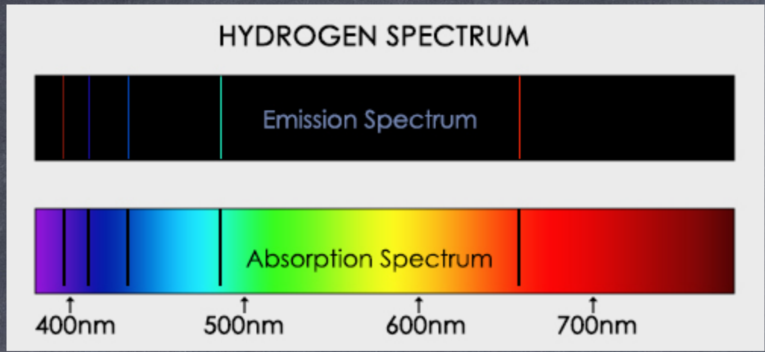
PHY127 FS 2024

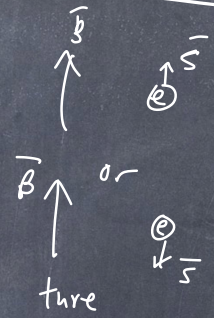
Prof. Ben Kilminster
Lecture April 26th, 2024

Last week:

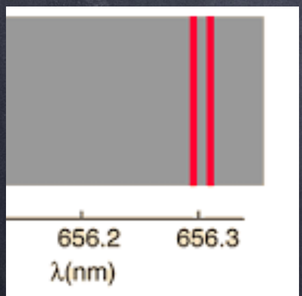
Fine structure is 4th quantum number, m_s



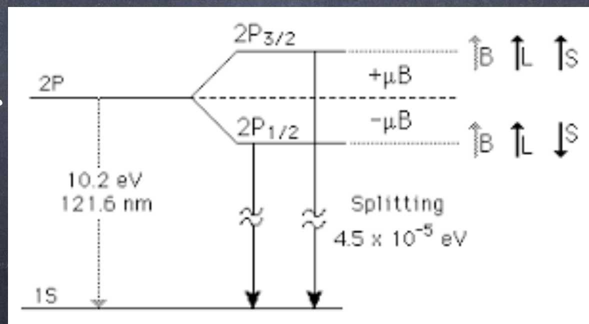
From spin of electron when atom is in a magnetic field.



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



2p line is actually split into two energy levels

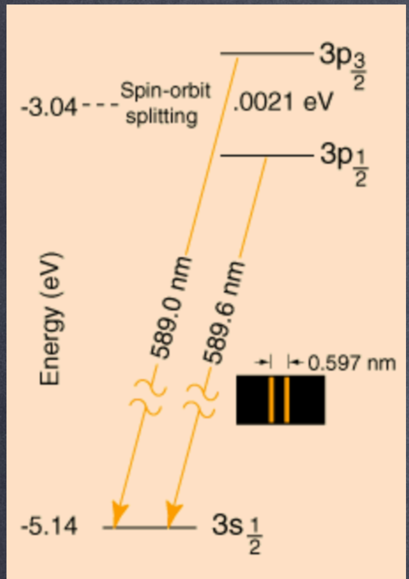


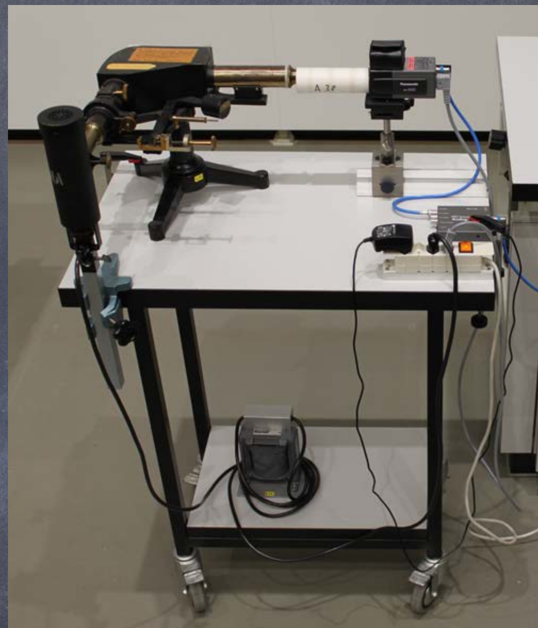
"Fine" structure = detailed structure

"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)

Experiment to see the effect of electron spin on the energy spectrum of Sodium (Na).





$\Delta E = 0.0021 \text{ eV}$

ΔE is due to the magnetic energy from the electron spin

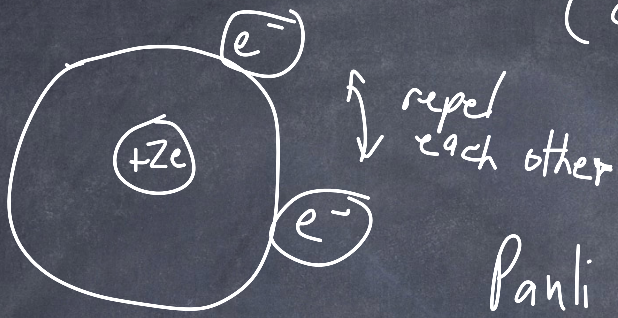
$\Delta E = \mu_e B = g \mu_B B$ $\quad$ ($g \sim 2$ for electrons)

we find that $B = \frac{\Delta E}{2\mu_B} = 18$ Tesla (very high by lab standards)

This B is the internal magnetic field from the electron spin that produces this splitting

Atoms with many electrons:

He



(cannot be solved exactly with the Schroedinger equation)

Pauli exclusion principle:

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

This is a rule that applies to all "fermions": particle that has a spin of $\frac{1}{2}\hbar$.

Fundamental fermions (like electrons) have a spin of $\frac{1}{2}$. (we often omit the "$\hbar$").

Can have spin of $+\frac{1}{2}$ or $-\frac{1}{2}$

Fermions are the particles that compose matter.

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

$+\frac{1}{2}$ ↑ $\qquad$ $-\frac{1}{2}$ ↓

Applied to the hydrogen atom (with one electron)

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

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

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

So the rules for atomic electron structure:

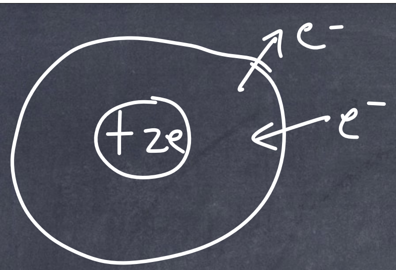
1) Electrons tend to occupy the lowest available energy levels.

2) Electrons have unique set of quantum numbers.

Consider Helium: According to our principles, the first & second electrons occupy:

$\left(1, 0, 0, +\frac{1}{2}\right)$

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



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 the n-values as shells.

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

And ℓ values as sub-shells:

$\ell =$	0	1	2	3	...
sub-shell $=$	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) state, the third electron must be in the $n=2$ (L-shell) state. So

Li is described as: $1s^2 2s^1$

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

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

For each m: two values of m_s

For each ℓ: $(2\ell+1)$ values of m $\quad 2(2\ell+1)$

ordered by energy level

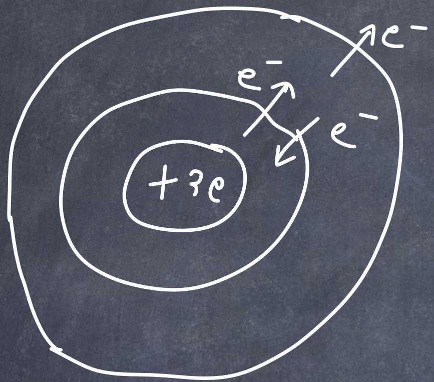
lowest energy states are filled first

n	ℓ	sub-shell	sub-shell capacity	total electrons in all sub-shells
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
…	…	…	…	…

4s lower energy than 3d due to screening

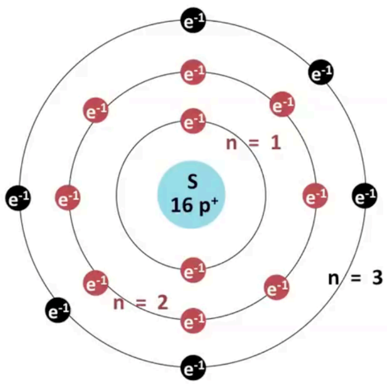
Aside on screening:

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, $Z_{effective} = Z_{eff} = +1e$

What is the effective nuclear charge felt by an electron in the n = 3 shell of sulfur?



Example:

Sulfur has $Z = 16$:

$$1s^2 2s^2 2p^6 3s^2 3p^4$$

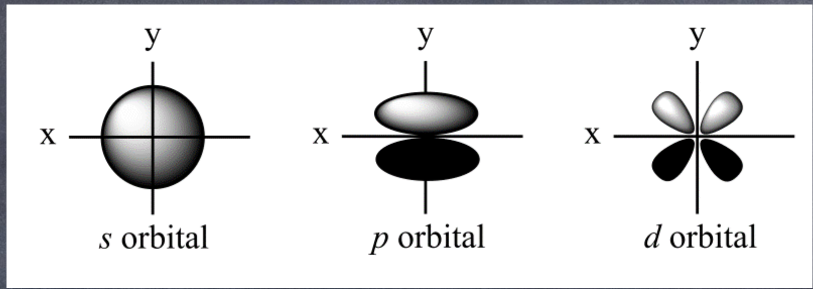
An electron at $n=3$ is shielded from the 16 protons by the inner shell electrons.

$$Z_{eff} = Z - \#\text{inner-shell electrons}$$

$$= 16 - 10$$

$$Z_{eff} = 6$$

Note: screening is a bit more complicated than this due to shape of orbits:



⋮
4p
3d
$\boxed{4s}$
3p
energy ↑ 3s
2s
1s

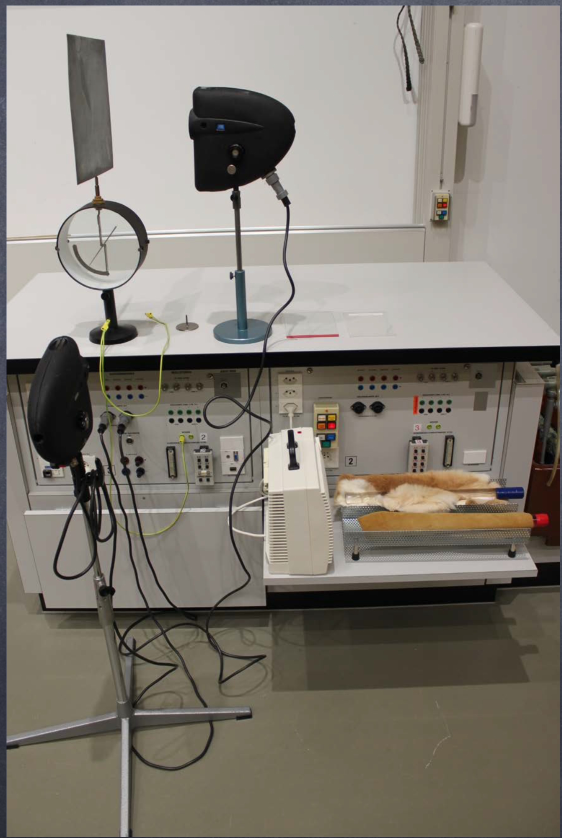
Note: 4s is bound with less energy than the 3d.

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.

A bit of an aside on detecting radiation

Photoelectric effect we already learned :

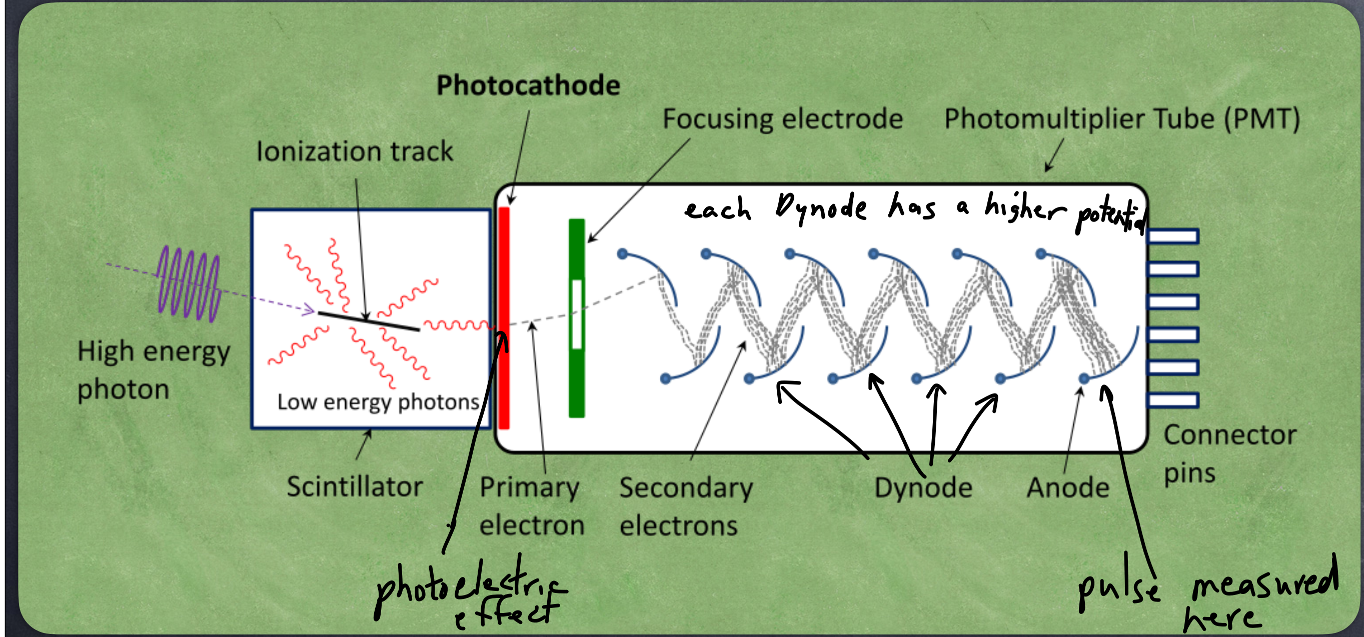


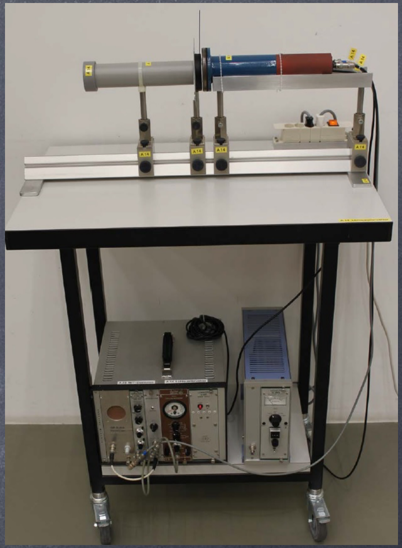
Light can free electrons if photons have enough energy to overcome binding energy

Radiation: we start with visible light detection

(PMT)

Photomultiplier tube causes cascade of electrons from one photon





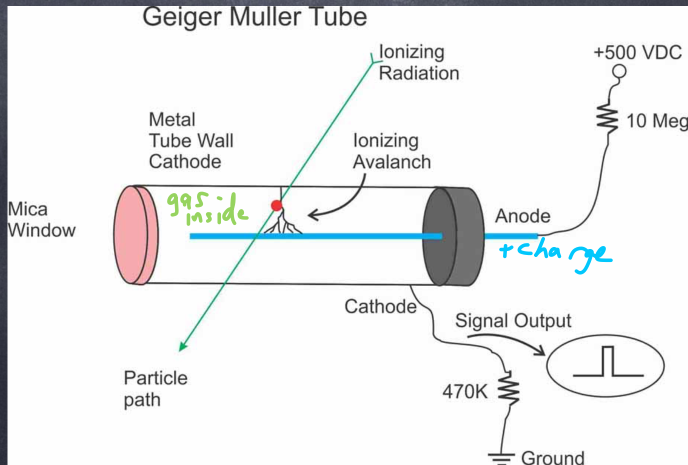
we hear a "click"

Charged particle radiation

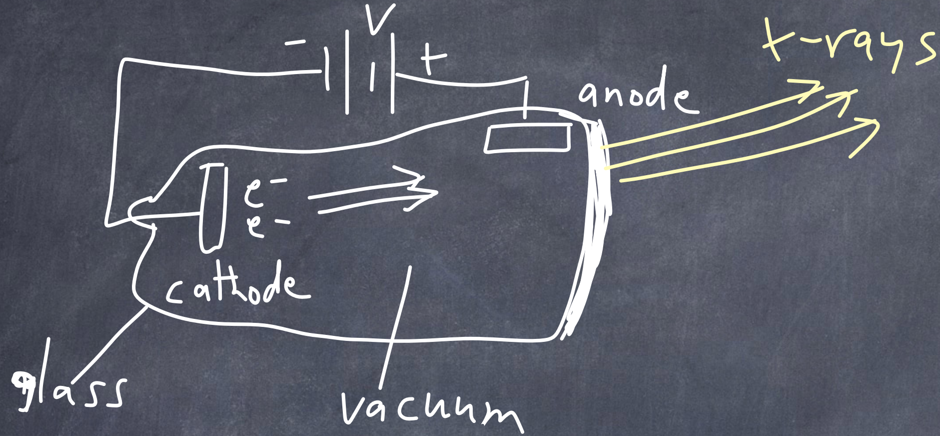
Radium & Uranium decay producing charged radiation (alpha particles or Helium nuclei)

Geiger counter

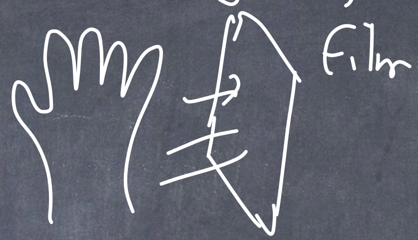
charged particle ionizes gas producing electrons and ions. As they are accelerated to anode, secondary electrons are produced.
Recorded as a pulse or a "click".

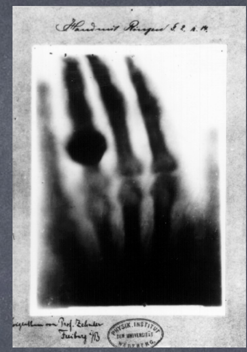


Discovery of the x-ray



Roentgen, 1895

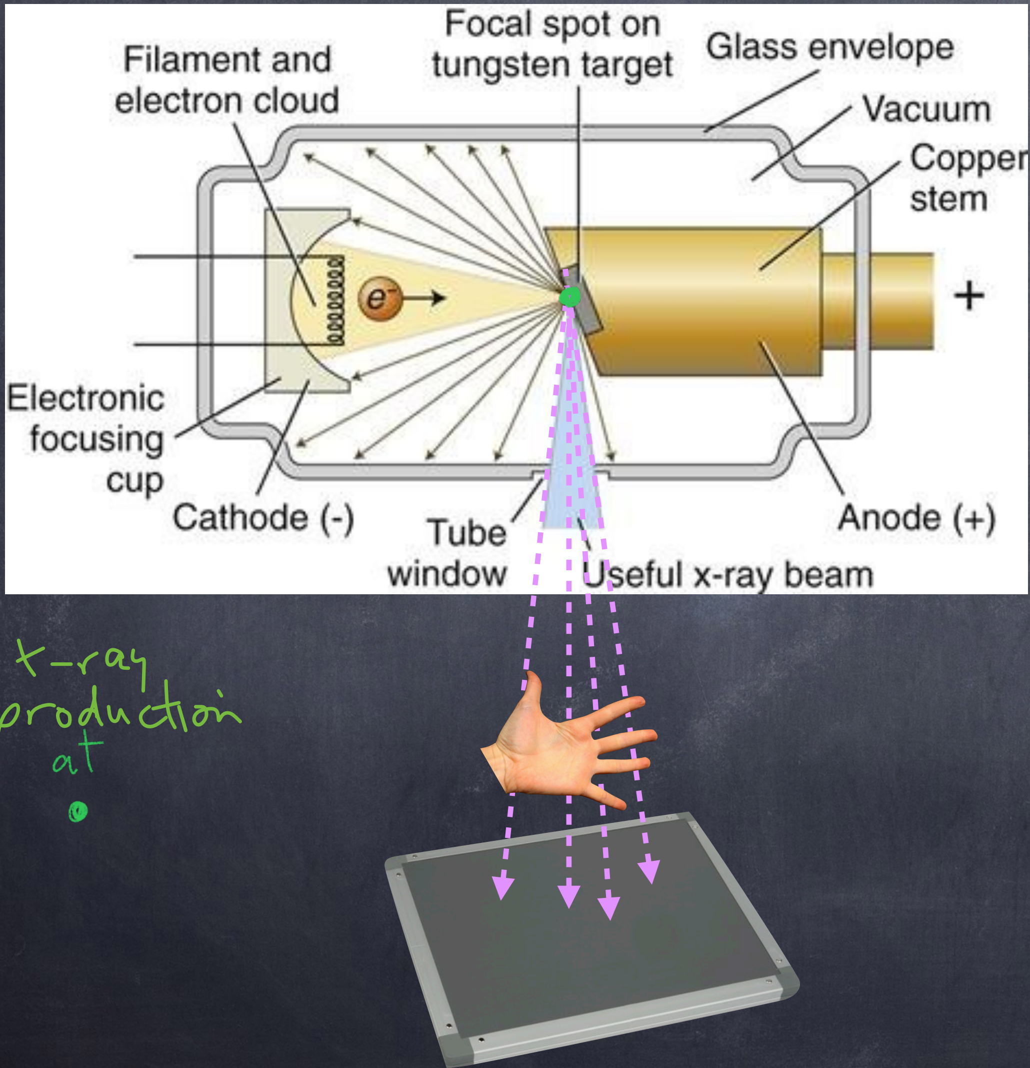




First "medical" x-ray

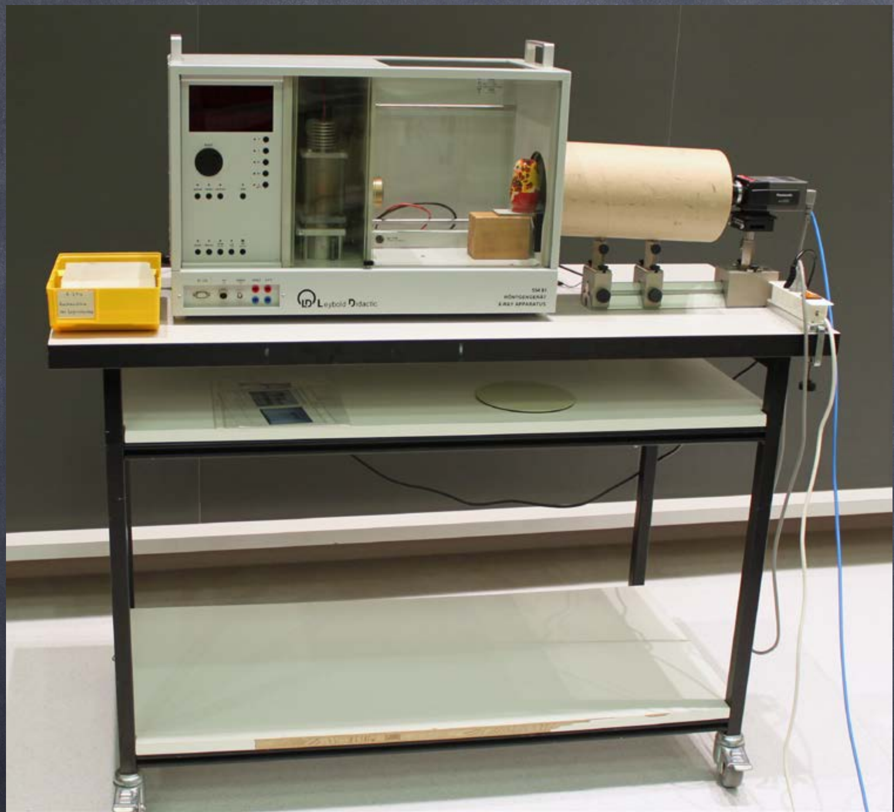
Roentgen's wife:
"I have seen my death."

Modern x-ray tube:

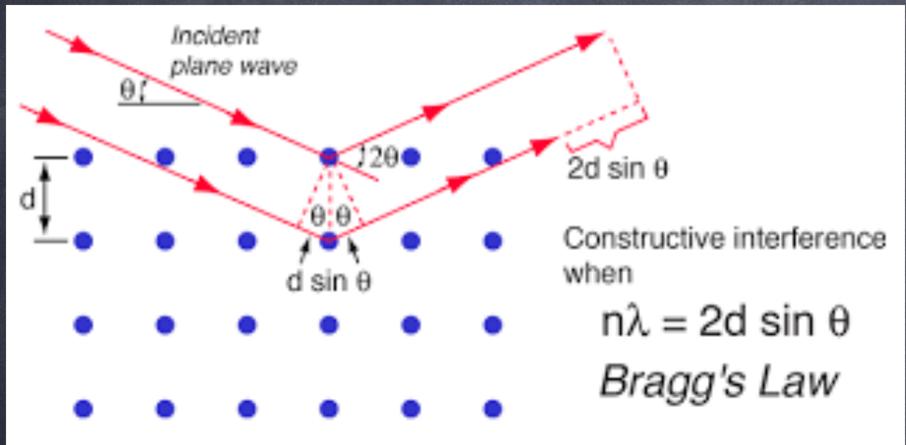


x-ray
production
at

Fun with x-rays in class:



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



Experiment in class:

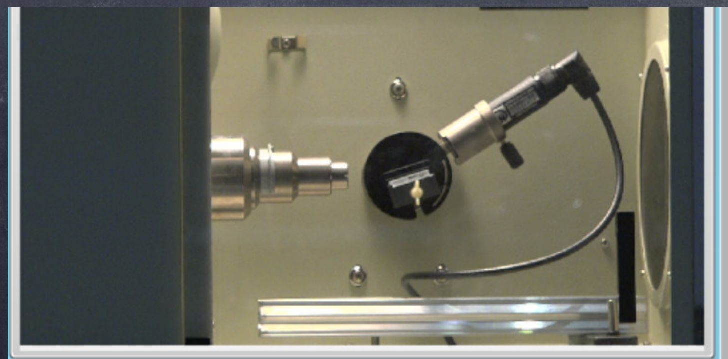
Crystal: Natrium-Chlorid:
Netzebenenabstand 282 pm
Reflexionswinkel für die Molybdän-K α-Strahlung der Wellenlänge 71 pm: σB = 7.24°.

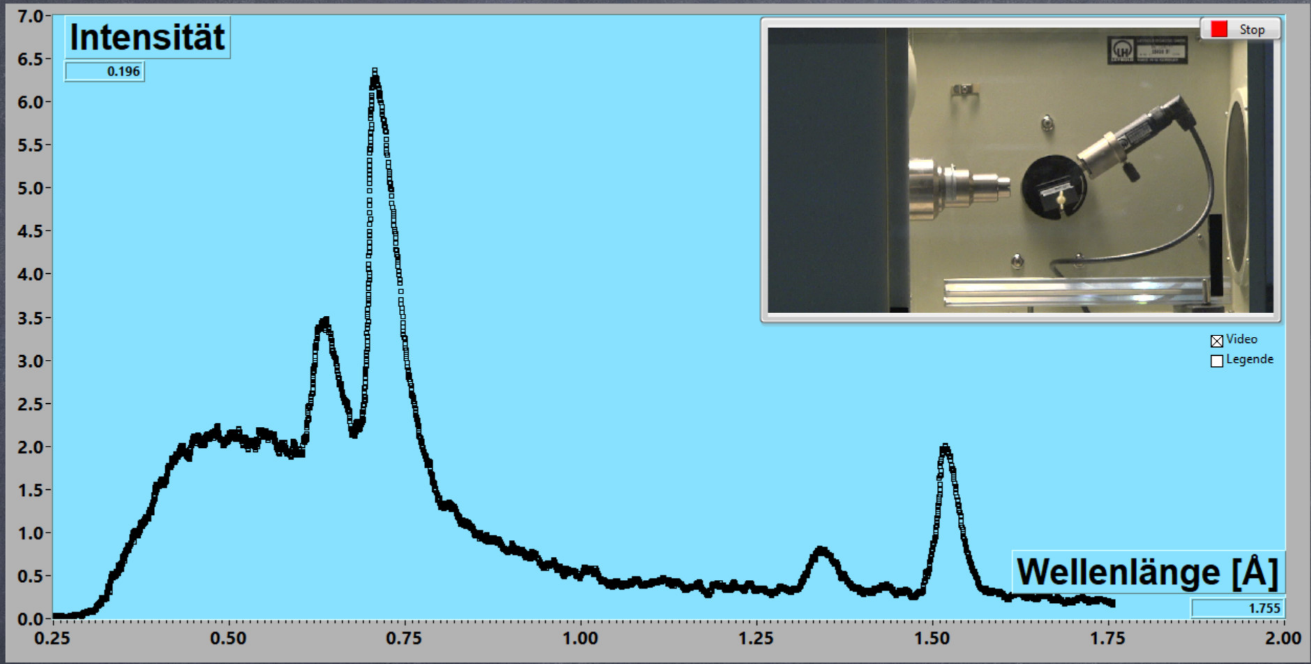
λ depends on θ

detector rotates in θ

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

interference maxima
(n=1 here)





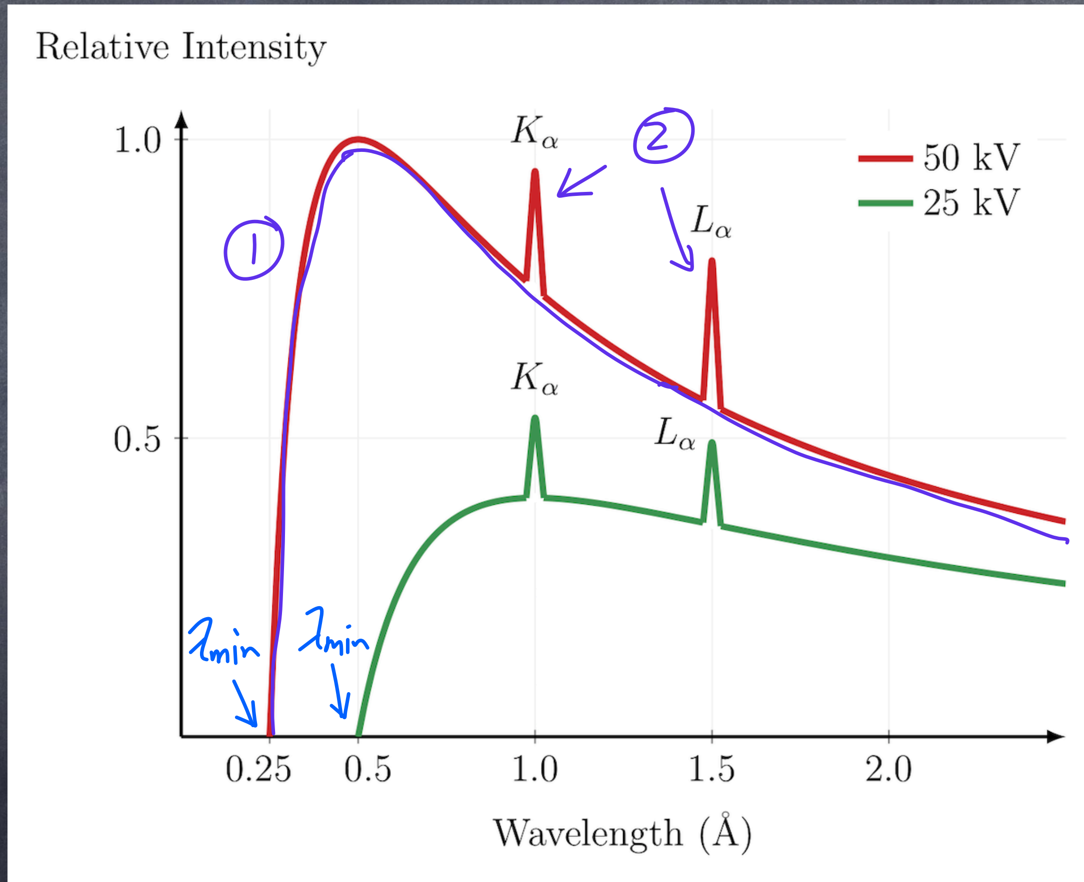
n=1 n=2

what is this structure?

x-ray production! 2 components:

1. Bremmstrahlung
2. characteristic x-rays (atomic excitations)

x-ray wavelength spectrum



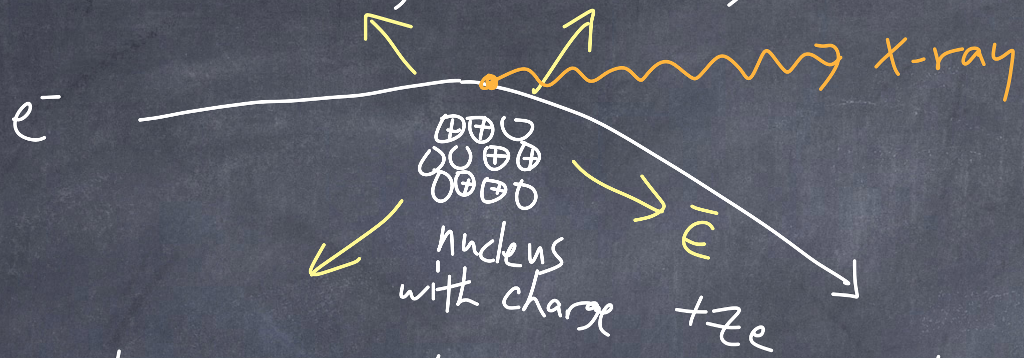
voltage of the electrons that are accelerated to produce the x-rays.

Å = 1E-10 m

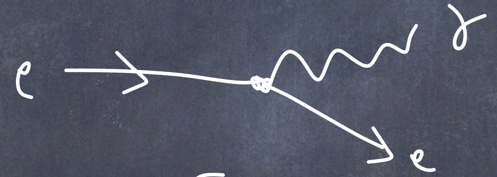
Angstrom

← 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 diagrams

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

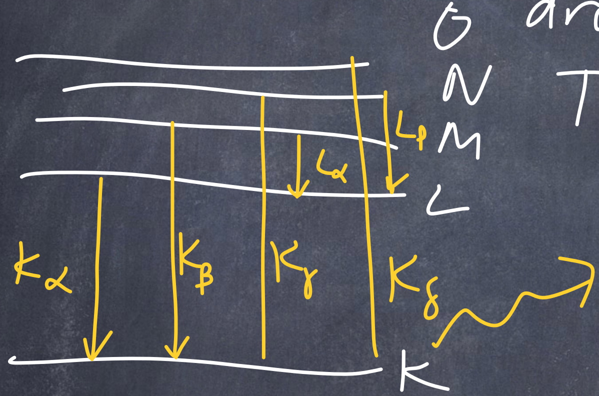
Then $\quad E = h\nu = \dfrac{hc}{\lambda} = U = eV$

so for a voltage V, the minimum wavelength of the x-ray is $\lambda_{min} = \dfrac{hc}{eV}$ (This is the cutoff wavelength)

② characteristic x-rays:

1) accelerated electrons hit inner orbital electrons of our atom, knocks it out.

2) once the inner electron is removed, electrons from higher energy levels drop down & fill the vacancy.



This energy difference becomes the energy of an emitted x-ray.

To estimate the photon energy of the characteristic x-rays, we can't simply use

$$\Delta E = \frac{hc}{\lambda} \quad \text{where} \quad \frac{1}{\lambda} = RZ^2\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$$

we instead need to use Z_{eff} because of screening

X-rays

energy for medical applications lies between 30 keV – 150 keV

	30 keV	150 keV
	mammography	high-kilovoltage radiology
these correspond to	10^{-10} m (λ)	10^{-12} m (λ)

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

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

Thomson scattering:

① photon, frequency, ν — electron

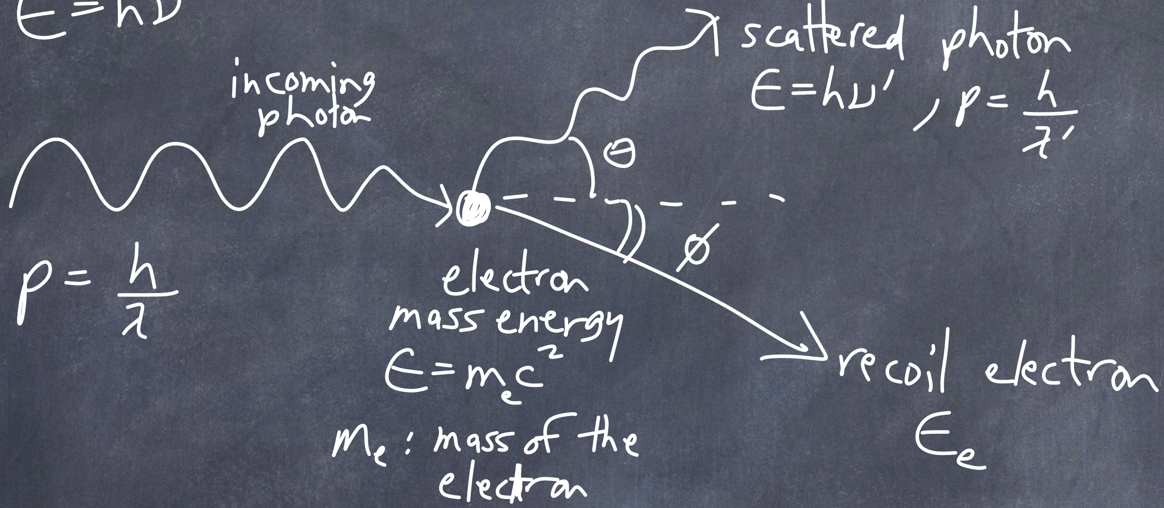
② electron oscillates at frequency, ν

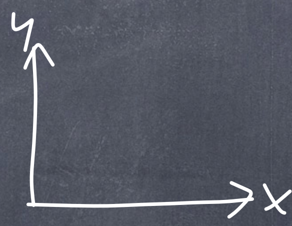
③ emits a photon at the same frequency ν

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

$E = h\nu$

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



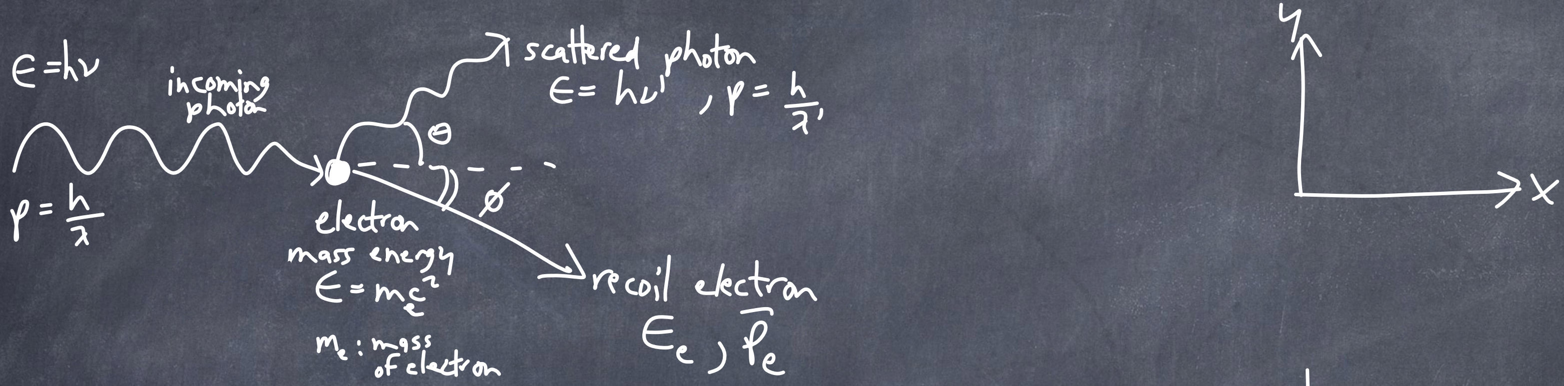


$$\boxed{\Delta\lambda = \lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)}$$

Compton effect

(Derivation of this formula next in case you are curious how) start of derivation!

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

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

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

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

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 $\frac{h}{m_e c}$ is called the Compton wavelength of the electron,

$$\lambda_c = \frac{h}{m_e c} = 2.43 \,E{-3} \text{ nm}$$

Only for wavelengths of X-rays equal to λ_c or smaller, is Compton scattering observed.

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

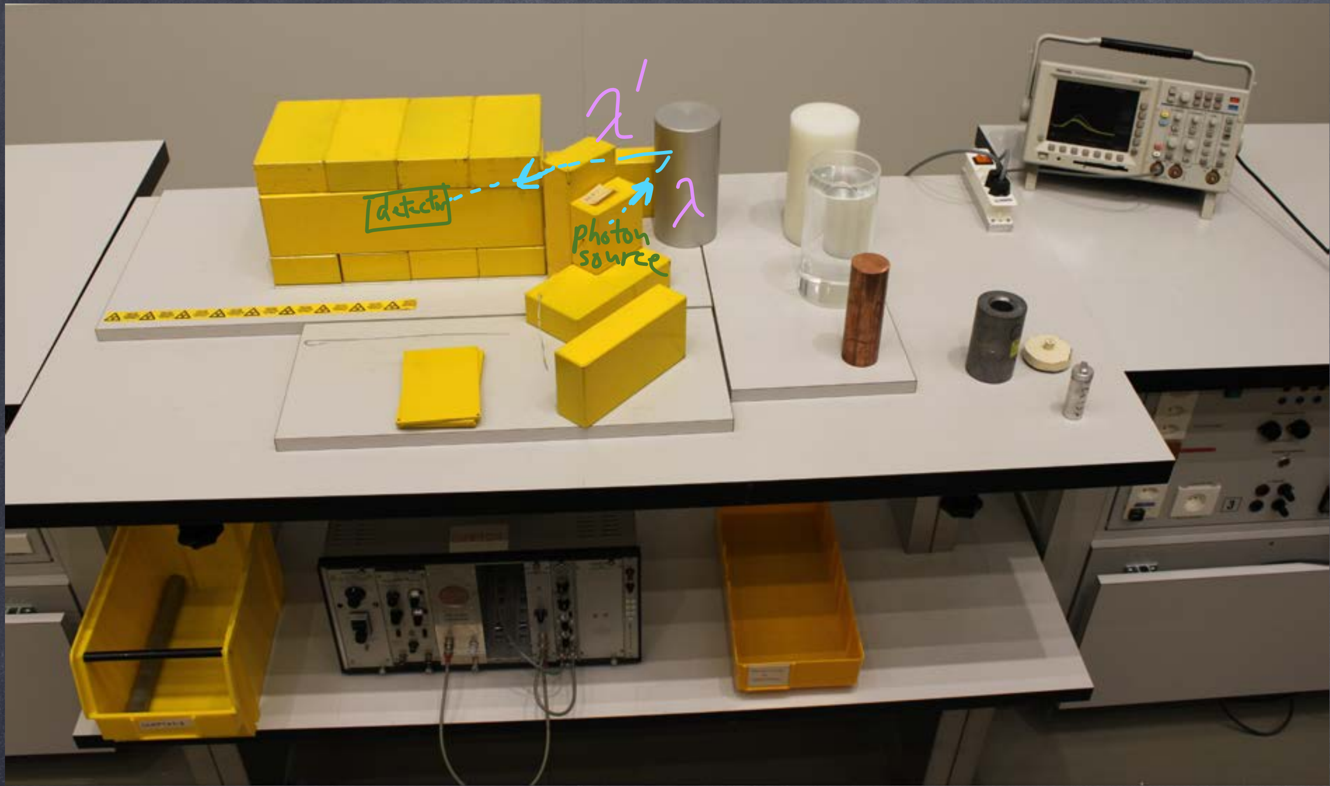
the maximum $\frac{\Delta\lambda}{\lambda} \sim 10^{-5}$

For an X-ray, $\lambda \sim 0.07$ nm,

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

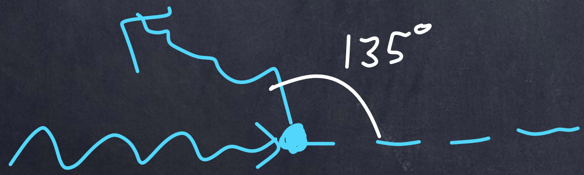
So the compton effect is only important for X-rays, gamma energies (not visible, infrared, UV, ...)

Compton effect experiment



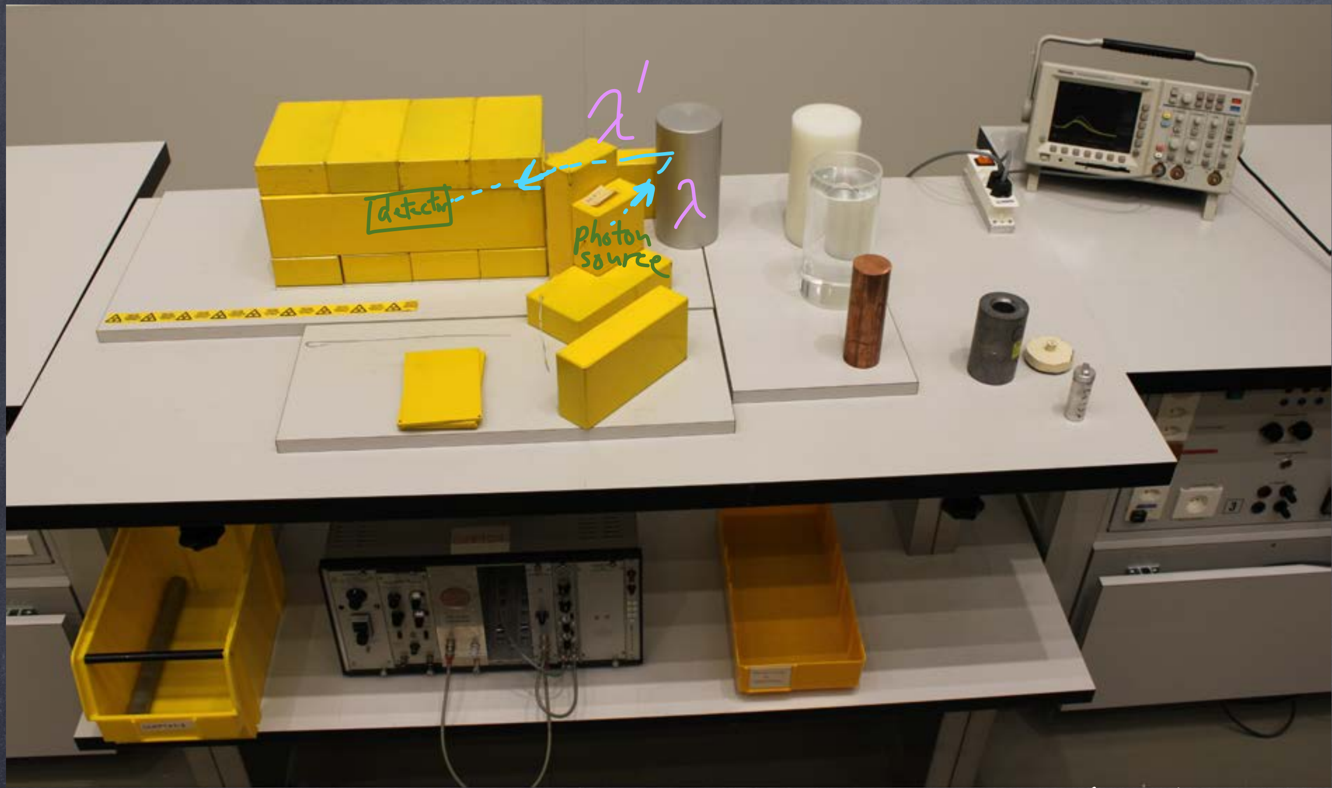
^{137}Cs source emits electrons (512 keV) and photons (662 keV) (gamma rays)

we can stop the electrons with aluminum



From the Compton formula, we could get the wavelength λ' of the scattered gamma rays

Compton effect experiment



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

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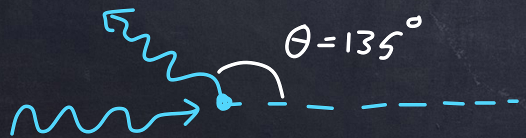
photon $E = 662\,\text{keV} \rightarrow \lambda = 0.019\,\text{E-10 m} = 0.019\,\text{Å}$ (Angstroms)

$$\frac{h}{m_e c} = 0.0243\,\text{Å}$$

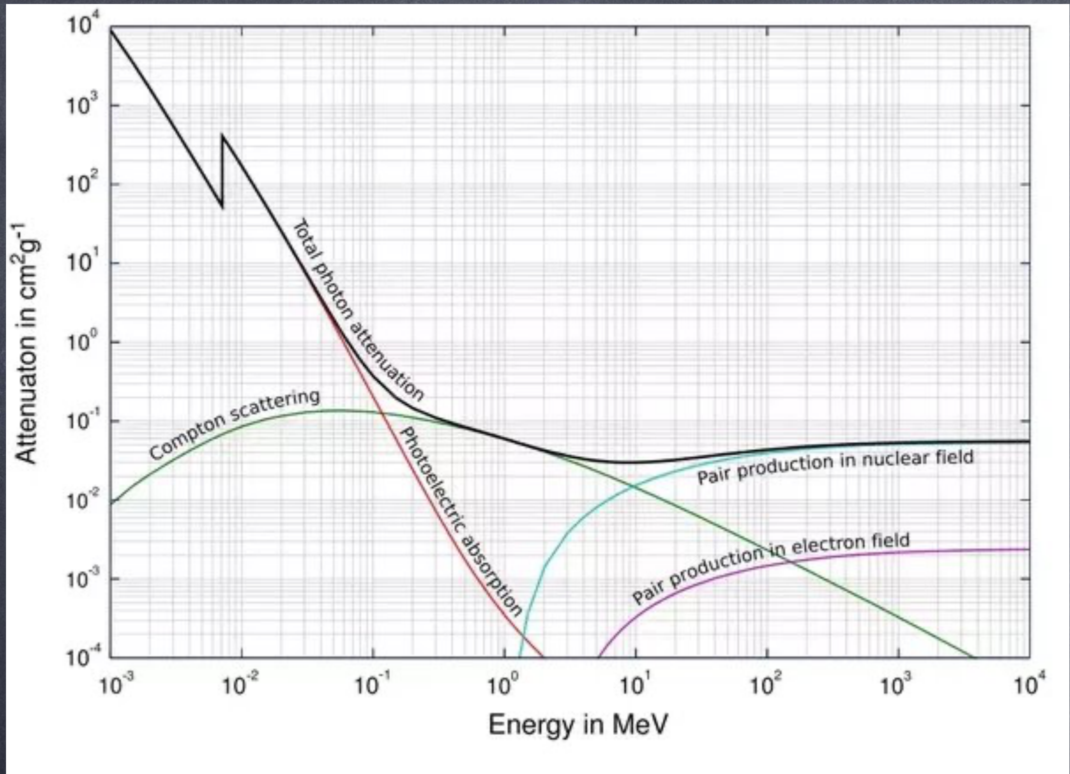


$$\lambda' = \lambda + \frac{h}{m_e c}(1 - \cos\theta)$$

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

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

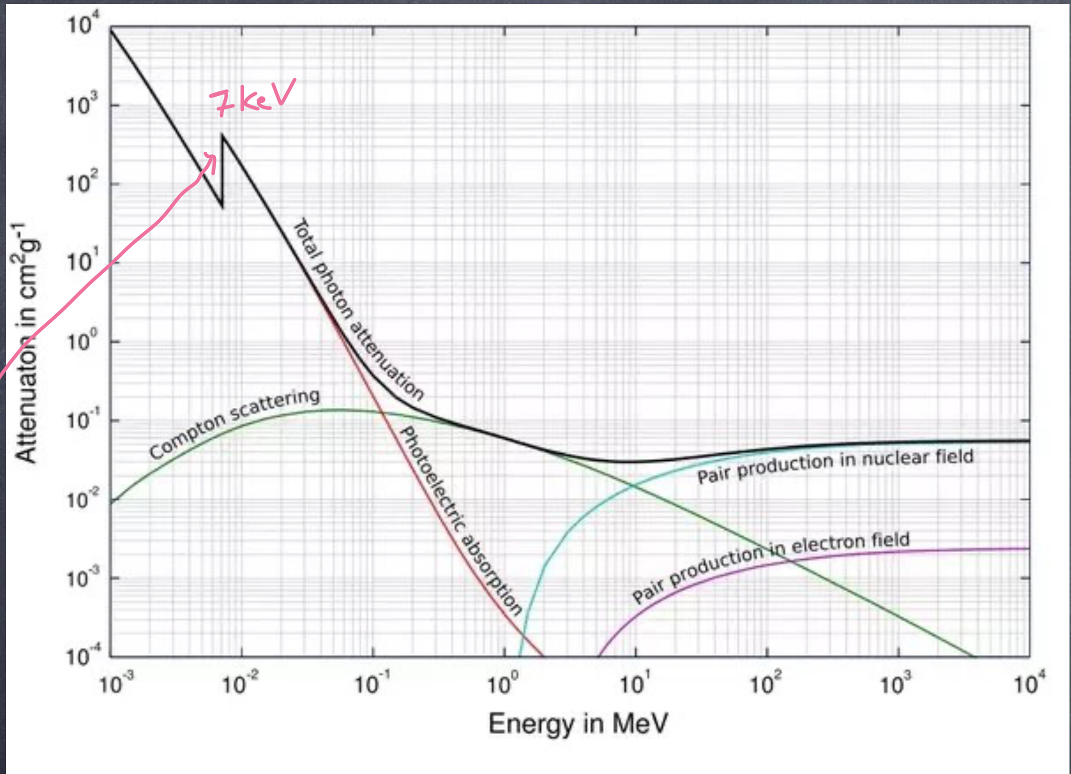
How photons lose energy as a function of their initial energy.



pair production

$\gamma \to e^+ e^-$

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.) Here we see the K-shell absorption edge.

Database of K-absorption edges for different materials here :

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

There was a question after class: If energy levels for atoms with a spin-up or spin-down electron are the same,

then why is there splitting of energy levels due to fine structure?

To be clear, energy levels are only the same when $\ell = 0$, such as the ground state, where $n=1$, $\ell=0$.

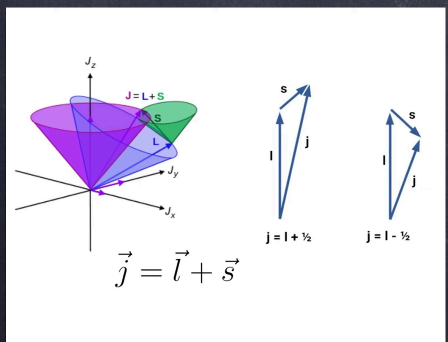
This is because the splitting of energy levels comes from adding the orbital angular momentum (quantum number, ℓ) with the spin, s.

To add $\bar{\ell} + \bar{s}$, we add or subtract the magnitudes:

$j = |\ell| + |s|$ and $j = |\ell| - |s|$

the total magnitude is $|j|$:

Adding $\bar{\ell} + \bar{s}$



Examples:

If one adds $\ell = 1$ and $s = \pm\frac{1}{2}$,

we get $j = |1| + |\pm\frac{1}{2}| = \frac{3}{2}$ and $j = |1| - |\pm\frac{1}{2}| = \frac{1}{2}$

So $|j| = |\frac{3}{2}| = \frac{3}{2}$ and $|j| = |\frac{1}{2}| = \frac{1}{2}$

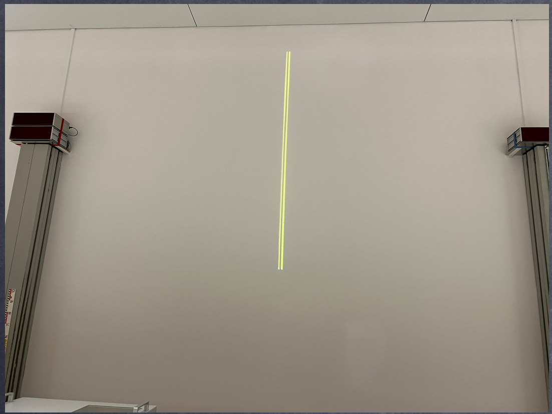
These different $|j|$ have different energy levels.

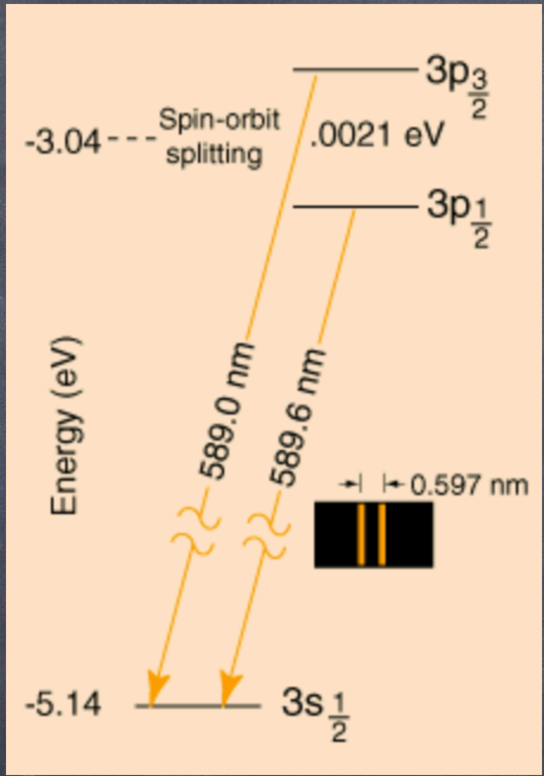
If one adds $\ell = 0$ and $s = \pm\frac{1}{2}$,

we get $j = |0| + |\pm\frac{1}{2}| = \frac{1}{2}$ and $j = |0| - |\pm\frac{1}{2}| = -\frac{1}{2}$

These same $|j| = \frac{1}{2}$ have the same energy levels.

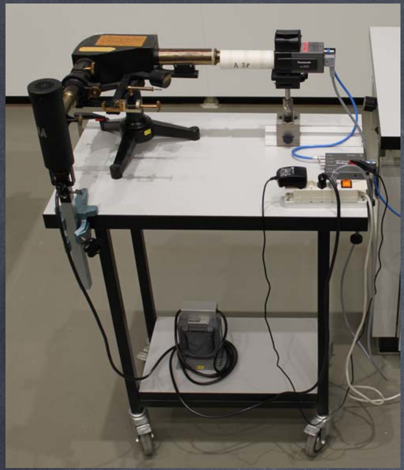
Sodium doublet



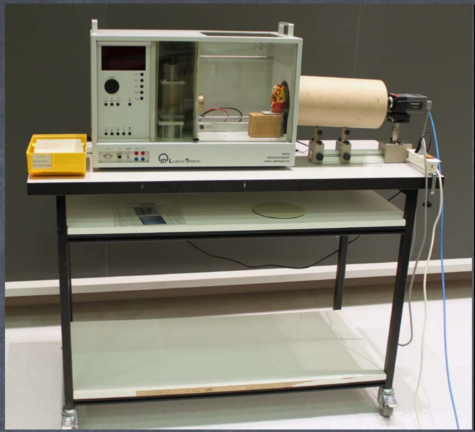


2 energy levels for $\ell=1$ (p subshell)

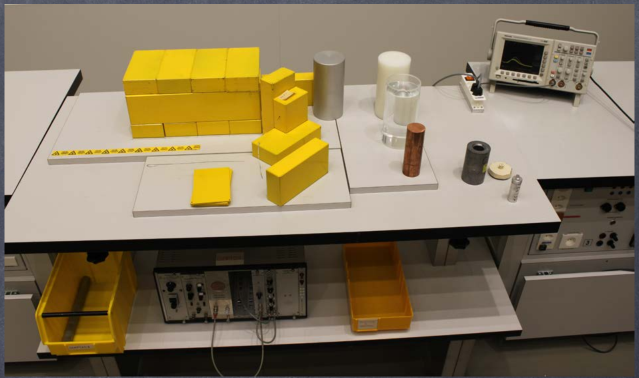
1 energy level for $\ell=0$ (s subshell)



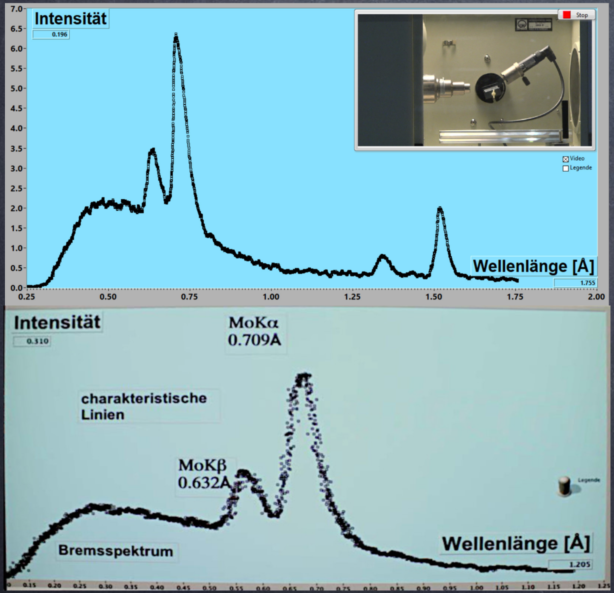
A38



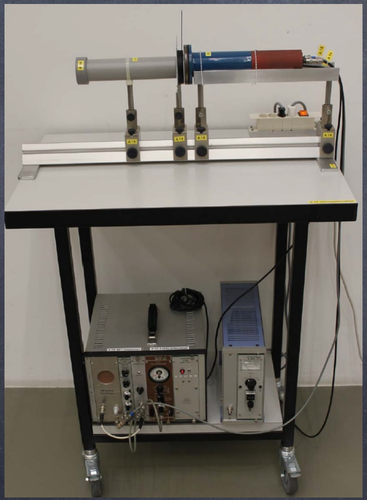
A24



A3



A25



A14

ES90