AGNAGN seminar chapter 11. Heavy Elements and High-energy Effects 11.1-11.3

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11.1 Introduction

So far, we have discussed

- Photoionization of H^0, He^0.
- HII region, galactic nebulae.

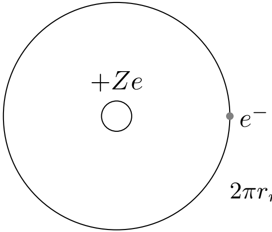
In this chapter, we will describle physical process with **higher energies**

- X rays, gamma rays, cosmic rays
- From AGN, supernova remnants.

And this time, the roles of the **heavy-element** atoms and ions become important.

8.2 Relativistic effect

Let's consider the classical Bohr's model of Fe^{+25} (only 1 electron).



$$2\pi r_n = n\lambda_{\rm d} = n\frac{h}{mv_n}$$

After simple calculation, we get

$$v_n = \frac{Ze^2}{4\pi\varepsilon_0\hbar}\frac{1}{n} \quad \xrightarrow{n=1} \quad v_1 \simeq 0.19c \tag{1}$$

As you can see, for high ionization stages of heavy elements, the electron orbital velocities can approach c.

→ The effect of special relativity is not negligible.

Relativistic effect

- $\Delta S = 1$ transitions become more likely.
- $J = 0 \to J = 0$ transitions occur (usually forbidden with E1).

Strict calculations of these transitions require relativistic quantum mechanics (Dirac equation).

$$i\gamma_\mu \partial^\mu \psi(x) - m\psi(x) = 0 \tag{2}$$

According to Dirac equation, 1st order corrected energy is

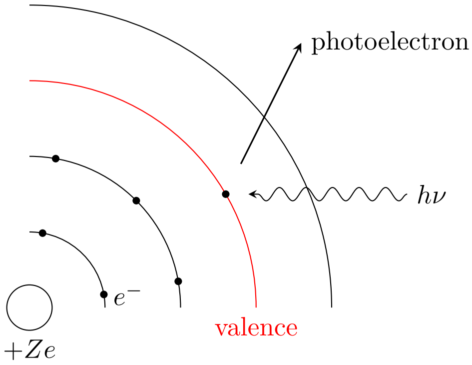
$$E_{n,j} \simeq -\frac{Z^2 \cdot 13.6\text{eV}}{n^2}\left[1 + \frac{(Z\alpha)^2}{n^2}\left(\frac{n}{j+1/2} - \frac{3}{4}\right)\right] \tag{3}$$

Note that

- Eigen energies depend on j (degeneracy is resolved).
- Correction term is proportional to $Z^4 \to$ effective when heavy Z.

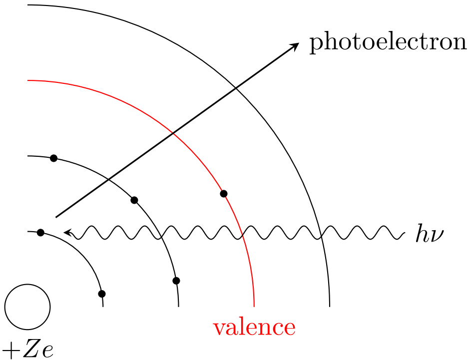
11.2 Photoionization (so far)

We have considered the photoionization of the outermost electron in previous chapters.
We call "the outermost shell" as **valence** shell.

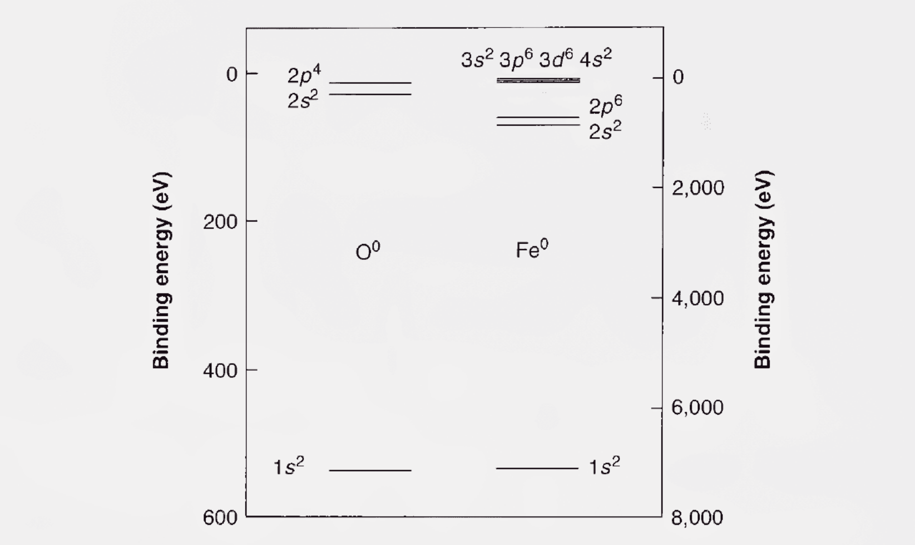


11.2 Inner-shell photoionization

This time, we are going to discuss the photoionization of inner-shell electrons.



11.2 Energy level structures (O, Fe)



In 0^{th} order, energies and their eigenstates are the same as hydrogen-like atom

$$E_n = -\frac{Z^2}{n^2} 13.6\text{eV}, \quad |\psi\rangle = |n, l, m\rangle \tag{4}$$

Also there exists the freedom of spin states, and 2 electrons (with different spin sign) can have the same quantum number (n, l, m).

$$|\psi_1\rangle = |n, l, m\rangle \otimes |\uparrow\rangle, \quad |\psi_2\rangle = |n, l, m\rangle \otimes |\downarrow\rangle \tag{5}$$

where $|\uparrow\rangle = |1/2; +1/2\rangle, |\downarrow\rangle = |1/2; -1/2\rangle$.

shell notation

$$L(2p^6) \quad \Leftrightarrow \quad |2, 1, (-1, 0, 1)\rangle \otimes |\uparrow, \downarrow\rangle \tag{6}$$

which designate $n = 1, 2, 3, \cdots$ as K,L,M (shell), $l = 0, 1, 2, \cdots$ as s, p, d (subshell) and display the number of electrons as superscript.

11.2 Fine structure

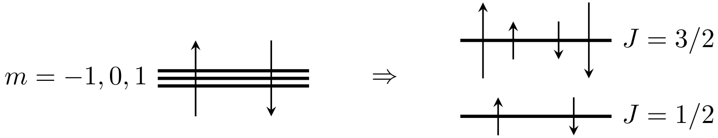
Contribution of subshell structures (e.g. spin-orbit coupling) is not negligible.

example 1.)

$L(2s^2) \Leftrightarrow |2,0,0\rangle \otimes |\uparrow,\downarrow\rangle$. Coupled angular momentum $J = \dfrac{1}{2}$ and resulting states $|n,l,J,J_z\rangle = |2,0,1/2,\pm 1/2\rangle$. We denote this as $L_1(2s_{1/2})$

example 2.

$L(2p^6) \Leftrightarrow |2,1,(-1,0,1)\rangle \otimes |\uparrow,\downarrow\rangle$. Coupled angular momentum $J = \dfrac{1}{2}, \dfrac{3}{2}$ and resulting states $|n,l,J,J_z\rangle = |2,1,1/2,\pm 1/2\rangle\, , \left|2,1,3/2,(-\frac{3}{2},-\frac{1}{2},\frac{1}{2},\frac{3}{2})\right\rangle$



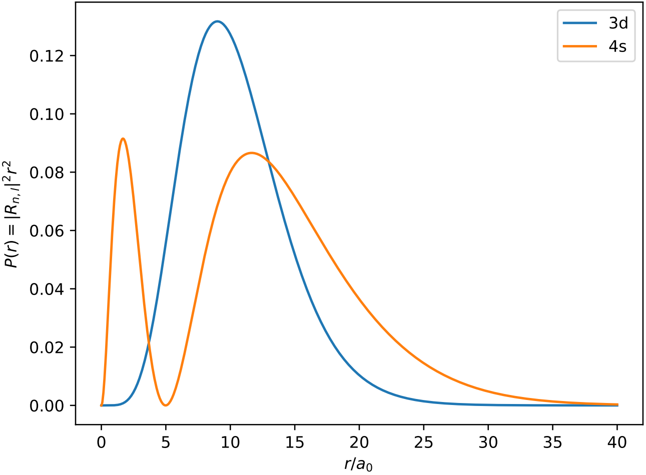
and we denote these coupled states as $L_2(2p_{1/2}), L_3(2p_{3/2})$ respectively.

11.2 Order of the subshell

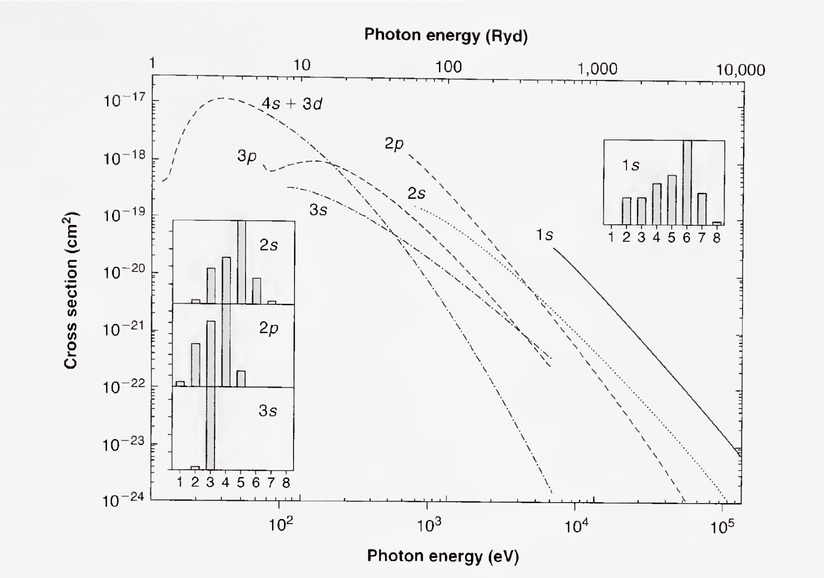
In ideal hydrogen, larger n leads to larger energy E_n.
Howevere, in reality, some **reversals** occur because of the electron-electron interaction.

- In the case of an element with N valence shell (e.g. Fe), the M shell and the $4s^2$ electrons of the N shell have **comparable energies**.
- This is because the 4s electrons are in " plunging " orbits
  - hence are subject to a larger effective nuclear charge
  - and become more stable (tightly bounded).
- The normal order of filling subshells

$$1s, 2s, 2p, 3s, 3p, 4s, 4p, 5s, 4d \tag{7}$$


3d
4s
0.12
0.10
0.08
0.06
0.04
0.02
0.00
$P(r) = |R_{n,l}|^2 r^2$
0
5
10
15
20
25
30
35
40
r/a_0

11.2 Cross sections(Fe)



11.2 Quiz !

If an ionizing photon with $h\nu = 1$keV interacts with Fe, which electron (state) is likely to be ionized ? Rearrange the following states,

$$1s, 2s, 2p, 3s, 3p, 3d + 4s$$

You can refer to the cross section in the previous slide.

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You can refer to the cross section in the previous slide.

Answer

By drawing $h\nu = 1\text{keV} = 10^3\text{eV}$ line in the Cross section figure, you will get

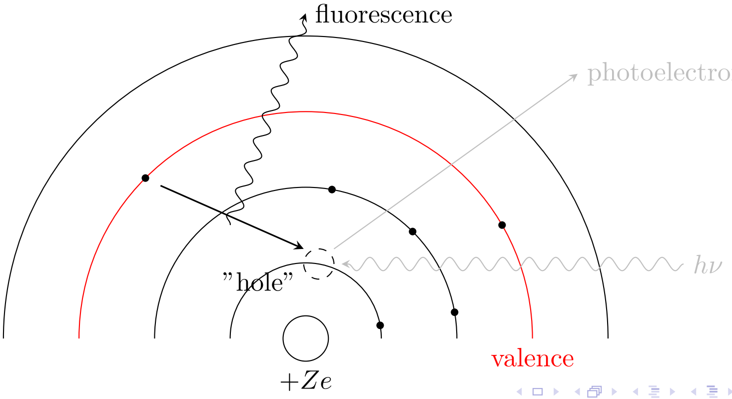
$$2p, 2s, 3p, 3s, 4s + 3d \tag{8}$$

and $1s$ cannot be ionized.

11.2 Inner shell fluorescence emission

According to the cross section, it is inferred that

- a photon is more likely to **remove an inner-shell electron** rather than a valence one.
- Then, an inner-shell vacancy or "hole" appears, which is immediately filled by outer electrons.
- Photons are emitted during this process. (This is called **fluorescence**)



11.2 Inner shell fluorescence emission

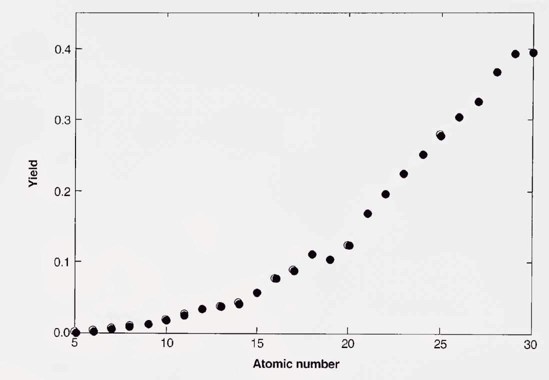
Major fluorescence line ; $2p \rightarrow 1s$ or $L \rightarrow K$, is called Kα line.
Actually, Kα line consists of two line $L_2 - K, L_3 - K$ line according to the fine structure.

11.2 Fluorescence yield

Here we define **fluorescence yield Y** as

$$Y = \frac{\#(\text{holes which are filled})}{\#(\text{total holes})} \tag{9}$$

Its dependence on Z is



11.2 Fluorescence yield

Rough estimate on the dependency $Y(Z)$.
Consider the simplest situation in which $Y \propto A$(transition probability).

- Since $E_n \approx -Z^2 13.6\text{eV}/n^2 \propto Z^2$, $h\nu = \Delta E \propto Z^2$
- According to Fermi's golden rule,

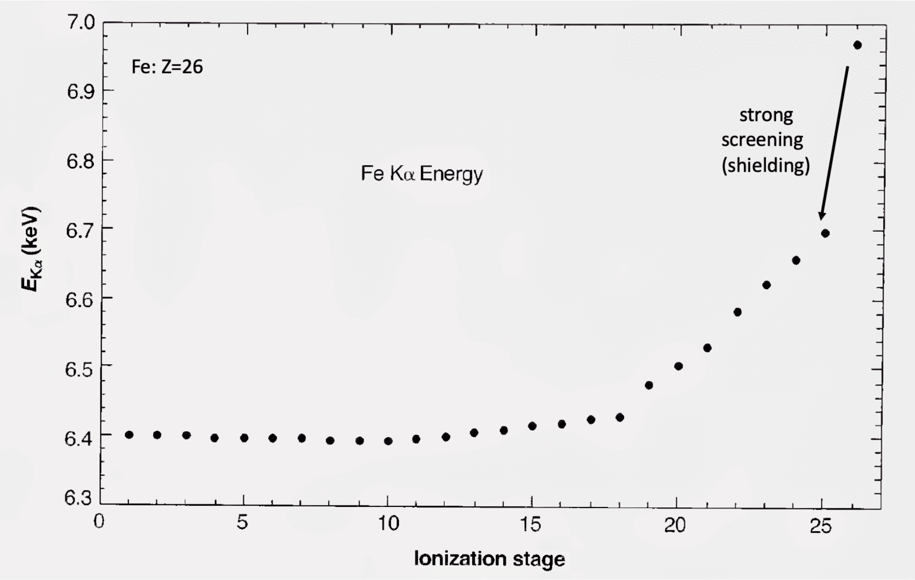
$$A = \frac{4}{3}\frac{\omega^3}{c^3} |\langle f|\boldsymbol{E} \cdot \hat{\boldsymbol{r}}|i\rangle|^2 \tag{10}$$

- Also, $r \propto 1/Z$ according to Bohr's model.
- Then, $A \propto \omega^3 r^2 \propto Z^6 Z^{-2} = Z^4$

So, decay rate A and resulting yield Y increases dramatically as atomic number Z increases.

Fluorescence emissivity

$$4\pi j_l = n_{ion} h\nu_l Y_l \int_{\nu_1}^{\infty} \frac{4\pi J_\nu}{h\nu} \sigma_\nu d\nu \tag{11}$$


Fe: Z=26
Fe Kα Energy
strong
screening
(shielding)
$E_{K\alpha}$ (keV)
Ionization stage
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
0
5
10
15
20
25

11.2 Fluorescence dependence on ionization stage

- Fe XXVI, emitted by the one-electron ion, has a Kα energy of 6.97keV.
- For Fe XXV, with two electrons, Kα energy drops to 6.72keV because of the **screening** (or shielding) effect by the other $1s$ electron.
- In the same way, $2s, 2p$ electrons screen the nuclear and the effective charge decreases.
- $3s, 3p, 3d$ electrons have too small overlap integral to effectively screen the nuclear.

Quiz !

Calculate Fe XXVI Kα energy by using hydrogen-like eigen energy $E_n = -\frac{Z^2}{n^2} \cdot 13.6\text{eV}$. Why does this result deviate from 6.97 keV?

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Quiz !

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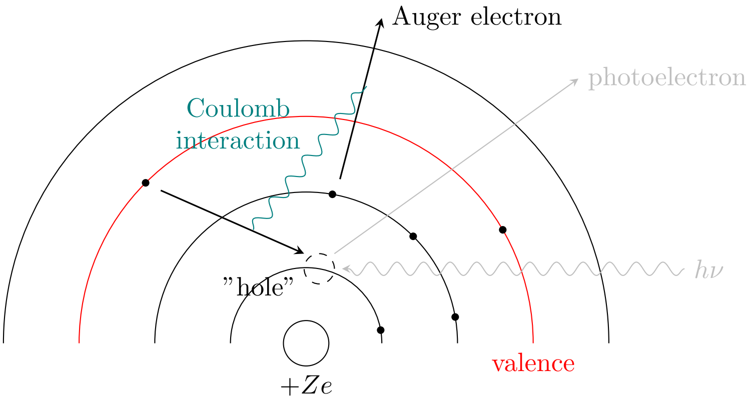
answer

$Z = 26,\ E_{\mathrm{K}\alpha} = -Z^2\left(\frac{1}{2^2} - \frac{1}{1^2}\right) \cdot 13.6\text{eV} = 6.9\text{keV}$. Deviation comes from special relativity (as it was mentioned earlier).

- Fluorenscence : When the "hole" is filled by outer electrons, photons with the energy difference ΔE are emitted.
- In stead of the emission, the ejection of outer electrons do occur (**Auger effect**). Ejected electrons are called **Auger electrons**.



11.2 Auger electron energy

Quiz !

Now we consider Fe ($Z = 26$) with hydrogen-like eigen energy $E_n = -\frac{Z^2}{n^2} 13.6\text{eV}$. When one $1s$ electron is photoionized and $1s$ "hole" is created, outer electron ($2p$) will fill the "hole" and another outer electron ($2p$) will be ejected.
How much kinetic energy will the Auger electron have when it leaves the potential of nuclear?
How about O ($Z = 8$) ?

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How much kinetic energy will the Auger electron have when it leaves the potential of nuclear?
How about O ($Z = 8$) ?

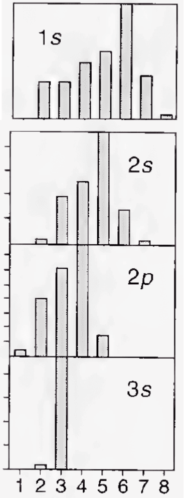
answer
Energy conservation

$$Z^2\left(\frac{1}{1^2} - \frac{1}{2^2}\right)13.6\text{eV} = \frac{Z^2}{2^2}13.6\text{eV} + K \tag{12}$$

$K_{\text{Fe}} = 4.6\text{keV}, K_{\text{O}} = 440\text{eV}$

11.2 Auger electron and ionization stages

How many Auger electrons are ejected at one "hole" ?



11.2 Auger electron and ionization stages

According to the probability distributions of the number of Auger electrons,

- K shell vacancies typically result in the ejection of 6 electrons.
- The removal of a $1s$ electron of Fe^0 typically produces ions Fe^{+7}.

High ionization states are produced by one Auger effect.

The Auger effect is one of the main physical processes responsible for producing highly ionized states in heavy elements

11.3 Physical Processes at Still Higher Energies

We have discussed

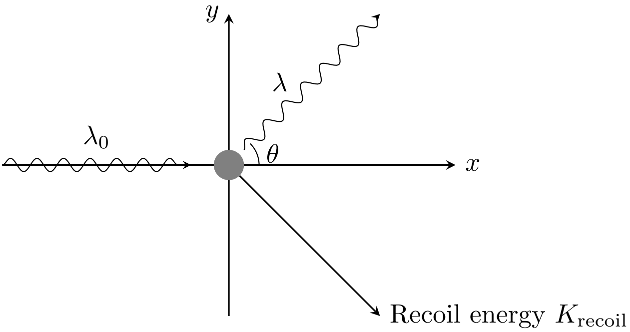
- Inner-shell photoionization
- Fluorescence emission
- Auger effect

These effects play an important role when injected photon has $10^2 \sim 10^3$ eV.

From now on, we will put focus on still higher energy region.

- Compton effect
- Pair production
- Secondary ionization
- Cosmic ray

11.3.1 Compton effect



Compton effect : a process in which photons are scattered by an electron. Its cross section is known as the Thomson electron-scattering cross section $\sigma_{\rm T} = 0.66 \times 10^{-24}{\rm cm}^{-2}$.

At restframe of an electron, photon with λ_0 is scattered by the electron and becomes λ, fly with angle θ.

11.3.1 Compton effect

Compton fomula

$$\lambda - \lambda_0 = \frac{h}{mc}(1 - \cos\theta) \tag{13}$$

is derived using energy and momentum conservation (special relativity).

But in reality, electrons move according to a thermal velocity distribution. Average energy shift by the Compton effect is

$$\left\langle \frac{\delta(h\nu)}{h\nu} \right\rangle = \frac{4kT}{mc^2}, \quad \text{where} \quad \frac{3}{2}kT = \left\langle \frac{1}{2}mv^2 \right\rangle \tag{14}$$

(you can derive this according to Lorentz transformation.)

11.3.1 Compton effect

If $kT > h\nu$, the photon can gain energy following the collision, termed inverse Compton scattering.

During one scattering process, net average heating (or cooling) is

$$\langle \Delta E_{\mathrm{elec}} \rangle = h\nu \frac{h\nu - 4kT}{mc^2} \tag{15}$$

and this results in the whole net heating under the radiation field J_ν

$$H_{\mathrm{Comp}} = n_e \int \frac{4\pi J_\nu}{h\nu} \sigma_{\mathrm{T}} \langle \Delta E_{\mathrm{elec}} \rangle \, d\nu \tag{16}$$

Kinetic energy of the electron increases during Compton scattering (**Compton recoil**).
Recoil energy is

$$K_{\text{recoil}} = h\nu_0 - h\nu = hc\left(\frac{1}{\lambda_0} - \frac{1}{\lambda}\right) \tag{17}$$

$$= \frac{hc}{\lambda_0}\left(1 - \frac{1}{\lambda/\lambda_0}\right) = h\nu_0\left(1 - \frac{1}{1 + \frac{h\nu_0}{mc^2}(1 - \cos\theta)}\right) \tag{18}$$

Typically,

$$K_{\text{recoil}} \approx h\nu_0\left(1 - \frac{1}{1 + \frac{h\nu_0}{mc^2}}\right) \tag{19}$$

Compton recoil ionization

If the recoil energy K_{recoil} is greater than the ionization potential $\chi_0 \approx 13.6 \cdot Z^2 \text{eV}$,

$$K_{\text{recoil}} = h\nu_0 \left(1 - \frac{1}{1 + \frac{h\nu_0}{mc^2}} \right) > \chi_0 \tag{20}$$

ionization by Compton recoil will occur.
And you get following ionization condition.

$$h\nu_0 > \frac{\chi_0 + \sqrt{\chi_0^2 + 4\chi_0 mc^2}}{2} \tag{21}$$

example)

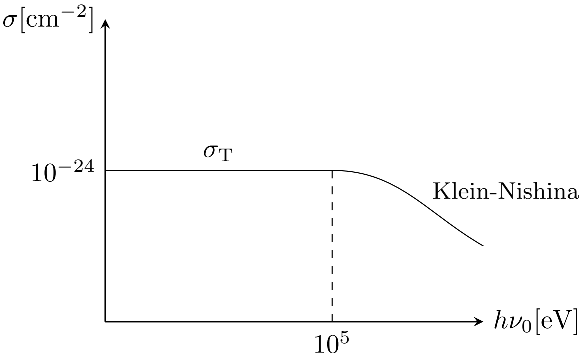
$Z = 1, \chi_0 = 13.6\text{eV} \ll mc^2 = 511\text{keV}$. Then, the condition becomes

$$h\nu_0 > \frac{\chi_0 + \sqrt{\chi_0^2 + 4\chi_0 mc^2}}{2} \approx \sqrt{\chi_0 mc^2} = 2.6\text{keV} \tag{22}$$

11.3.1 Compton cross section

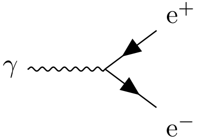
Cross section of Compton effect is roughly the same as Thomson electron-scattering cross section $\sigma_{\mathrm{T}} = 0.66 \times 10^{-24}\mathrm{cm}^{-2}$.
But the difference cannot be neglected when the energy is quite high.
In high energy region, cross section is given by **Klein-Nishina formula**

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{\alpha}{2\pi}\right)^2 \frac{h^2}{2m^2c^2} \frac{\lambda_0^2}{\lambda} \left[\frac{\lambda}{\lambda_0} + \frac{\lambda_0}{\lambda} - \sin^2\theta\right], \quad \sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} d\Omega \tag{23}$$



11.3.2 Pair production

When a photon has energy greater than $2mc^2 \approx 1$Mev, energy conservation allows it to decay into $e^+ - e^-$ pair.



- $e^+ - e^-$ pair are **virtual** (they cannot become a real pair in a vacuum) because of momentum conservation.
- If the pair is near the nuclear, it can transfer momentum to the nuclear and become a real pair.
- The typical cross section of pair production $\sim 10^{-27}\text{cm}^{-2}$
- Pair eventually annihilates and forms two photons , each having 0.511 MeV (This is called **annihilation line**).

11.3.3 Secondary ionization

Energy of

- Auger electrons
- $e^+ - e^-$ pair
- photoelectron by strong radiation

is far larger than that of thermal electrons (kT).

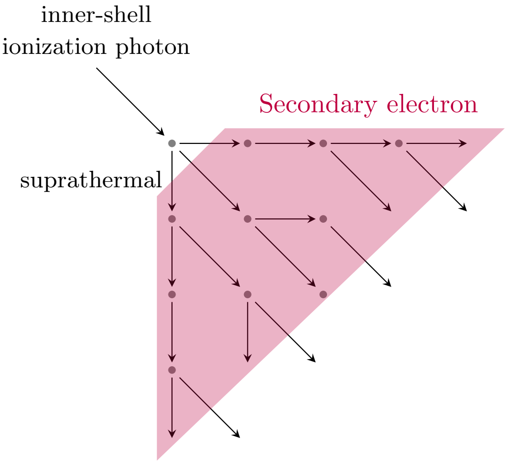
Under ionized gas environment

These "suprathermal" electrons are gradually thermalized during collisions with surrounding thermal electrons.

Under neutral gas environment

- These "suprathermal" electrons collide with atoms → collisional ionization.
- They can create a **second suprathermal electron** if it collisionally ionizes an atom.

11.3.3 Secondary electron shower



Neutral atoms are ionized and secondary suprathermal electrons are produced one after another.

The ionization fraction

$$x := \frac{n(\mathrm{H}^+)}{n(\mathrm{H})} \tag{24}$$

determines the importance of secondary ionization.

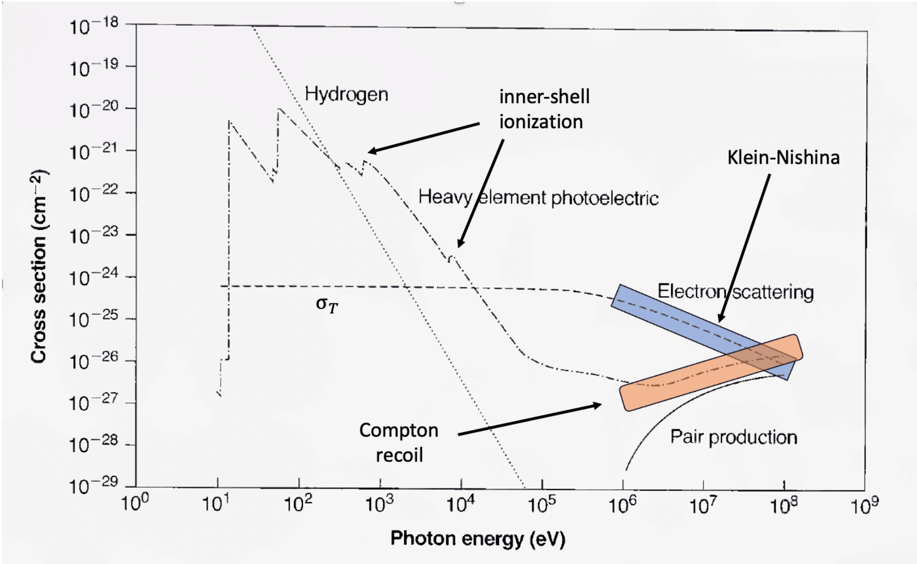
- If $x > 0.9$, most kinetic energy goes into heat.
- If $x \ll 0.9$, much of an energetic primary electron's energy goes into secondary ionization(40%) and excitation(40%), and less into heat (14%).

11.3.4 Cosmic rays

Cosmic ray : nuclei and electrons with relativistic energies ($\lesssim$ 10GeV).

- Distribution function $n(E) \propto E^{-2.4}$
- Lower-energy cosmic rays cannot be directly observed from the Earth, but synchrotoron radiation indirectly infers the exisitance of them.
- Cosmic rays ionize neutral atoms rather than heat them.
- The H^0 ionization rate is approximately $2 \times 10^{-17} s^{-1}$
- Typical energy of electrons ionized by cosmic rays is 35eV(suprathermal).
- That suprathermal electron will then create secondary electrons.

11.3.5 Total opacity



11.3.5 Total opacity

The sources of opacity vary across different energy ranges.

- Low-energy range (< 54eV): $\mathrm{H}(13.6\mathrm{eV}), \mathrm{He}(24.6, 54\mathrm{eV})$, grain
- Middle-energy range ($54\mathrm{eV} < h\nu < \mathcal{O}(\mathrm{keV})$): Inner-shell ionization (→Auger effect, fluorescence)
- High-energy range($100\mathrm{keV} < h\nu < \mathcal{O}(\mathrm{MeV})$): Compton recoil, pair production

Column density

$$\tau_\nu = a_\nu N(\mathrm{H}) = 1 \quad \rightarrow \quad N(\mathrm{H}) = a_\nu^{-1} \approx 10^{24}\mathrm{cm}^{-2} \tag{25}$$

High-energy processes become very important for relatively large column densities (above $10^{24}\mathrm{cm}^{-2}$)