LC Quantum Mechanics Lecture Notes

MSci Physics w/ Particle Physics and Cosmology
University of Birmingham

Year 1, Semester 1
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Lectures Index

Fri 03 Oct 2025 12:00

Lecture 1 - Atomic Structure

1 Atomic Structure

1.1 What is the course?

- Quantum mech is weird and unintuitive, we will build up a case in the course for why this weird theory was necessary and why we're confident it works.

- Each week will be a self-contained concept and/or historical experiment, working up to the Shroedinger Equation and wave-particle duality.

- Names and dates do not need to be memorised.

- Recommended text: University Physics (Young and Freedman).

- Office hours: 13:00 − 13:50 Fridays (immediately post-lecture), Physics East Rm 207.

1.2 Atomic Structure

What actually is an atom? What does it actually look like inside?

Early Clues

- Periodic Table (Mendelev, 1989), periodic patterns in elements properties.

- Radioactivity (Becquerel, 1896, Curie 1898)

- Atoms emit and absorb specific discrete wavelengths, (Balmer, 1884)

- Discovery of the Electron (Thompson 1897). Cathode rays - heating metal in a vacuum with an electric field above it, to strip away electrons from the metal.

    - This showed electrons were negatively charged and extremely light (1/2000th of the atomic mass).
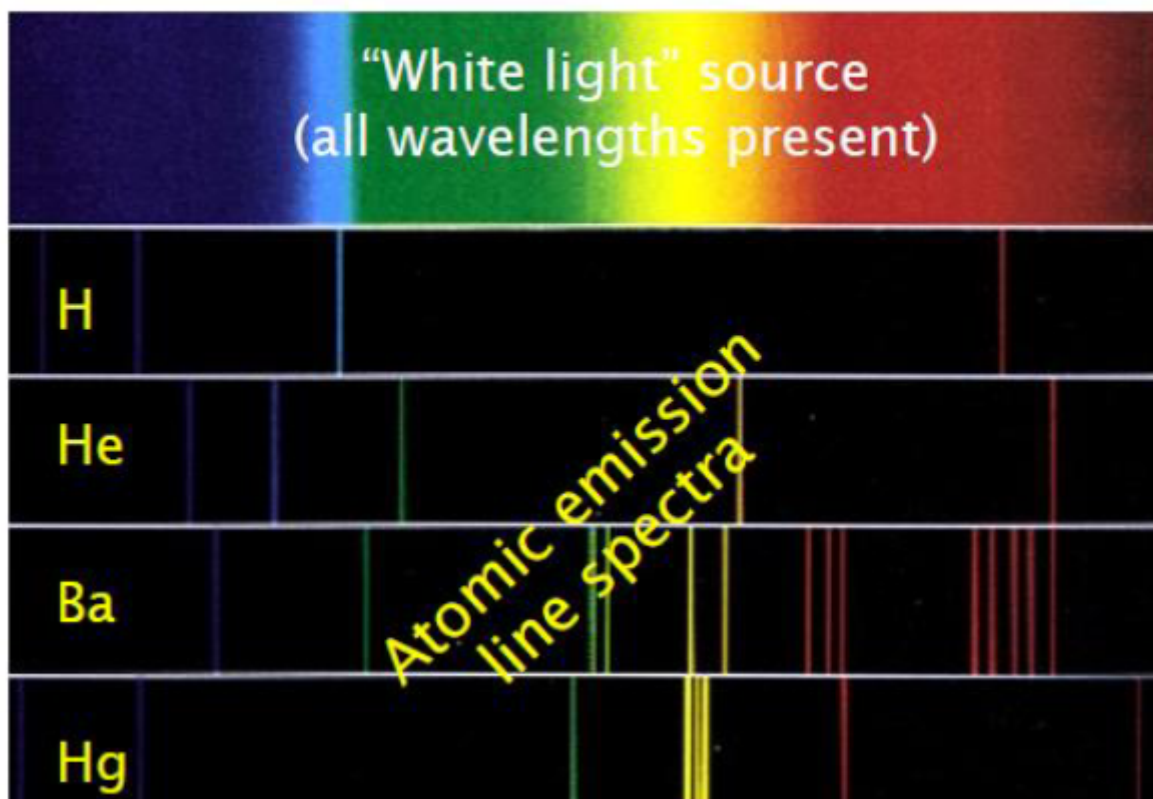
Atoms emit/absorb light at discrete wavelengths

Figure 1.1: Absorption Spectra

1.3 Plum Pudding Model

A solid, uniform lump of positively charged matter, approximately 10^{-10}m across. This had evenly distributed negative charges (electrons) scattered throughout.

1.4 Discovery of the Nucleus

Geiger and Marsden (1908-1913), fired alpha particles (He nuclei) at thin gold foil and measured the deflection / scattering.

The alpha particles had a mass of 4u, a charge of $+2e$ and an energy of approximately 5MeV.

They found that most α were scattered only by small angles, but (surprisingly) a small number were scattered right back towards to emitter (through $\theta > 90 \deg$). The distribution of the angles is approximately Normally distributed, with a mean of 0. Only approximately 1 in 8,000 fired αs were scattered by $\theta > 90$ ("back-scattering").

Can this be explained with the Plum Pudding Model? No, it cannot. This was used to demonstrate that atoms cannot be evenly distributed.

2 Demonstrating by Calculation

Lets work out the work done to take an α from infty to the pudding centre. If the electrostatic repulsion is not enough to overcome this, we cannot stop the α and cannot back scatter.
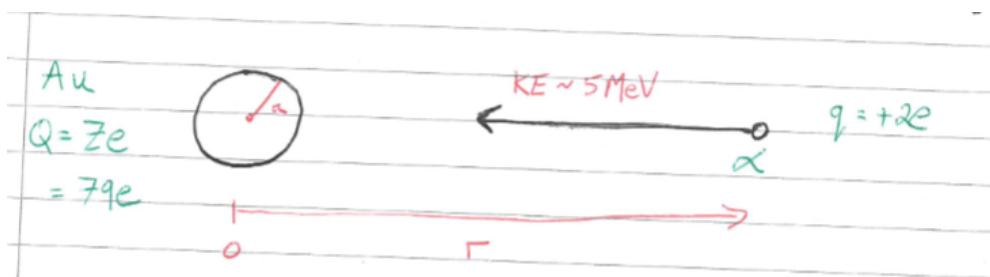
Figure 1.2: The experiment

2.1 Assumptions

- The atom stays still.

- Ignore the gold electrons (this is fine, as they would cancel some positive charge and make repulsion weaker, which would be even worse. If we can't do it without them, it would be equally impossible to do it with.)

2.2 Recap and Eqns

Coulomb Potential Energy is:

$$u(r) = \frac{qQ}{4\pi\epsilon_0 r}$$

Force is:

$$F(r) = -\frac{du}{dr} = \frac{qQ}{4\pi\epsilon_0 r^2}$$

Change in potential energy $(u_2 - u_1)$ is work done:

$$\int_{u_1}^{u_2} du = -\int_{r_1}^{r_2} F(r) dr$$

From outside the atomic radius, we treat the atomic pudding as a point charge of charge Q. From inside the atomic radius, we treat it as a smaller point charge $Q'(r)$, where we only consider the charge inside the portion of the pudding where $a < r$, where a is the current position inside the sphere and r is the atomic radius.

If charge is spread uniformly, the total charge is proportional to the volume of the sphere. So:

$$\frac{Q'}{Q} = \frac{\frac{4}{3}\pi r^3}{\frac{4}{3}\pi a^3}$$

$$Q' = Q\frac{r^3}{a^3}$$

Inside the Pudding

$$F = \frac{qQ'}{4\pi\epsilon_0 r^2}$$

$$F = \frac{qQr^3}{4\pi\epsilon_0 r^2 a^3}$$

$$F = \frac{qQr}{4\pi\epsilon_0 a^3}$$

$$F = \frac{qQ}{4\pi\epsilon_0 a^3} \times r$$

Hence inside, $F \propto r$

Outside the Pudding

$$F = \frac{Qq}{4\pi\epsilon_0 r^2}$$

4

$$F = \frac{Qq}{4\pi\epsilon_0} \times \frac{1}{r^2}$$

Hence outside, $F \propto \frac{1}{r^2}$

To integrate, we are therefore integrating the area under this (almost) triangle:
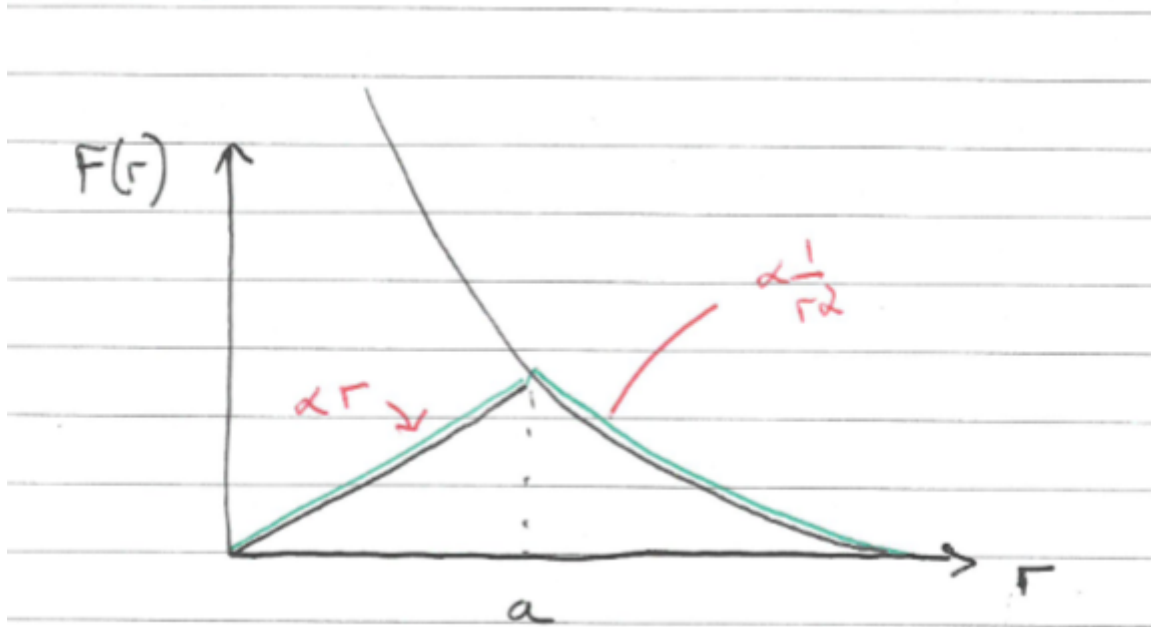

Figure 1.3: Radius vs electrostatic repulsion force

$$\Delta u = -\int_{r_1}^{r_2} F(r)\, dx$$

Splitting into two sections (prior to, and after the point where r = atomic radius, $r = a$), and integrating across all r (as we are attempting to work out the work done to bring an α from infinity to the charge, at which point distance is 0):

$$= -\int_{\infty}^{a} \frac{qQ}{4\pi\epsilon_0 r^2}\, dx - \int_{a}^{0} \frac{qQr}{4\pi\epsilon_0 a^3}\, dx$$

$$= -\frac{qQ}{4\pi\epsilon_0} \int_{\infty}^{a} \frac{1}{r^2}\, dx - \frac{qQ}{4\pi\epsilon_0 a^3} \int_{a}^{0} r\, dx$$

$$= -\frac{qQ}{4\pi\epsilon_0} \lim_{x\to\infty} \int_{x}^{a} \frac{1}{r^2}\, dx - \frac{qQ}{4\pi\epsilon_0 a^3} \int_{a}^{0} r\, dx$$

$$= -\frac{qQ}{4\pi\epsilon_0} \lim_{x\to\infty} \left[-\frac{1}{r} \right]_{x}^{a} - \frac{qQ}{4\pi\epsilon_0 a^3} \left[\frac{1}{2} r^2 \right]_{a}^{0}$$

$$= -\frac{qQ}{4\pi\epsilon_0} \left(-\frac{1}{a} - 0 \right) - \frac{qQ}{4\pi\epsilon_0 a^3} \left(\frac{1}{2} 0^2 - \frac{1}{2} a^2 \right)$$

$$= -\frac{qQ}{4\pi\epsilon_0} \left(-\frac{1}{a} \right) - \frac{qQ}{4\pi\epsilon_0 a^3} \left(-\frac{1}{2} a^2 \right)$$

$$= \frac{qQ}{4\pi\epsilon_0 a} + \frac{qQa^2}{8\pi\epsilon_0 a^3}$$

$$= \frac{qQ}{4\pi\epsilon_0 a} + \frac{qQ}{8\pi\epsilon_0 a}$$

$$= \frac{qQ}{4\pi\epsilon_0 a} + \frac{1}{2}\frac{qQ}{4\pi\epsilon_0 a}$$

$$= \frac{3}{2}\frac{qQ}{4\pi\epsilon_0}$$

As required! Plugging in values gives us:

$$\Delta u = \frac{3}{2}\frac{(2e)(79e)}{4\pi(8.854\times10^{-12})\times10^{-10}}$$

$$= 5.45\times10^{-16}J = 3.41KeV$$

This is much less than the kinetic energy of the 5MeV alpha particle, therefore (as this value is maximum work done against the repulsive force) a plum pudding could not backscatter a 5MeV alpha particle. However, since $\Delta u \propto 1/a$, a smaller volume of charge could. How small, however?

$$\Delta u = 5\text{MeV} = -\int_\infty^{r_{max}} \frac{qQ}{4\pi\epsilon_0 r^2}\, dr$$

$$-5\text{MeV} = \frac{qQ}{4\pi\epsilon_0}\int_\infty^{r_{max}} \frac{1}{r^2}\, dr$$

$$-5\text{MeV} = \frac{qQ}{4\pi\epsilon_0}\lim_{x\to\infty}\left[-\frac{1}{r}\right]_x^{r_{max}}$$

$$-5\text{MeV} = \frac{qQ}{4\pi\epsilon_0}\left[-\frac{1}{r_{max}} - \lim_{x\to\infty}\frac{1}{x}\right]$$

$$-5\text{MeV} = \frac{qQ}{4\pi\epsilon_0}\left[-\frac{1}{r_{max}}\right]$$

$$5\text{MeV} = \frac{qQ}{4\pi\epsilon_0 r_{\mathsf{max}}}$$

Substitution and rearrangement gives $r_{\mathsf{max}} = 4.5\times10^{-14}m = 45fm$. We accept the 10^{-10}m $= 100,000$fm figure as the total width of the atom, but this demonstrates that there must exist a nucleus of no larger than 45fm.

2.3   Next Idea: The Solar System Model

Therefore, the next idea was an orbiting solar system model, where electrons orbit in fixed paths around a central nucleus. However, accelerating charges (i.e. a charge in circular motion) radiates energy, so this orbiting electron would be on a decaying path to crash into the nucleus. We can observe this does not happen, so need another idea…

Bohr made two postulates:

- The electron in hydrogen moves in a set non-radiating circular orbit.

- Radiation is only emitted or absorbed when an electron moves from one orbit to another.

This works (at least for hydrogen) and explains the absorption spectra, but for now lacks a physical grounding.

Fri 10 Oct 2025 12:00

Lecture 2 - The Ultraviolet Catastrophe

In this lecture:

- How classical theories fail to explain black body radiation ("The Ultraviolet Catastrophe").

- How quantising light into photons gives predictions that fit this observation.

1   Black Body Radiation

A 'black body' is an idealised perfect object, that does not reflect, and absorbs internally all light (regardless of wavelength) incident upon it. No light is transmitted, so nothing shines out the other side. The object is perfectly black.

All bodies emit electromagnetic energy, usually outside the visible portion of the spectrum. For example, Paul Hollywood (and other humans) emit at about 300 Kelvin, which is infrared (at the temperature which night vision goggles are tuned to).

For the black body, emission spectrum is **only** from this thermal emission (no reflection, no fluorescence, etc). Hotter objects are brighter and bluer (hotter means higher energy, and therefore a shorter wavelength)
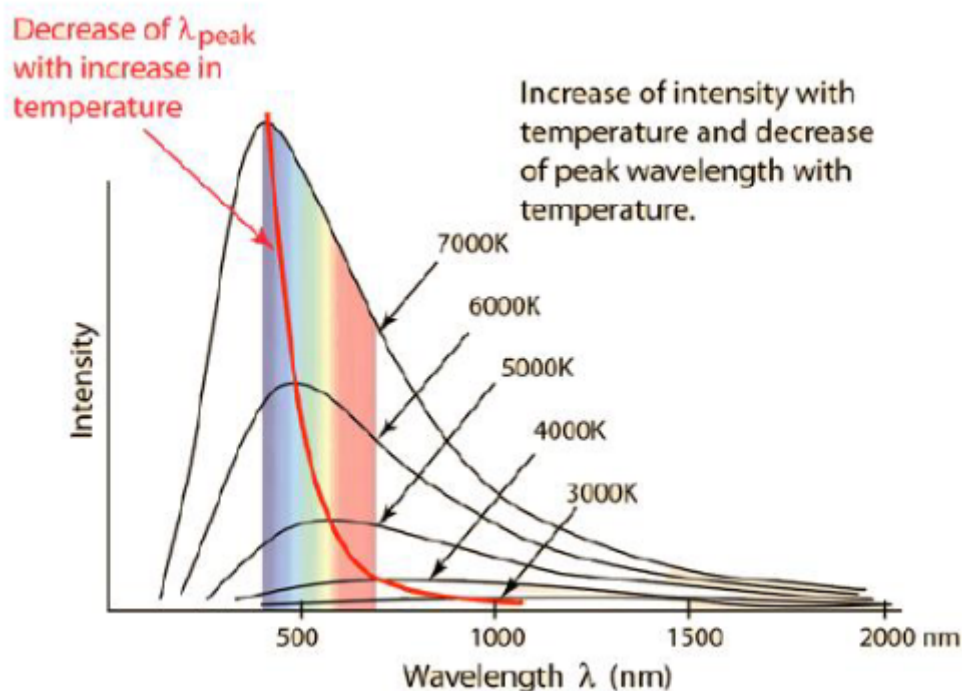

Figure 2.1: Observed Emission Spectra

However, we run into a problem. If we plot the spectra predicted by classical thermodynamics, vs the observed spectra for a given temperature object, the classical prediction gets it totally wrong, especially at shorter wavelengths.
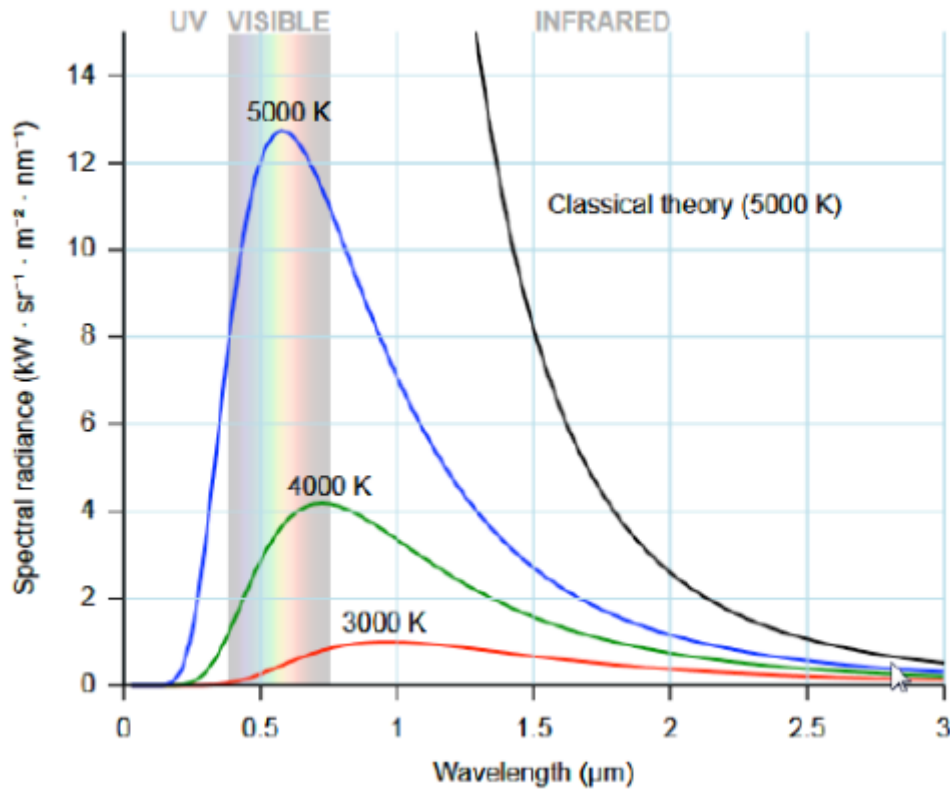
Figure 2.2: Predicted and Observed Spectra for 5000K (and Observed for 4k K and 3k K)

1.1   Notation

$I(\lambda)$ is the intensity per wavelength for an emitted wavelength λ. I is the total intensity across all wavelengths per unit time (in W/m^2, power per unit area).

$$I = \int_0^\infty I(\lambda)\, d\lambda$$

I is the total area under the $I(\lambda)$ curve, i.e. the sum of intensity per wavelength, across every wavelength.

2   The Ultraviolet Catastrophe

2.1   Empirical Results

The Stefan-Boltzmann Law gives $I = \sigma T^4$, where σ is the Stefan-Boltzmann constant, $\sigma = 6.57 \times 10^{-8} W m^{-2} K^{-4}$

Wien's Displacement Law gives $\lambda_{\text{peak}} = \frac{b}{T}$, where $b = 2.898 \times 10^{-3} Km$.

2.2   Why does classical mechanics break?

Lets model the $I(\lambda)$ spectrum by slotting standing waves into a cavity. Inside the blackbody, EM waves form standing waves (in a limited number of possible configurations).

We can simplify by considering a 1D cavity of length L. We can consider 'cavity modes' as the possible standing waves that can exist in this cavity. As we know the wave is bound at each end, the displacement at each end of the cavity must be 0. Therefore, the only possible waves must obey this, and these are cavity modes.
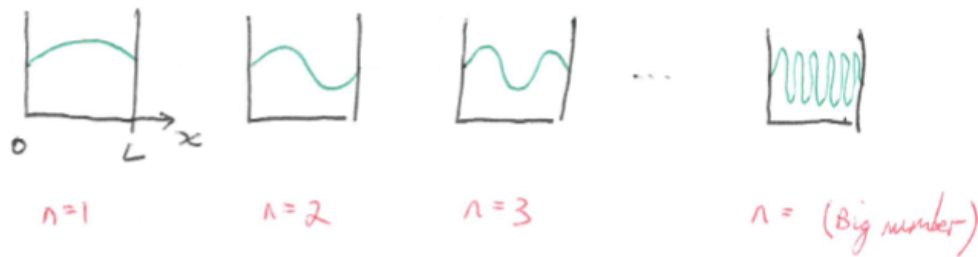
Figure 2.3: Possible cavity modes

The amplitude $a(x)$ can be given by this:

$$a(x) = \sin\left(\frac{n\pi x}{L}\right), \qquad n = 1, 2, 3, \ldots n \quad \text{(mode number)}$$

And by inspection from the figures:

$$\lambda = \frac{2L}{n}$$

And therefore the number of nodes per wavelength is:

$$n(\lambda) = \frac{2L}{\lambda}$$

So, classically:

$$I(\lambda) \propto \frac{n(\lambda)}{\lambda} \times k_B T \propto \frac{1}{\lambda^2}$$

Where the first term is the density of nodes at lambda, and the second is the average energy of nodes. As we head to UV and $\lambda \to 0$, $I(\lambda) \to \infty$... which is not accurate. This is the UV Catastrophe!

2.3   Where did it go wrong?

The issue was assuming that all cavity modes have average energy $k_B T$ - the "Equipartition Theorem" (which we'll meet in later courses).

In brief: the probability distribution of energies is a "Boltzmann Distribution":

$$p(E) = \frac{\exp\left(-\frac{E}{k_B T}\right)}{k_B T}$$

Average energy:

$$\bar{E} = \int_0^\infty E p(E)\, dE = k_B T$$

Which the UV Catastrophe says is incorrect...We therefore need another model to replace the idea of the Boltzmann Distribution.

2.4   Plank's Hypothesis

A rather desperate Plank hypothesised that energy was quantised, i.e. it comes in discrete packets, called quanta. The energy of these quanta is proportional to frequency. This was radical at the time, even though we accept it now.

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

Where $h = 6.626 \times 10^{-34} Js$ is Plank's constant.

Sticking this into the Partition Function from statistical mechanics (which we will properly encounter later on, for now don't worry!), we get an average energy:

$$\bar{E}(\lambda) = \frac{hc/\lambda}{\exp(hc/\lambda k_B T) - 1}$$

Looking at limits:

$$\text{For } \bar{E}(\lambda \rightarrow \infty): \quad \frac{hc}{\lambda k_B T} << 1$$

And the Taylor Series of e^x:

$$\exp\left(\frac{hc}{\lambda k_B T}\right) \approx 1 + \frac{hc}{\lambda k_B T} + \dots$$

Yields:

$$\bar{E}(\lambda) \approx \frac{hc/\lambda}{1 + (hc/\lambda k_B T) - 1} = k_B T$$

This is a good sign, because it means that Plank's Hypothesis holds the correct classically predicted and empirically observed behaviour for higher wavelengths.

Now what about lower wavelengths, where the classical behaviour broke?

$$\text{For } \bar{E}(\lambda \rightarrow 0): \quad \exp\left(\frac{hc}{\lambda k_B T}\right) \rightarrow \infty \quad \text{(very quickly)}$$

$$\text{For } \bar{E}(\lambda \rightarrow 0): \quad \frac{hc}{\lambda} \rightarrow \infty \quad \text{(slower)}$$

Therefore, in the expression:

$$\bar{E}(\lambda) = \frac{hc/\lambda}{\exp(hc/\lambda k_B T) - 1}$$

The numerator and denominator both tend to infinity, but the denominator does so much faster. Therefore (and this can be done in a less handwavy manner via L'Hopital):

$$\bar{E}(\lambda \rightarrow 0) \rightarrow \frac{1}{\infty} \rightarrow 0$$

Which recovers the behaviour at UV wavelengths, so no Catastrophe!

3   Conclusion

- This strange quantisation hypothesis actually fits the data.
- Quantising energy means that the average energy of each cavity mode is wavelength dependant, and not fixed $k_B T$ as seen at larger wavelengths.
- This solves the UV Catastrophe!

Thu 17 Oct 2025 12:00

Lecture 3 - Particle Nature of Light

In this lecture:

- The photoelectric effect.

- Compton scattering.

Which are two examples where classical theory (light as a wave) break down.

1   The Photoelectric Effect

When shining ultraviolet light on a metal surface, electrons are emitted. This is the photoelectric effect.

Why are we not bombarded by electrons in daily life? For the electron to fly off, we must be in a vacuum. Otherwise, it'll immediately strike an air molecule and be absorbed.

Photoelectric Effect Background

- Discovered by Hertz, 1887

- Thomson (1889) went further, so did Lenard (1902) and others.

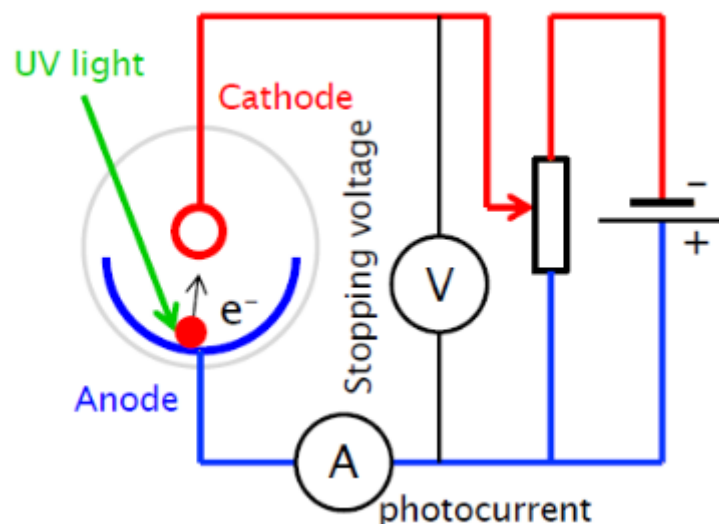- Einstein won his Nobel Prize for explaining this, not from relativity.

Figure 3.1: A circuit diagram for measuring the photoelectric effect.

The above setup would be encased in a glass ball (containing a vacuum), with a setup like this:
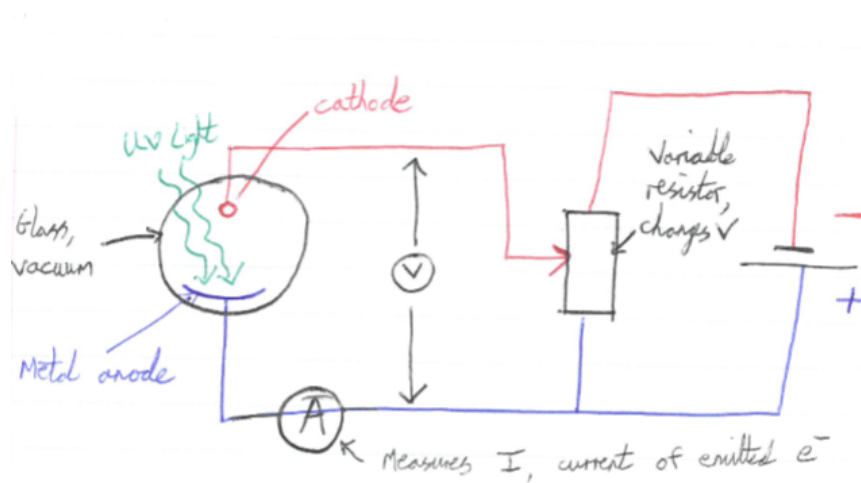
Figure 3.2: Experimental Setup

1.1   Results

Result One - Changing Intensity

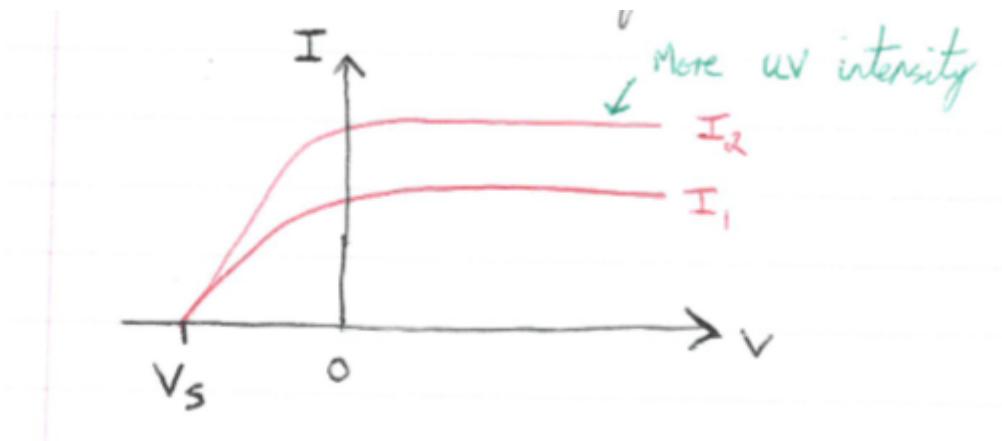For fixed UV wavelength, increasing the intensity of light increases the measured photocurrent:

Figure 3.3

- Increasingly negative potential the cathode decreases photocurrent. At some potential v_s (the "stopping potential") this current drops to zero.

- Potential does not affect electron emission, however adding potential causes an electric field which effectively blows electrons back towards the anode. The stopping potential is when this electric field is perfectly strong to prevent electrons from reaching the cathode and causing a current.

- The fact this can happen consistently (i.e. no current means no electrons made it through) implies that there must be some maximum kinetic energy these electrons can have ($KE_{max} = eV_S$).

- The stopping potential is independent of UV intensity. More UV makes current increase, but does not change stopping potential (i.e. it does not give more energy to each electron, they each have the same energy). This does not make sense classically. Classically we would expect adding more energy to cause emitted electrons to have more energy, therefore changing the stopping potential.
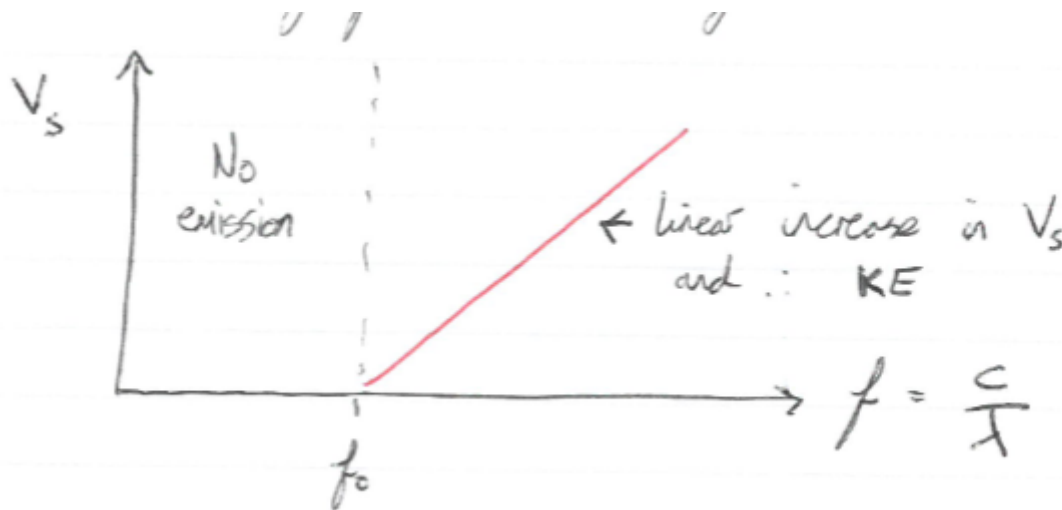
Result Two - Changing Wavelength

Figure 3.4

We have to reach some baseline threshold frequency f_0 before we see any photocurrent. After this, increasing wavelength increases photocurrent (and hence KE of emitted electrons) linearly.

- For a given metal, we find the threshold frequency f_0, below which there is no emission of electrons (no current). If below the frequency f_0, intensity is irrelevant. This contradicts classical mechanics which would suggest that turning up the light intensity would supply more (and potentially sufficient) energy.

- Above the threshold, the energy of individual emitted photons depends on UV frequency and not intensity (by result one).

1.2   Conclusions

Classically

Classically, we expect energy to be proportional to intensity, $\therefore v_s$ should increase with greater intensity. We also expect there to be no link between between frequency and energy, hence no threshold frequency. We'd expect no threshold frequency, instead being a time delay as electrons "soak up" energy to reach the required threshold.

In theory, great, in practice *this is not observed.*

Einstein's Proposal

Energy in light comes from photons with energy $E = hf$. There is a minimum energy required for an electron to be able to escape from the metal. This minimum energy is called the work function ϕ.

$$KE_{\text{max}} = hf - \phi = eV_s$$

Now:

- Higher intensity means more of the same particles (more photons), but the energy of each is unchanged.

- $E = hf$ so frequency changes energy (as observed).

- The Bohr model says that an electron can only have certain electron energy transitions when the correct energy is supplied (an electron cannot gradually soak up energy). This explains why there is a cutoff below the work function, and no observed time delay (as the "soaking up" that causes the delay does not happen). Either an incoming photon has sufficient energy, or it does not. Having more photons does not help.

- The first incoming photons immediately releases an electron (assuming the incoming light has sufficient energy), therefore there's no time delay.
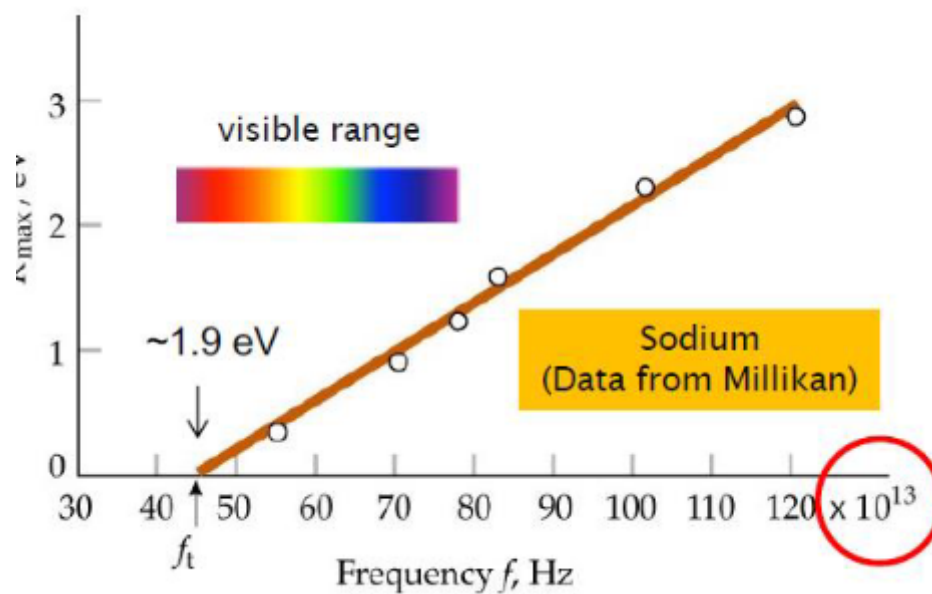
1.3 In Practice

Figure 3.5: Sodium photocurrent measurements by Robert Millikan

2 Compton Scattering

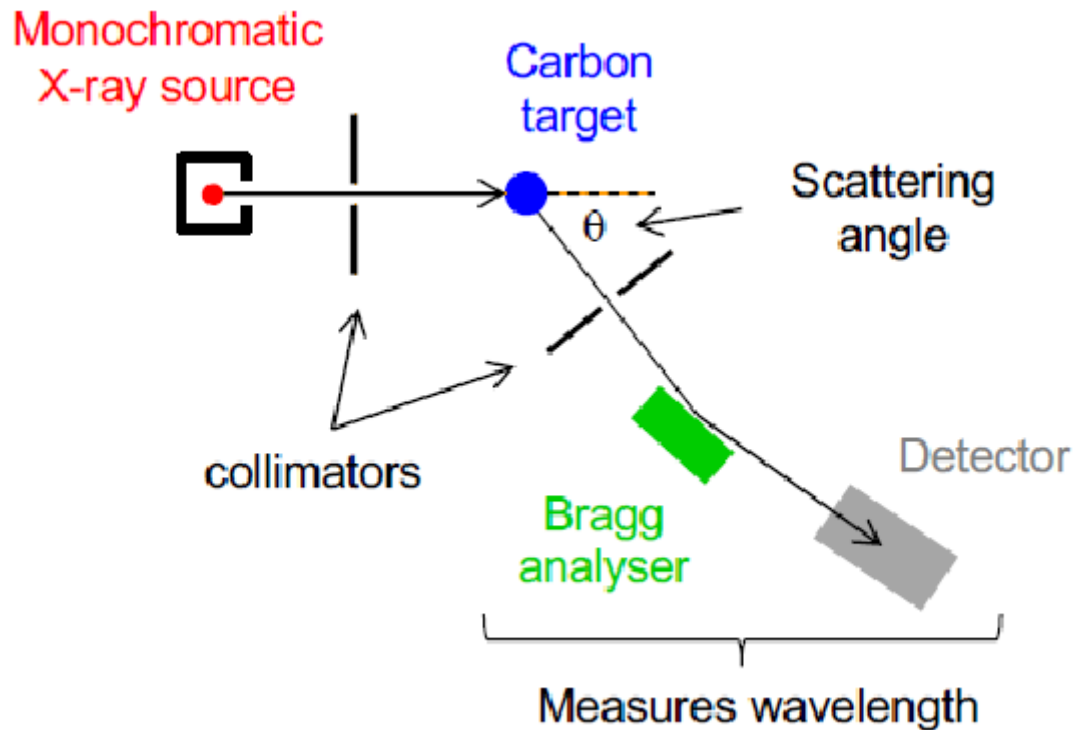Compton Scattering is the scattering of x-rays off carbon atoms.

Figure 3.6: A Compton Scattering experimental setup.

The surprising result is that two wavelengths were observed (not just the original) - λ_1, λ_2, where λ_1 is the original and λ_2 is different. Classically this is hard to explain and λ should not change.

The difference between these two wavelengths increases with scattering angle θ. This can be explained if the x-ray beam is a stream of photons, but not classically.

Possible options when a photon collides:

- Elastic: No loss of energy, hence no change in wavelength.

- Inelastic: Change of energy, so the wavelength also changes. An electron is fired out of the target, carrying energy and momentum, so the photon loses energy.
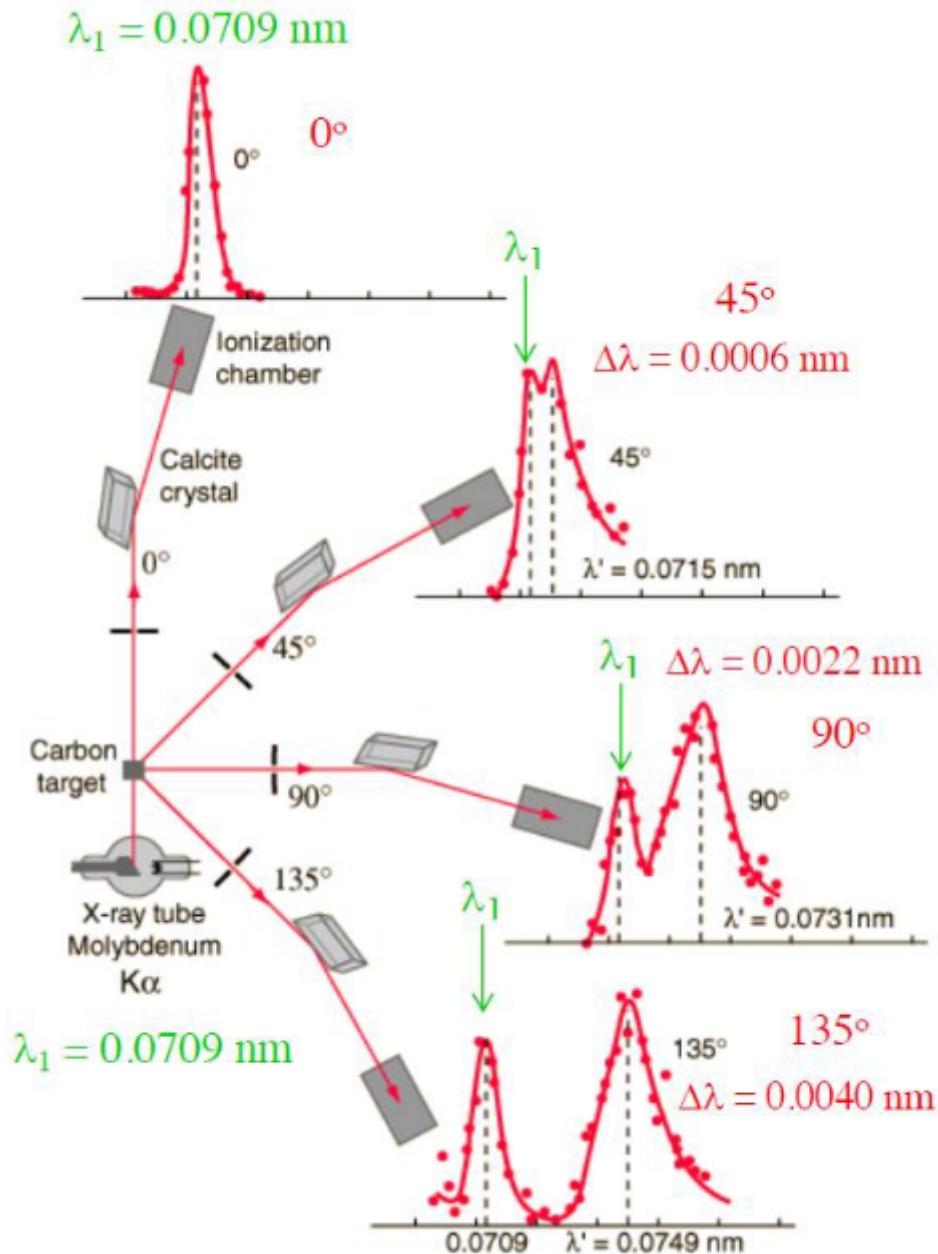

Figure 3.7: The observed results

3   Deriving Compton's Equation

Given an incoming photon with with energy E_1, wavelength λ_1 and momentum $\underline{p}_1$. This strikes a carbon atom and is deflected by angle θ. There is also an emitted electron at angle ϕ which must be in the opposite direction (angled up vs down) to conserve momentum. The new deflected photon has E_2, λ_2, $\underline{p}_2$.

We must consider relativistic effects here given the high speed ($E^2 = p^2c^2 + m^2c^4$)

Figure 3.8

3.1 Setup

For a massless photon ($m = 0$):

$$E = pc$$

And:

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

So:

$$p = \frac{h}{\lambda} \tag{3.1}$$

3.2 Conservation and Relativity

Conserving momentum (underlines omitted for speed):

$$p_1 = p_e + p_2$$

$$p_e = p_1 - p_2$$

Squaring both sides:

$$p_e^2 = p_1^2 + p_2^2 - 2p_1 \cdot p_2$$
$$p_e^2 = p_1^2 + p_2^2 - 2p_1 p_2 \cos\theta \tag{3.2}$$

And then by conservation of energy:

$$E_1 + E_e = E_2 + E_e'$$

Where E_1 is the incoming photon energy, E_e is the energy of the electron at rest in atom before collision, E_2 is the deflected photon energy and finally E_e' is the deflected electron's energy.

Using this:

$$p_1 c + m_e c^2 = p_2 c + \sqrt{p_e^2 c^2 + m_e^2 c^4}$$
$$\implies p_1 - p_2 + m_e c = \sqrt{p_e^2 + m_e^2 c^2}$$

And squaring both sides:

$$(p_1 - p_2)^2 + \cancel{m_e^2 c^2} + 2m_e c(p_1 - p_2) = p_e^2 + \cancel{m_e^2 c^2}$$

Substituting in Eqn 3.2 for p_e^2

$$(p_1 - p_2)^2 + 2m_e c(p_1 - p_2) = p_e^2$$
$$(p_1 - p_2)^2 + 2m_e c(p_1 - p_2) = p_1^2 + p_2^2 - 2p_1 p_2 \cos\theta$$

And rearranging:

$$(p_1 - p_2)^2 + 2m_e c(p_1 - p_2) = p_1^2 + p_2^2 - 2p_1 p_2 \cos\theta$$
$$p_1^2 + p_2^2 - 2p_1 p_2 + 2m_e c(p_1 - p_2) = p_1^2 + p_2^2 - 2p_1 p_2 \cos\theta$$
$$-2p_1 p_2 + 2m_e c(p_1 - p_2) = -2p_1 p_2 \cos\theta$$
$$-p_1 p_2 + m_e c(p_1 - p_2) = -p_1 p_2 \cos\theta$$
$$m_e c(p_1 - p_2) = -p_1 p_2 \cos\theta + p_1 p_2$$
$$m_e c(p_1 - p_2) = p_1 p_2 (1 - \cos\theta)$$

Substituting Eqn 3.1:

$$m_e c(p_1 - p_2) = p_1 p_2 (1 - \cos\theta)$$
$$m_e c \left(\frac{h}{\lambda_1} - \frac{h}{\lambda_2} \right) = \frac{h}{\lambda_1} \frac{h}{\lambda_2} (1 - \cos\theta)$$
$$m_e c \left(\frac{h}{\lambda_1} - \frac{h}{\lambda_2} \right) = \frac{h^2}{\lambda_1 \lambda_2} (1 - \cos\theta)$$
$$m_e c \left(\frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right) = \frac{h}{\lambda_1 \lambda_2} (1 - \cos\theta)$$
$$m_e c \left(\frac{\lambda_1 \lambda_2}{\lambda_1} - \frac{\lambda_1 \lambda_2}{\lambda_2} \right) = h(1 - \cos\theta)$$
$$m_e c (\lambda_2 - \lambda_1) = h(1 - \cos\theta)$$
$$(\lambda_2 - \lambda_1) = \frac{h}{m_e c} (1 - \cos\theta)$$

Which is the Compton Equation. This shows that the change in wavelength is proportional to $1 - \cos\theta$.

4   Conclusions

The photoelectric effect and Compton scattering are two more physical phenomena that cannot be explained using traditional classical mechanics with EM waves alone. They both require assuming photons of energy $E = hf$ to be adequately explained.

Fri 24 Oct 2025 12:00

Lecture 4 – Atomic Energy Levels and Atomic Spectra

In this lecture:

- The spectra of light emitted and absorbed by electrons in:
  - Hydrogen (simple)
  - Larger atoms (not simple…)
- Electronic shells and orbits.

1 Spectra

The Bohr Model says that electrons in an atom can hold discrete values "levels" of energy. As electrons go up or down these levels they must absorb or will emit a photon. This emission causes a discrete spectra of emitted frequencies, unique to the element causing it.
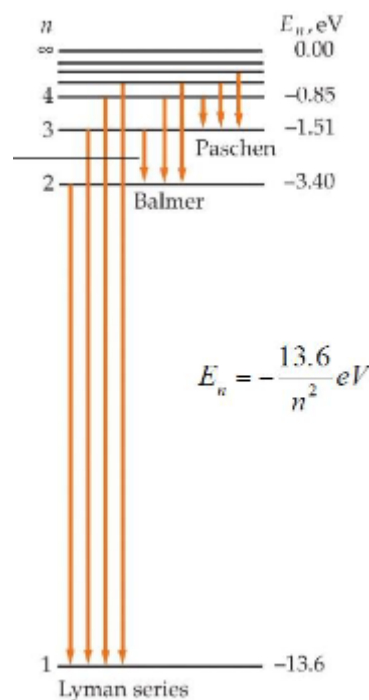

Figure 4.1: Example emission spectra.

Each of the transitions from one energy level to another have a discrete change in energy (measured in eV), therefore each transition will have a discrete wavelength of produced photons.

From the Bohr model, he postulated (from experimental observations) that light can *only* be absorbed or emitted when an electron goes up or down a discrete energy level (excitation or relaxation). The lowest energy level is known as the "Ground State" ($n = 1$).

It is important to note that the transitions in energy levels are not spatial - changing the energy level of an electron does not physically change its position (despite what the diagrams may imply).
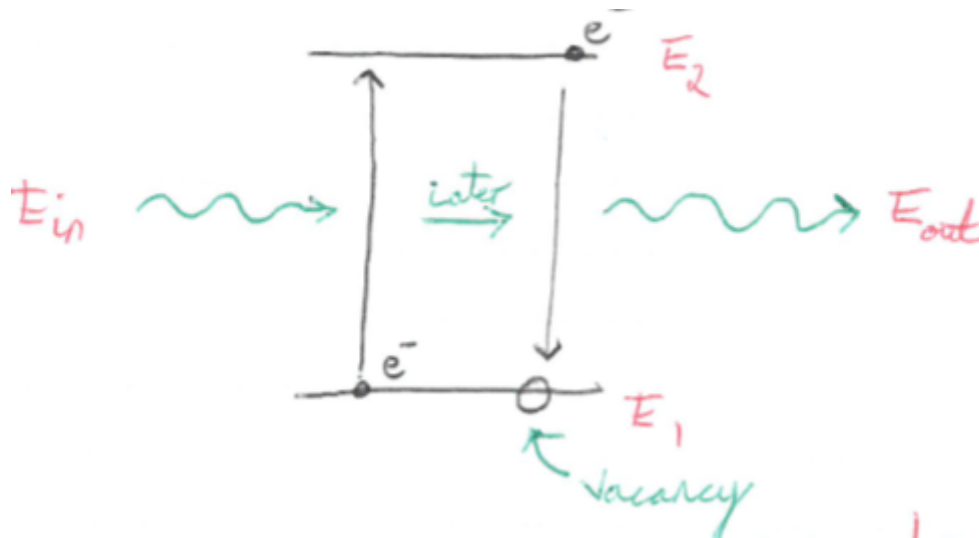
2 Absorption and Emissions

Figure 4.2

An electron is excited up an energy level, leaving a vacancy behind. Some time after, the electron drops back down into the ground state, emitting the energy in terms of a photon. By conservation of energy:

$$E_{\text{in}} = E_{\text{out}} = E_2 - E_1 = hf = \frac{hc}{\lambda}$$

Notably, the energy of the photon that initially triggered the excitation is given by $E_\gamma = E_2 - E_1$

3 Atomic Hydrogen

Atomic Hydrogen is by far the simplest example we can deal with (given the single proton and single electron). This single electron is 'orbiting[1]' the nucleus at some distance r.

The potential energy of this electron is:

$$v(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

This P.E. is negative, so the electron is trapped in a potential well and must be supplied with energy to escape, assuming no K.E. We also know (if we take into account kinetic energy too):

$$E = T + V$$

Where E is total energy, T is K.E, V is P.E. If the total is negative, the electron is bound to the atom.

We can see from the equation for potential energy that $v(r) \propto -1/r$, which gives us the green line. Of the points on this green line, only some of them are actually discrete allowed orbits. The region at the top is called the continuum, which is where an electron has positive energy and has therefore left the nucleus.

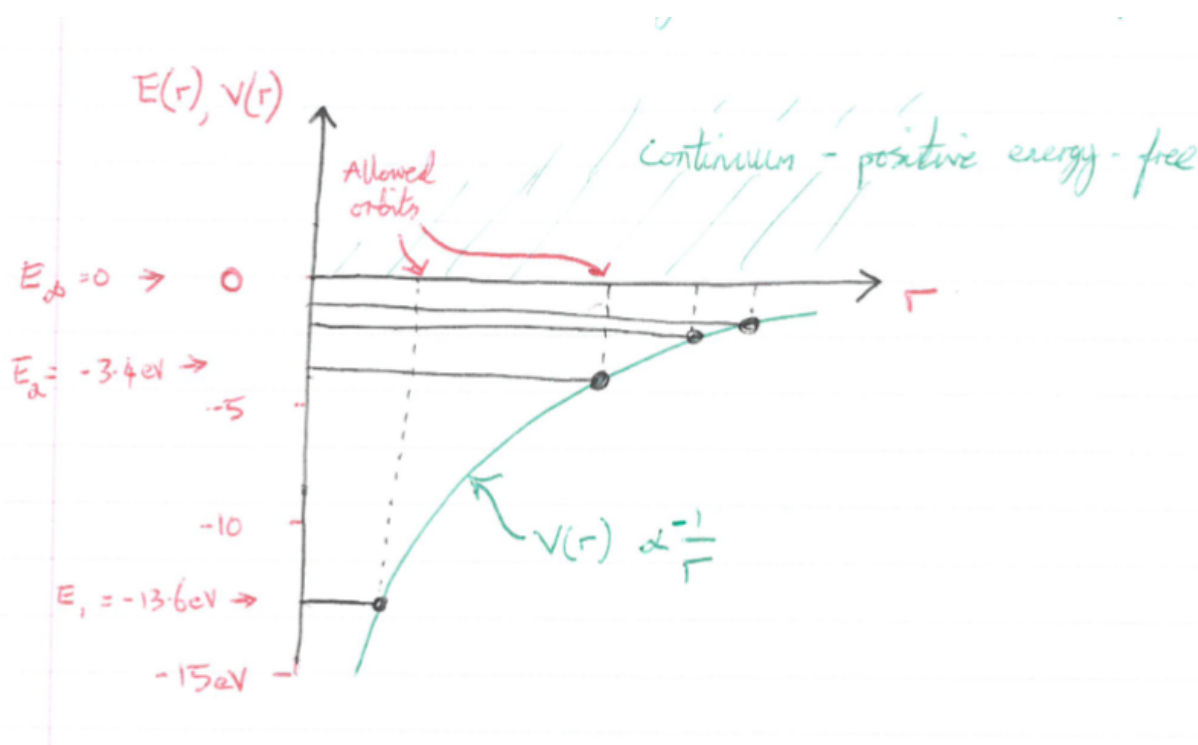[1]for the sake of argument, even if in practice it does not really

Figure 4.3

In Lec 08, we will properly derive from the Bohr model that the energy of each energy level is given by this:

$$E_n = \frac{-13.6eV}{n^2} \quad n = 1, 2, 3, \ldots, \infty$$

Note that if $n \to \infty$, $E_n \to 0$. Emission and absorption happens when an electron moves from two different energy levels ($m \to n$).

$$E_\gamma = E_n - E_m = 13.6(1/n^2 - 1/m^2)eV$$

$$\frac{hc}{\lambda} = E_n - E_m = 13.6(1/n^2 - 1/m^2)eV$$

Or, finally:

$$\frac{1}{\lambda} = \frac{13.6eV}{hc}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

The $\frac{13.6eV}{hc}$ term is known as the Rydberg constant.

3.1   Balmer Series

The 'Balmer Series' is a portion of the hydrogen emission spectra which happens to take place at visible wavelengths. It is specifically transition which take place to n = 2. To find these wavelengths, we set $n = 2$:

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

Moving from 3->2 gives us the Balmer Alpha line, for example.

4   Ionisation Energy of Hydrogen

The ionisation energy is the minimum energy required to kick an electron out of the ground state and into the continuum. This is just enough energy to barely make it free (i.e. when the continuum is reached the electron has 0 KE). Setting $n = 1, m = \infty$:
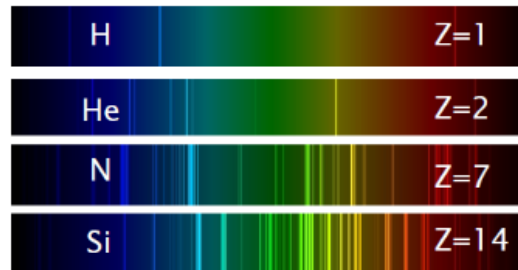
$$\frac{1}{\lambda} = R\left(\frac{1}{1} - \frac{1}{\infty}\right) = R$$

Where R is the Rydberg constant. Note: the energy levels can be very sharp, and they do not change (unless external stimuli like a strong external magnetic field are applied). We can therefore use this in e.g. atomic clocks.

5 Bigger Atoms

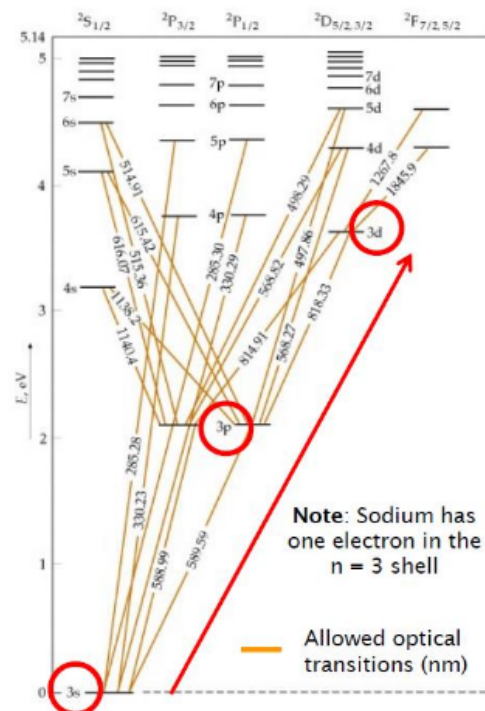Bigger atoms gets more complex than we can reasonably consider now.

Figure 4.4

Electrons begin interacting with each other and the nucleus in weird ways, and it becomes too messy to calculate easily. If there is only a single electron, we can still use the Bohr model, just with a different charge of the nucleus, and we multiply by Z^2 when calculating. If we have multiple electrons, there is no general formula and it becomes unpleasant. The energy levels become split into multiple possible orbitals, i.e for $n = 1$, 1s. For $n = 2$, 2s, 2p. For $n = 3$, $3s, 3p, 3d$ (where s, p, d are different electronic orbitals).

5.1 Spin

Electrons also have an intrinsic quantum property called 'spin', with a value $\frac{1}{2}$. They are fermions with two spin states (up, down). Note that spin is quantum, and has no relation to a physical geometric spin. The maximum occupancy of each level is $2n^2$ (i.e. the 1s state has space for one electron of each spin, i.e. one spin up and one spin down).

6   More Complexity...

- **Fine Splitting**: Electrons are moving, so have non-zero angular momentum. A moving charge creates a magnetic field, which changes the energy of the other electrons.

- **Hyperfine Splitting:** The nucleus also has a spin, they can be parallel (i.e. both have the same spin), or antiparallel, where the electron and the nucleus have opposing spins. These two configurations have slightly different energies (difference of $5.9\mu eV$). The parallel state is metastable, with a half life of 10 million years. There is so much hydrogen in the galaxy that radioastronomers can use this decay, and by detecting it they can image the location of hydrogen in the universe.

Fri 31 Oct 2025 12:00

Lecture 5 - X-Ray Production and Diffraction

In this lecture:

- Production of x-rays

- How to measure their wavelength

- Bragg scattering of x-rays by crystals and Bragg conditions.

1   Production of X-Rays

From the blackbody spectra lecture, we saw that something becoming hotter affects the wavelength of emission. Surely we, therefore, can just heat something hot enough for the peak of the emission spectra to be in the x-ray range?

Unfortunately not, this works, but would need the black body to be 1MK.

The more practical alternative to to fire high energy electrons (keV range) into a metal target in a vacuum.

2   What are they?

Electromagnetic radiation (light) outside of the visible spectrum. It sits beyond the UV portion.

Approximately 0.1keV ($\lambda = 10nm$) to 100keV ($\lambda = 0.01nm$), these are called soft and hard x-rays respectively.

3   Measuring Wavelength

How can we measure or select x-ray wavelengths? With visible light, we can use a prism to turn wavelength into an angle and measure the angle. However, a prism works for visible light because of its high refractive index. Unfortunately, for x-rays, $n \approx 1$ for all materials.

We therefore need some other way to split up wavelengths into angles, for which we can use a diffraction grating. Different wavelengths will be diffracted at different angles.

Another problem arises however…We need the slit separation d to be $d \approx \lambda$ for a diffraction grating to work. For x-rays, $\lambda \approx 10^{-10}m$, which is approximately the width of an atom. Good luck making that grating…

Luckily, nature has made these gratings for us — crystalline materials! Strontium titanate ($SrTiO_3$) has an approx 0.389nm spacing between strontium atoms. We can therefore use this crystal lattice as a diffraction grating.

4   X-Ray Diffraction from Crystals

We treat the x-rays as EM waves (and ignore weird photon stuff for now) and we assume that each atom scatters independently. We also assume that the atom absorbs the x-ray and later re-emits it, in all directions uniformly (at photon level, the emission is in a random direction, therefore we probabilistically treat it as in all).

We want to find the angles where *constructive interference* occurs. Zero intensity everywhere else due to very very high number of slots.

The Bragg Conditions determine where this interference happens. Consider a single plane of equally spaced atoms.
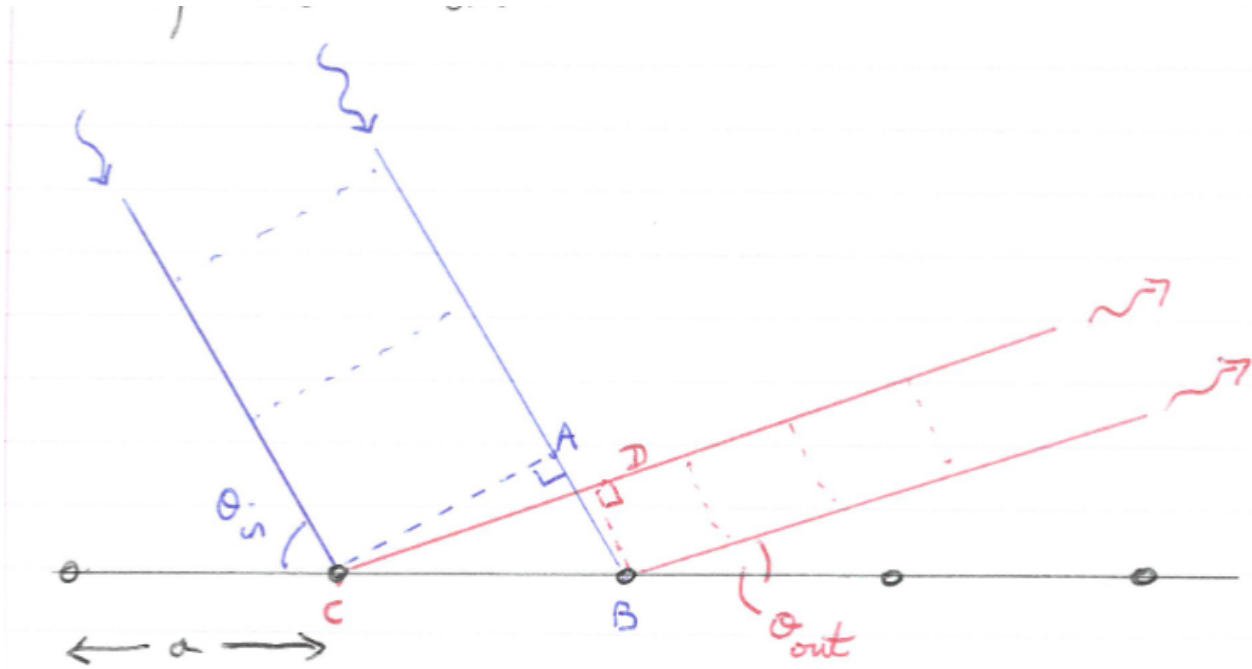
4.1   First Bragg Condition

Figure 5.1

The outgoing waves (red) are all in phase when the wavefronts line up perpendicularly. This happens when path lengths AB and CD are the same. So:

$$a \cos \theta_{in} = a \cos \theta_{out}$$

$$\theta_{out} = \theta_{in}$$

We disregard higher orders where:

$$\cos(\theta_{out} + 2n\pi) = \cos(\theta_{in} + 2k\pi), \quad n, k \in \mathbb{Z}^{+}$$

And we only consider the case where they are explicitly equal. Note that, so far, this is independent of wavelength (i.e. there is 'no dispersion'). This means we're not acting like a diffraction grating yet, more of a mirror.

4.2   Second Bragg Condition

Now we consider the inclusion of a second plane of atoms (we have some much larger number of n planes).
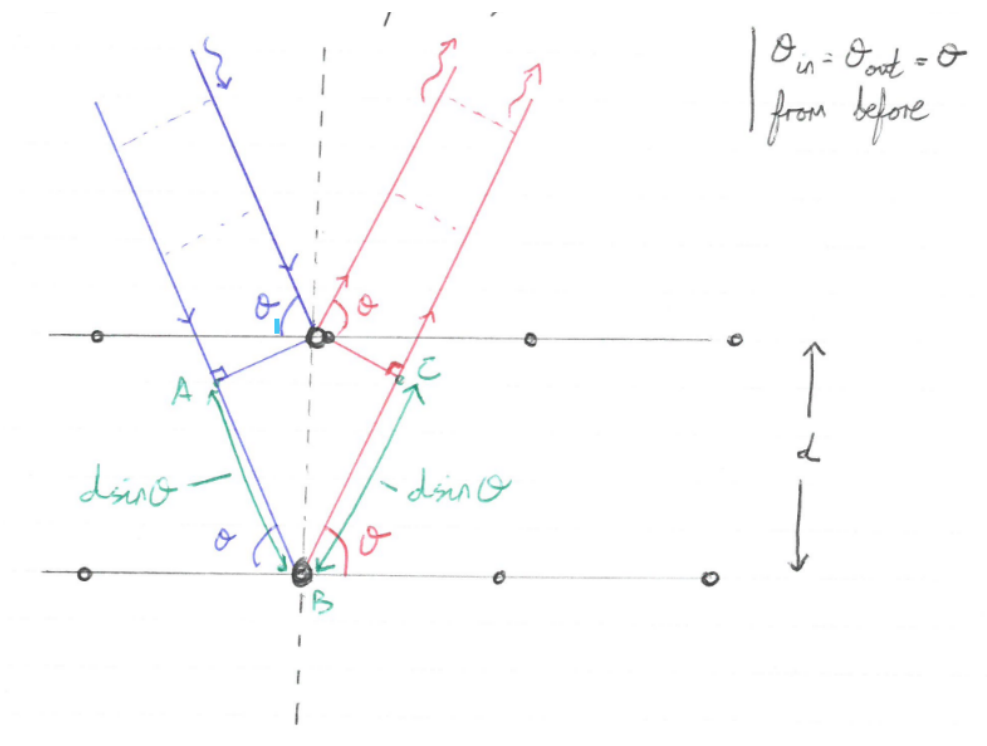
Figure 5.2

The ray which hits the lower plane travels further than the ray which hits the upper plane. For constructive interference to take place, this extra path difference must be an integer multiple of the wavelength. So:

$$AB + BC = 2d\sin\theta = n\lambda \quad n = 1, 2, 3, \dots$$

Where d is the separation of crystal planes. Note: This θ is not the beam deflection angle. It is the angle between the **horizontal** and the incoming beam.

This equation gives us different angles for different wavelengths, therefore we can select light (inc X-rays) of a certain wavelength by splitting multi-wavelength light into different angles, and physically selecting the one that we wish. This throws back to Lec 03, where a Bragg Analyser was used with a detector to measure the wavelength of the produced X-rays.

5   Uses

We can use this in two ways:

We can determine an unknown wavelength (or select a wavelength out of multi-frequency light) by varying θ and identifying the detection peak. Note that θ is here twice, the detector must also be moved, and therefore the total deflection angle is 2θ
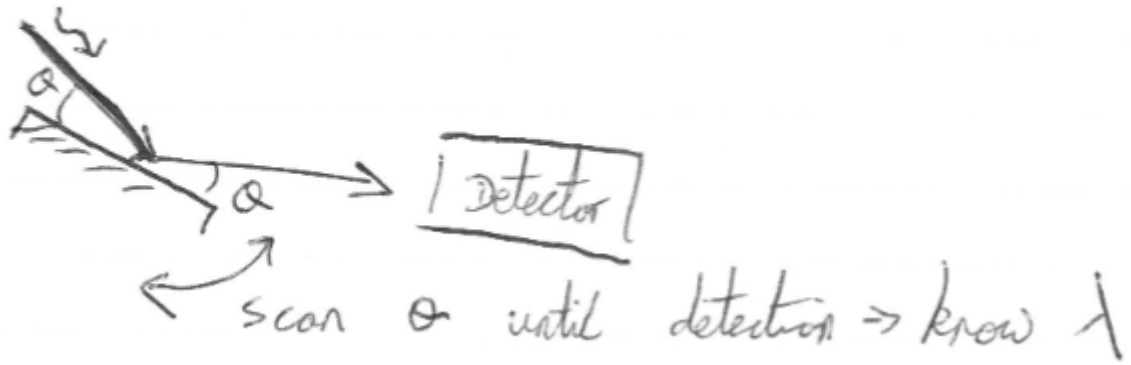
Figure 5.3

Alternatively, we can know lambda and fire at an unknown crystal to determine the atomic spacing. We can scan through 2θ and identify the angles where $n\lambda = 2d_i \sin\theta$ for various d_i. This leads us to x-ray crystallography, where we use x-rays to work out the structure of materials. Using crystals to measure or select an x-ray wavelength is called "wavelength dispersive x-ray spectroscopy".

Fri 07 Nov 2025 12:00

Lecture 6 - X-Ray Spectra

In this lecture:

- The production of X-rays - the spectrum created.

- Attenuation of X-rays in matter.

- Absorption of X-rays in materials, and 'absorption edges'.

1   Typical Tube Spectra

Key: **What spectrum do we get from a typical x-ray tube?**

As a reminder, the source is metal bombarded with high-energy electrons. This causes electron energy level changes in deep electron shells in the metal. This spectrum is characteristic of the anode (the thing being hit by the electrons) material.
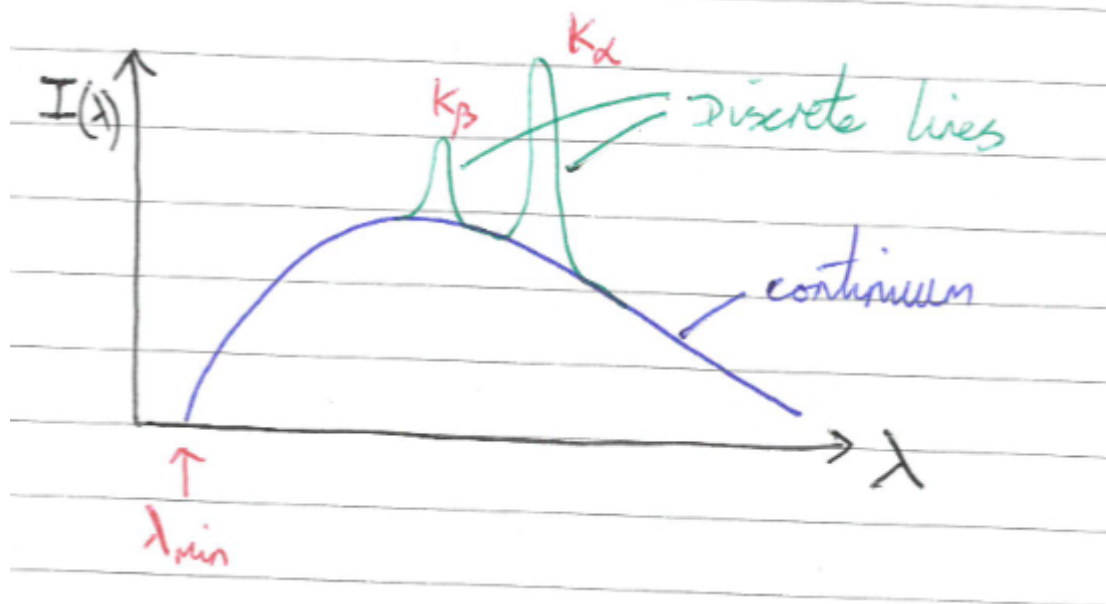

Figure 6.1: A typical x-ray spectra, with a background continuum and unique discrete peaks. Note there is some min λ

The continuous background curve is due to 'Bremsstrahlung', or 'braking radiation'.

2   Braking Radiation

Braking radiation is independent of anode materials. As an electron comes in at a high KE, it interacts with matter (charged nuclei etc) it is deflected and slows down. This lost KE is emitted as X-rays.
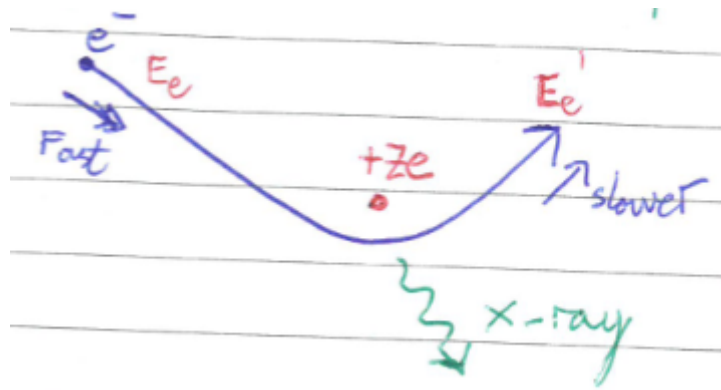
Figure 6.2

2.1   Lambda Min

By C.O.E:

$$E_{\text{x-ray}} = E_e - E_e' = \frac{hc}{\lambda}$$

If the electron came to a stop entirely, E'e would be minimised (braking radiation maximised). The minimum wavelength λ_{min} occurs at the highest x-ray energy, i.e. when E_e' is zero.

$$E_e - 0 = \frac{hc}{\lambda_{\text{min}}} = eV$$

$$\lambda_{\text{min}} = \frac{hc}{eV}$$

Where V is the accelerating voltage.

3   Discrete Lines

These arise from inner shell electron transitions. These, unlike Bremsstrahlung, are characteristic of the anode material. We can use this to investigate the anode material, or we can use different materials to build different x-ray tubes with different emission spectra.

4   Jargon

Note the following stupid jargon.

- m means the n = 1 energy level.
- l means the n = 2 energy level.
- et cetera.

Lets again consider the atomic energy levels (and their associated maximum occupancy):
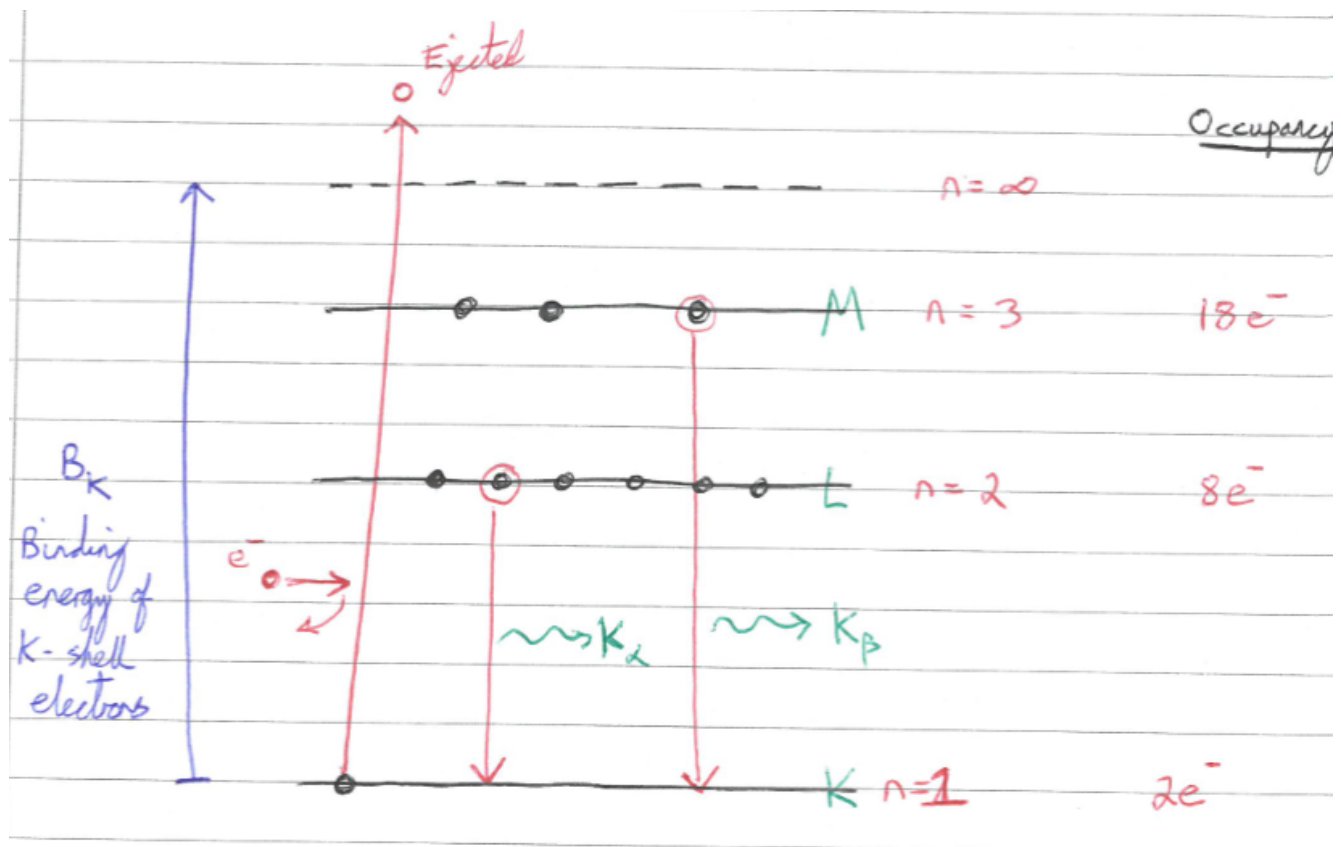
Figure 6.3

If the incoming energy eV is bigger than the binding energy B_k of the k-shell electrons, they can be ejected. This is called 'collisional ionisation'. The intention is to eject an electron from the n=1 shell. This leads to an open space in the n=1 shell (a 'hole'), and the atom will automatically settle into the lowest energy state, i.e. a higher level electron will drop down to fill the lower energy hole. This change in energy requires the emission of a photon.

This specific n = 2 to n = 1 state transition is called k_α (the k denoting 'to the 1st level'), while n = 3 to n = 1 would be k_β etc. Transitions from the third to the second would be L_α, etc etc.

k_α etc only appear if bombardment energy is sufficiently high to cause collisional ionisation. Lower energy lines will therefore appear sooner.
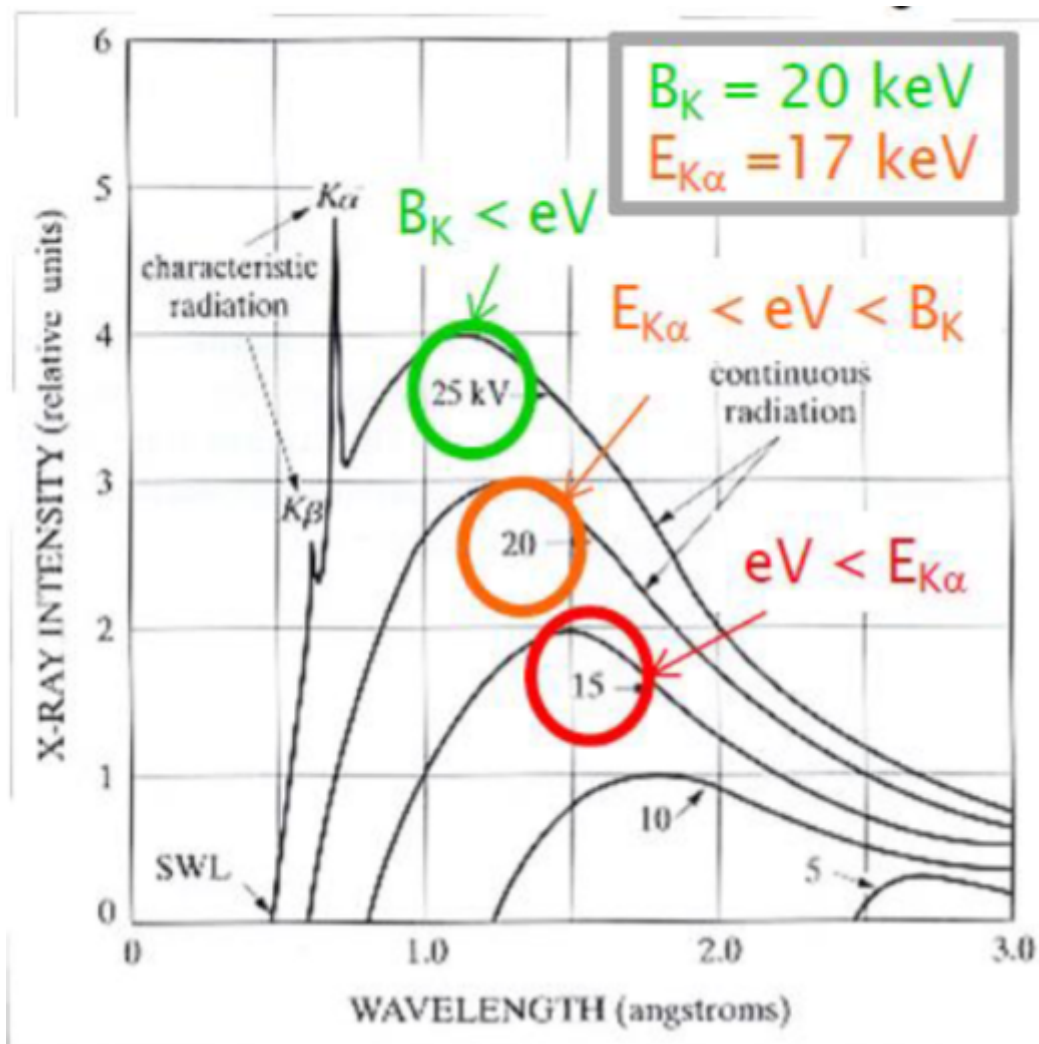
Figure 6.4: Molybdenum X-Ray Spectra (1 Angstrom = 1Å = 0.1nm)

Note that, while Bremsstrahlung is present consistently (albeit with a changing min wavelength where higher accelerating voltage leads to a higher energy x-ray and a lower min wavelength), the sharp spectra lines only appear at higher accelerating voltages where a sufficiently high threshold energy to trigger collisional ionisation is met.

5   X-Ray Absorption

As x-rays pass through a material, x-rays fall exponentially with distance travelled. Suppose we hit a material with x-rays of intensity I_0. These x-rays travel x distance units. The final intensity is:

$$I = I_0 e^{-\mu x}$$

Where μ, the attenuation coefficient, depends on the material and incoming energy.

$$\mu \propto \frac{1}{E_{\text{x-ray}}^3}$$

This hearkens back to the photoelectric effect.

Absorption drops as energy of the x-ray falls below the binding energy of a given shell.
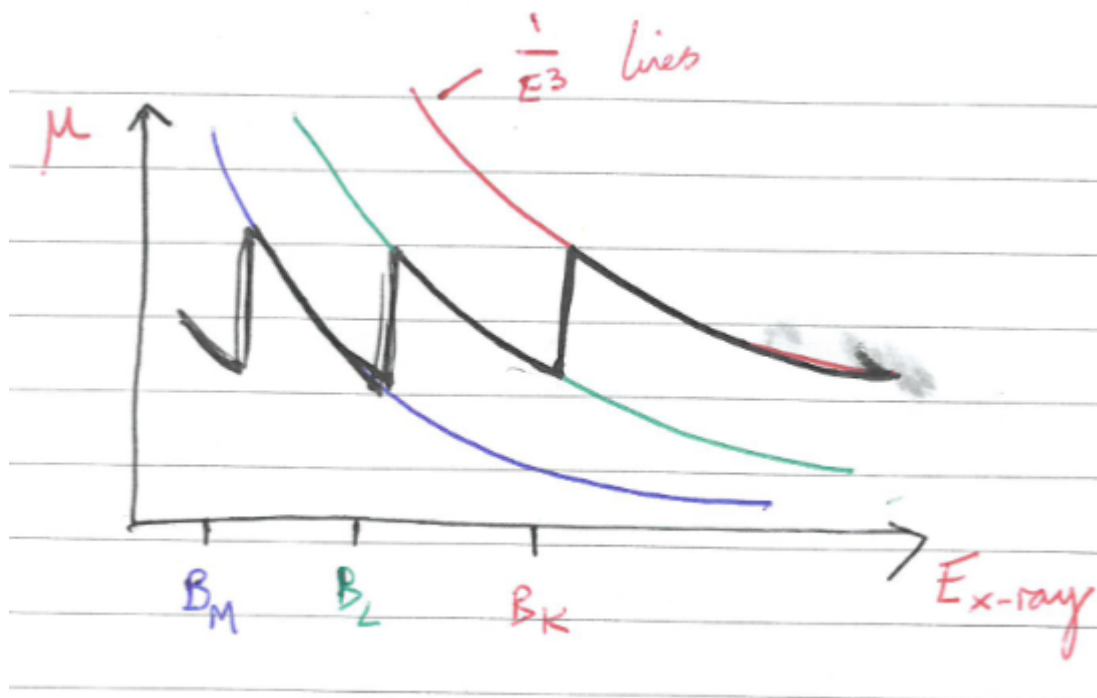
6   Absorption Edges

Figure 6.5: Absorption varying with x-ray energy.

Each line represents the $1/E^3$ value for a given energy shell. If we decrease energy and follow the red line along, we eventually hit the point where there is no longer sufficient energy for ejection from the k-shell. We then drop, and can now eject from everything except from the k-shell until we reach the point where we can no longer eject from the k-shell *or* the l-shell. We drop again, (blue line) and only have emission from all shells except for k and l.
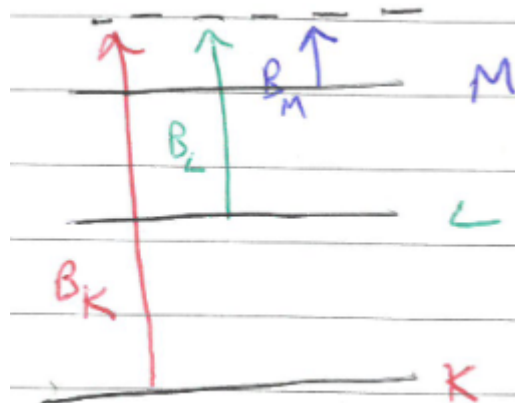
Note:

Figure 6.6

- Measuring these 'absorption edges' lets us determine what atom something is made of, and the associated electronic energy levels.

- Describing these as hard lines is inaccurate, there is (in reality) much more fine detail.

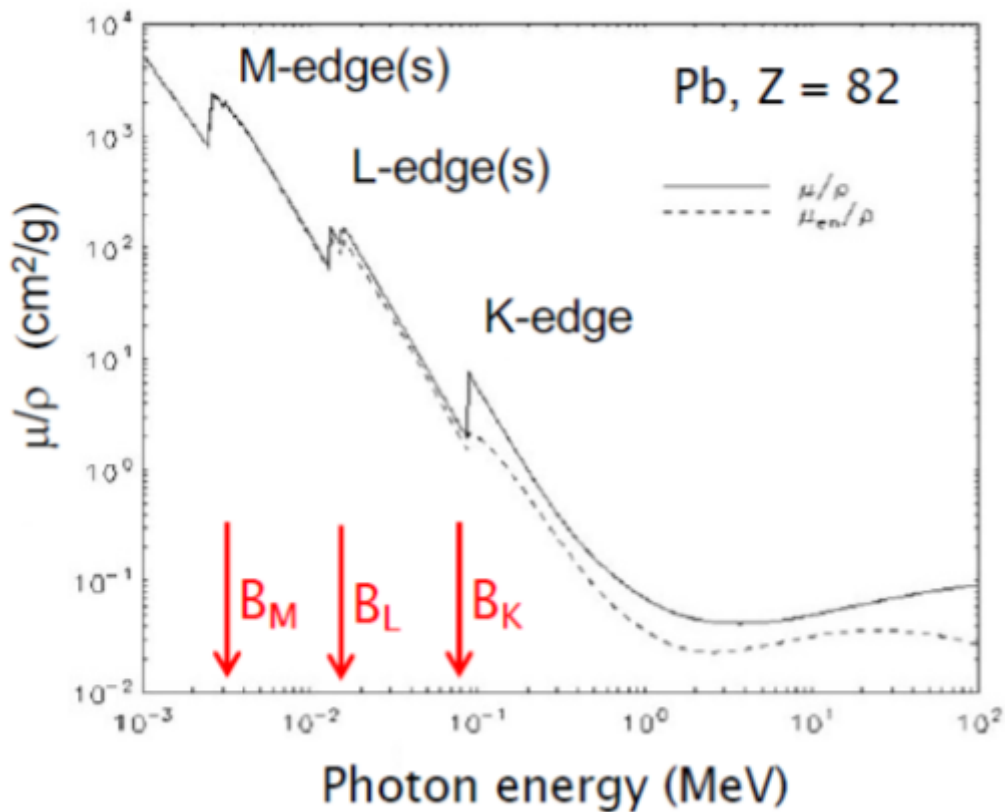- This process is called x-ray absorption spectroscopy.

Figure 6.7: Fine detail visible in absorption edges (especially visible on L-edge).

7 Moseley's Law

If you measure the frequency of k alpha for some material, it is equal to a constant times (Z-1) squared, where Z is the atomic number. This lets us identify elements:

$$f_{k\alpha} = (2.48 \times 10^{15})(Z - 1)^2$$

Note: the '- 1' appears because there will be a second electron 'left behind' in the k shell, which reduces effective nuclear charge by one. This is called screening or shielding.

Fri 14 Nov 2025 12:00

Lecture 7 - "Matter Waves"