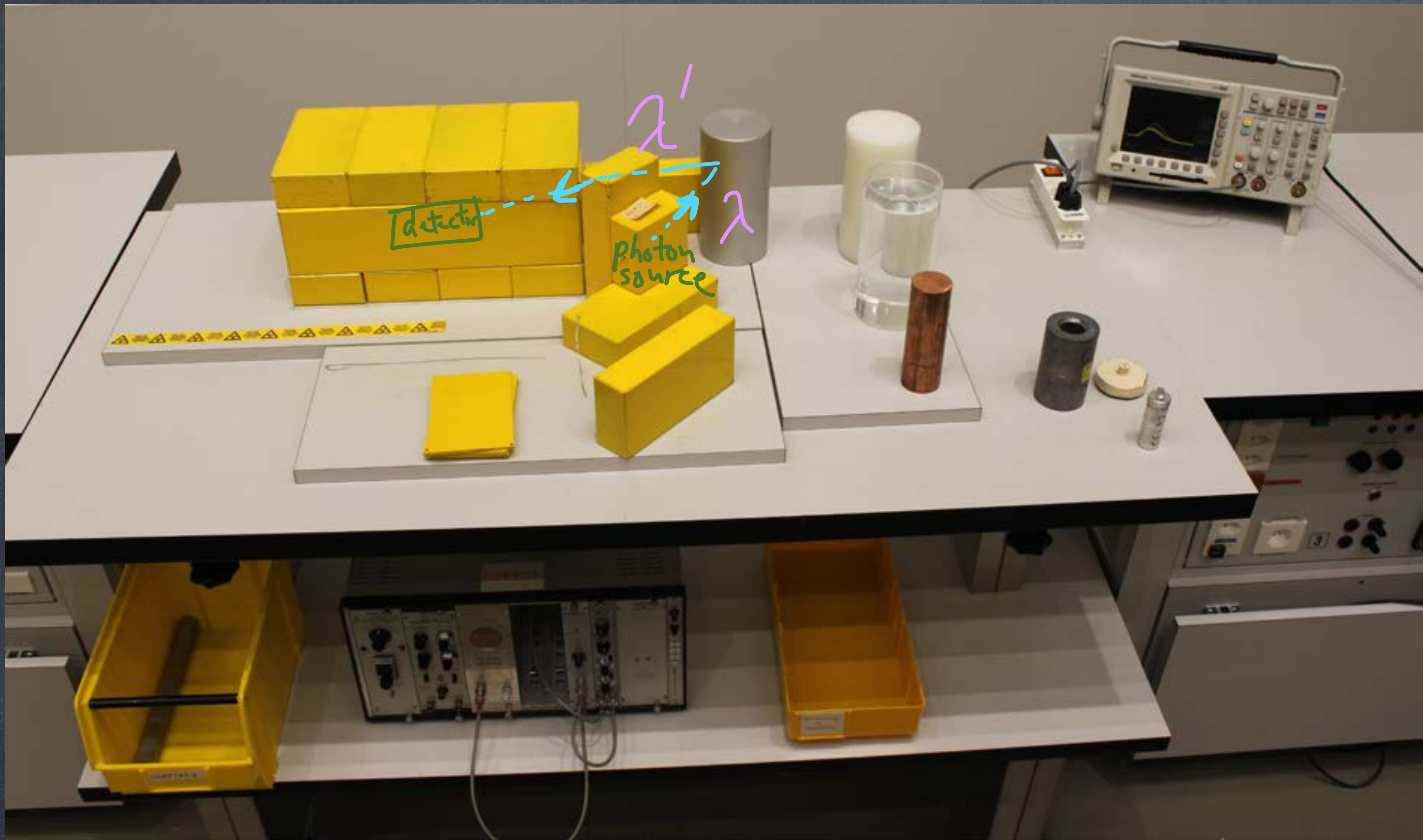
(Not visible, UV, infrared, ...)

Photoelectric effect we already learned :



Light can free electrons if it is has enough energy to overcome binding energy

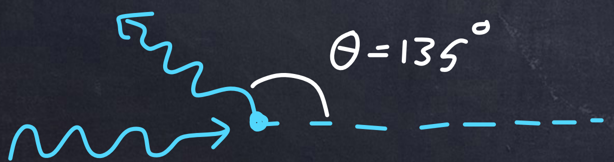
Compton effect experiment



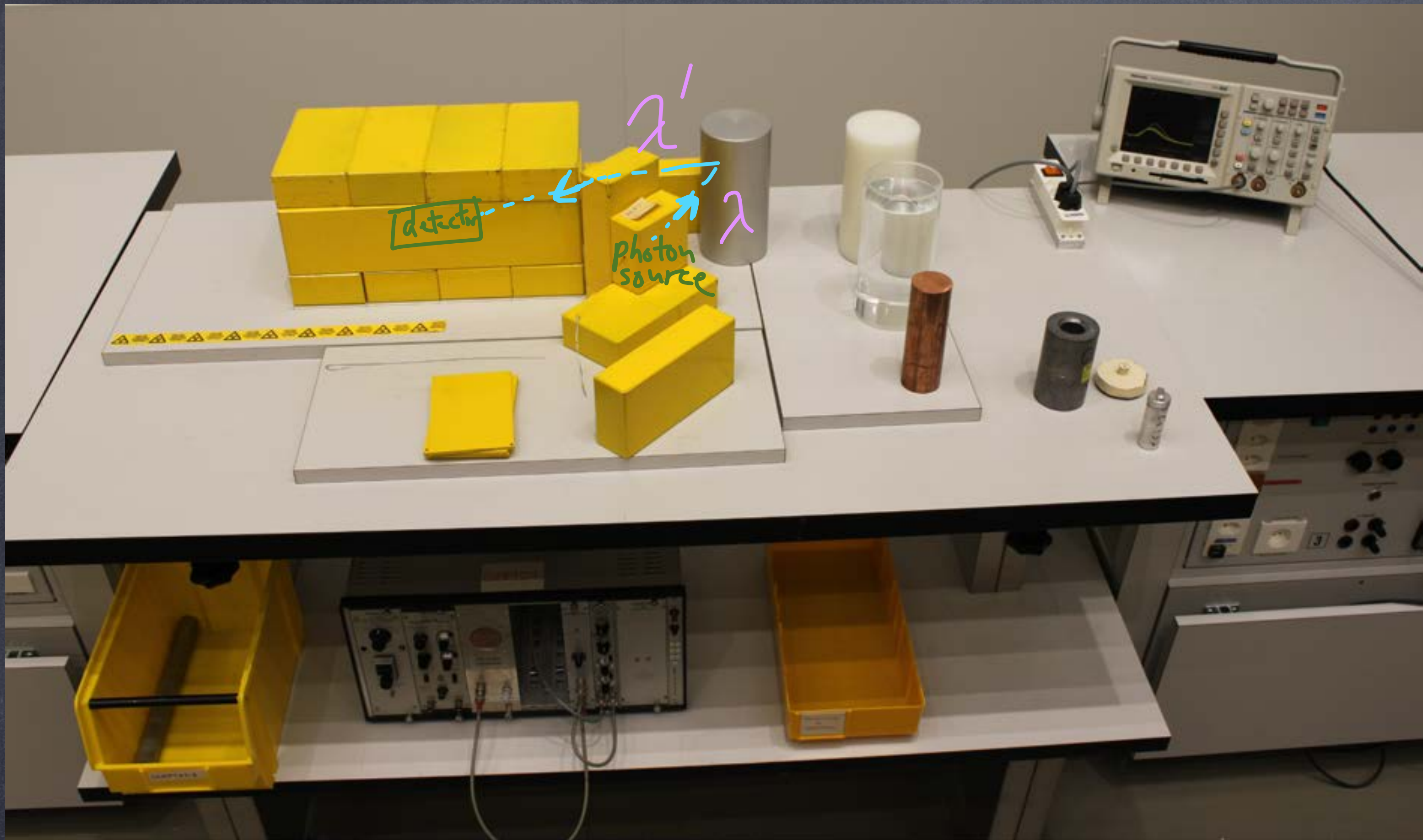
^{137}Cs source emits electrons (512 keV) and photons (662 keV)

we can stop electrons with aluminum

what is the wavelength of photons that are Compton scattered? (see next page)



Compton effect experiment

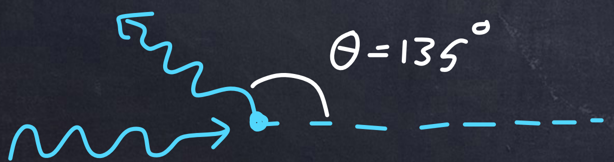


^{137}Cs source emits electrons (512 keV) and photons (662 keV)

we can stop electrons with aluminum

photon $E = 662\,keV \rightarrow \lambda = 0.019\,E{-10}\,m = 0.019\,Å$ (Angstroms)

$$\frac{h}{m_e c} = 0.0243\,Å$$

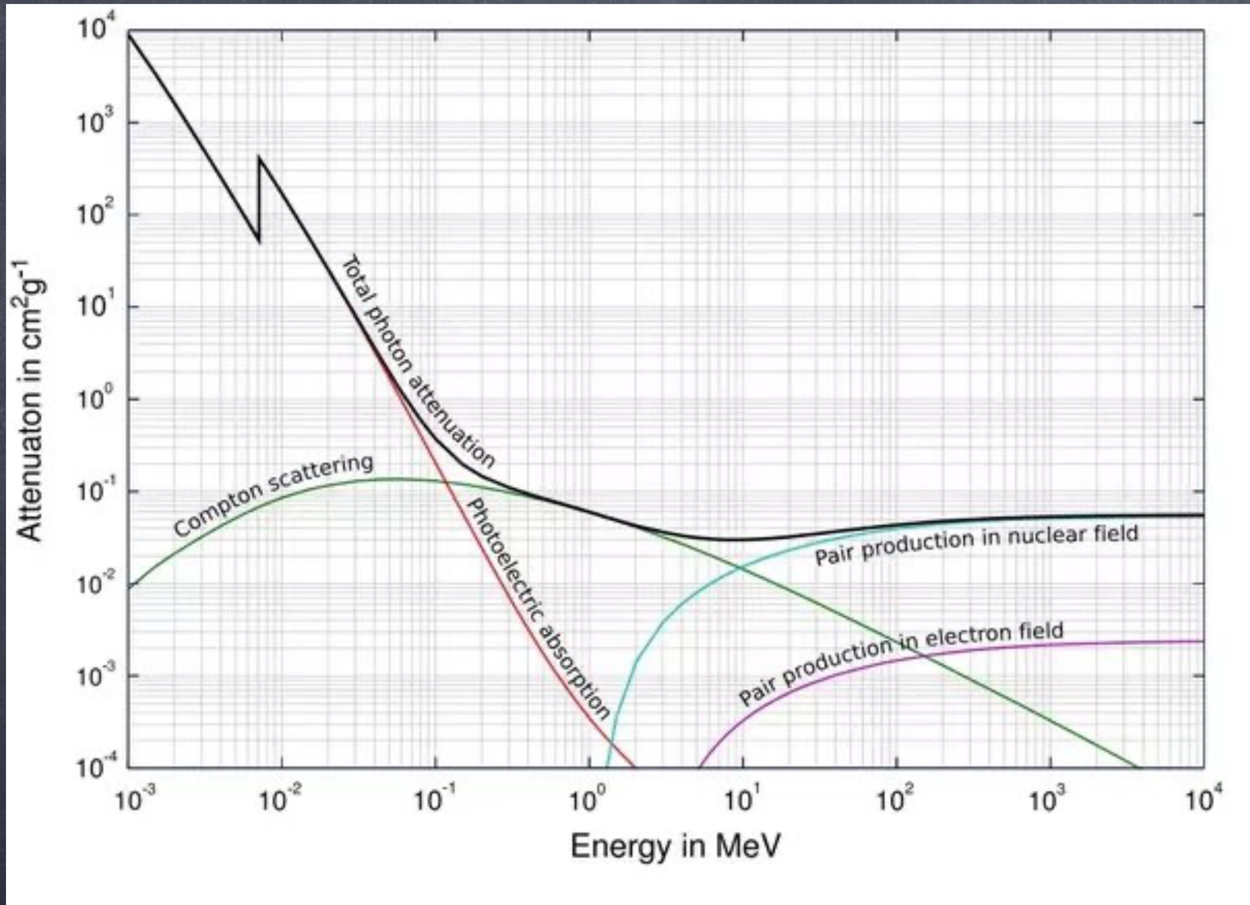


$$\lambda' = \lambda + \frac{h}{m_e c}(1-\cos\theta)$$

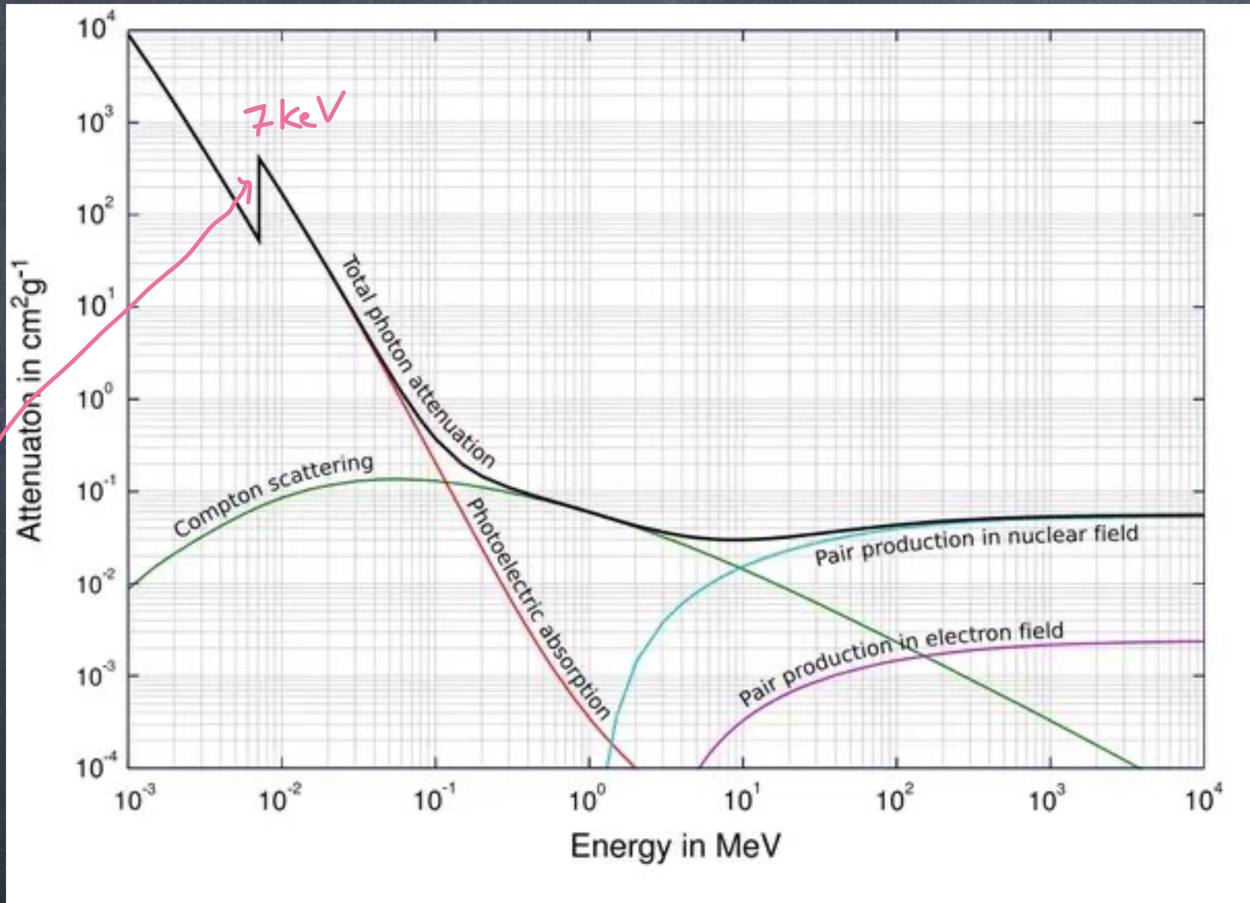
$$= (0.019\,E{-10}m) + (0.0243\,E{-10}m)(1-\cos 135°)$$

$$\lambda' = 0.06\,E{-10}\,m$$

How photons lose energy as a function of their initial energy.



How photons lose energy as a function of their initial energy.



From this plot, the K-absorption edge is ~7 keV. use this website to find out what material this is.

photoelectric absorption edge (higher interaction rate if photon has almost the same energy as an atomic energy shell.)

Database of K-absorption edges for different materials here :

http://skuld.bmsc.washington.edu/scatter/AS_periodic.html

Here we see the K-shell absorption edge.