Lecture 5 — Wave and particle beams.

1 What can we learn from scattering experiments

- **The crystal structure**, i.e., the position of the atoms in the crystal *averaged* over a large number of unit cells and over time. This information is extracted from Bragg diffraction.

- **The deviation from perfect periodicity**. All real crystals have a finite size and all atoms are subject to thermal motion (at zero temperature, to *zero-point motion*). The general consequence of these deviations from perfect periodicity is that the scattering will no longer occur exactly at the RL points (δ functions), but will be "spread out". Finite-size effects and fluctuations of the lattice parameters produce *peak broadening* without altering the integrated cross section (amount of "scattering power") of the Bragg peaks. Fluctuation in the atomic positions (e.g., due to thermal motion) or in the scattering amplitude of the individual atomic sites (e.g., due to substitutions of one atomic species with another), give rise to a selective reduction of the intensity of certain Bragg peaks by the so-called *Debye-Waller factor*, and to the appearance of intensity elsewhere in reciprocal space (*diffuse scattering*).

- **The case of liquids and glasses**. Here, crystalline order is absent, and so are Bragg diffraction peaks, so that all the scattering is "diffuse". Nonetheless, scattering of X-rays and neutrons from liquids and glasses is exploited to extract *radial distribution functions* — in essence, the probability of finding a certain atomic species at a given distance from another species.

- **The magnetic structure**. Neutron possess a dipole moment and are strongly affected by the presence of internal magnetic fields in the crystals, generated by the magnetic moments of unpaired electrons. Magnetic scattering of X-rays is much weaker, but modern synnchrotron techniques have turned it into a very powerful tool, highly complementary to neutron scattering.

It is important to stress that, in order to extract information about the *atomic* structure of a crystal, liquid or glass by diffraction, **the wavelength of the probe must be comparable or smaller than the interatomic distances**, which are typically a few Ångstroms (10^{-10} m, or 10^{-1} nm). Tab. 1 illustrates the typical wavelengths and energies employed for X-ray, neutron and electron diffraction.

In these sections, the most important formulas pertaining to scattering of different types of radiations from, electrons, nuclei and atoms are collected. Some detailed demonstrations are given in references [2, 3].

Table 1: Typical wavelenghts and energies employed for X-ray, neutron and electron diffraction. For electromagnetic radiation, $E = hc/\lambda$, with $hc = 12.4$ KeV $\cdot$ Å; for a non-relativistic particle beam, $E = \frac{2\pi^2\hbar^2}{m\lambda^2} =$, where $\frac{2\pi^2\hbar^2}{m} = 82$ meV $\cdot$ Å^2 for neutrons and 150 eV $\cdot$ Å^2 for electrons. A typical Transmission Electron Microscope (TEM) can operate at 200 KV raising the electron velocity to 70 % of the speed of light, and some state-of-the-art microscopes can reach the MV range; therefore, relativistic effects need to be taken into account in converting between energy and wavelength.

	λ	E
X-rays	0.1–6 Å	2–150 KeV
neutrons	0.3–10 Å	1–1000 meV
electrons	0.02–3 Å	20 eV–200 KeV

2 Thomson scattering of X-rays

Bragg diffraction of X-rays is primarily due to the scattering of X-ray from electrons bound to the atoms of the crystal structure. It is generally a very good approximation (we will look at *caveats* and exception later on) to employ the so-called Thomson formula (from J.J. Thomson, Nobel Prize 1906) to calculate the relevant scattering amplitudes and cross sections. This is a bit of a paradox, since the Thomson formula assumes *free* electrons, but the agreement with experiments in nonetheless very good.

2.1 Scattering from a free electron

Thomson scattering is a *classical* phenomenon, and can be explained as follows: as electromagnetic radiation impinges on a free electron, the oscillating electric field subjects it to an acceleration. The scattered radiation is the radiation emitted by the accelerated charge. The calculation can be done non-relativistically, provided that the charge is observed in a reference frame where its velocity is *small compared to that of light* The amplitude and polarisation of the scattered radiation depends on the angle ξ between the plane of polarisation and the plane of scattering, as well as on the scattering angle (Fig. 1). One can show that

$$\mathbf{E}(R,t) = -r_0\, E_0 \frac{e^{i(kR-\omega t)}}{R} \left[(\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}'_\sigma)\boldsymbol{\epsilon}'_\sigma + (\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}'_\pi)\boldsymbol{\epsilon}'_\pi \right] = -r_0\, E_0 \frac{e^{i(kR-\omega t)}}{R} \left[\cos\xi\, \boldsymbol{\epsilon}'_\sigma + \sin\xi\, \cos\gamma\, \boldsymbol{\epsilon}'_\pi \right] \tag{1}$$

where

$$r_0 = \frac{e^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-15} \text{ m} \tag{2}$$

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is the *classical radius of the electron.*

The incident polarisation is

$$\boldsymbol{\epsilon} = \cos \xi \, \boldsymbol{\epsilon}_\sigma + \sin \xi \, \boldsymbol{\epsilon}_\pi \tag{3}$$

and γ is the angle between the incident and scattered wavevector (this angle is also known, by longstanding diffraction convention, as 2θ). Based on eq. 1, we can make the following observations:
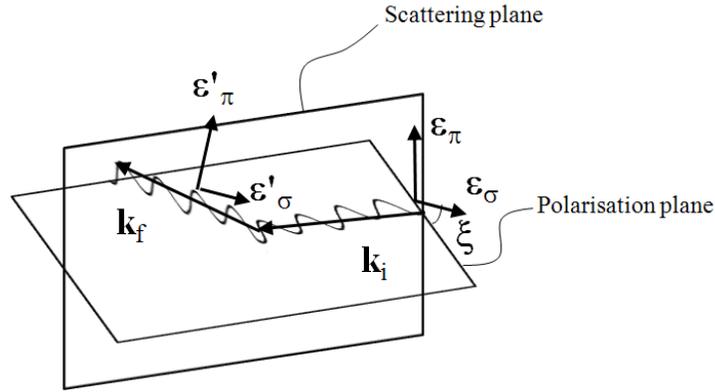

Figure 1: Diagram illustrating the conventional σ and π reference directions for the incident and scattered polarisation. Note that $\boldsymbol{\epsilon}_\sigma \cdot \boldsymbol{\epsilon}'_\sigma = 1$ *always*. Conversely, $\boldsymbol{\epsilon}_\pi \cdot \boldsymbol{\epsilon}'_\pi = \cos \gamma$ **depends on the scattering angle** γ, and **vanishes** for $\gamma = \pi/2$.

- A plane wave impinging on a quasi-free charge produces a scattered *spherical* wave $\dfrac{e^{i(kR-\omega t)}}{R}$, with an amplitude that in general depends on the scattering angle γ.

- If the incident wave is σ-polarised, the scattered wave is σ'-polarised, and has amplitude $\frac{r_0}{R} E_0$.

- If the incident wave is π-polarised, the scattered wave is π'-polarised, and has amplitude $\frac{r_0}{R} E_0 \cos \gamma$.

- The intensity of the scattered wave is zero for scattering of π polarisation at 90°.

- The scattered wave has a phase shift of π upon scattering (*minus* sign).

The instantaneous energy flux of the scattered wave is given by the Poynting vector:

$$\mathbf{S} = \mathbf{E} \times \mathbf{H} = \epsilon_0 c |\mathbf{E}|^2 \, \mathbf{n} \tag{4}$$

The *average* power radiated per unit solid angle in *both* polarisations is therefore

$$\frac{dP}{d\Omega} = R^2 \langle|\mathbf{S}|\rangle = \frac{\epsilon_0 c}{2} R^2 |\mathbf{E}|^2 = \frac{\epsilon_0 c \, r_0^2}{2} E_0^2 \left[\cos^2 \xi + \sin^2 \xi \, \cos^2 \gamma\right] \tag{5}$$

It can also be shown that the power radiated for an arbitrary final polarisation $\boldsymbol{\epsilon}'$ is

$$\left(\frac{dP}{d\Omega}\right)_{\boldsymbol{\epsilon}'} = \frac{\epsilon_0 c \, r_0^2}{2} E_0 \left[\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}'\right]^2 \tag{6}$$

As appropriate for a scattering process, it is convenient at this point to introduce the *cross section*, defined as the average power radiated per unit solid angle divided by the average incident power per unit area (power flux, Φ), which is

$$\Phi = \frac{\epsilon_0 c}{2} E_0^2 \tag{7}$$

The cross section into both final polarisation channels (i.e., if the scattered beam is measured *without* an analyser) is therefore

$$\frac{d\sigma}{d\Omega} = r_0^2 \left[\cos^2 \xi + \sin^2 \xi \, \cos^2 \gamma\right] \tag{8}$$

whereas for an arbitrary final polarisation $\boldsymbol{\epsilon}'$ is

$$\left(\frac{d\sigma}{d\Omega}\right)_{\boldsymbol{\epsilon}'} = r_0^2 \left[\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}'\right]^2 \tag{9}$$

For an *unpolarised* X-ray beam, for which all the angles ξ are equally represented, the cross section becomes

$$\frac{d\sigma}{d\Omega} = r_0^2 \left[\frac{1 + \cos^2 \gamma}{2}\right] \tag{10}$$

2.2   Thomson scattering from many quasi-free electrons

The Thomson formula can be easily extended to the case of multiple scattering centres, provided that the amplitude of the motion of each electron is small with respect to the wavelength. What

we aim to achieve is to find an expression for the X-ray scattering amplitude and cross section of **a multi-electron atom**. In this case, the radiation emitted by each electron at position $\mathbf{x}_i$ will be characterised by an approximately *time-independent* phase factor $e^{i\mathbf{k}\cdot\mathbf{x}_i}$, accounting for the fact that the charge is not at the origin, $\mathbf{k}$ being the wavevector of the incident radiation. Also, the radius R in eq. 1 needs to be replaced with individual radii R_i. Since the sample-detector distance (a few cm) is always much larger than distance between electron in an atoms (a few tenths of nm), we are in the so-called *Fraunhofer diffraction (or far-field) limit*. Assuming a continuous distribution of electrons, we arrive at the following formula for the scattering amplitude:

$$\mathbf{E}(R,t) = -r_0 E_0 \frac{e^{i(kR-\omega t)}}{R} \left[(\boldsymbol{\epsilon}\cdot\boldsymbol{\epsilon}'_\sigma)\boldsymbol{\epsilon}'_\sigma + (\boldsymbol{\epsilon}\cdot\boldsymbol{\epsilon}'_\pi)\boldsymbol{\epsilon}'_\pi\right] \int \rho(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}d\mathbf{x} \tag{11}$$

where $\boldsymbol{q} = \boldsymbol{k}_f - \boldsymbol{k}_i$ is the **scattering vector** and $\mathbf{k}_i$ and $\mathbf{k}_f$ are the incident and scattered wavevectors.[1] Note the important formula, valid for elastic scattering (we recall that $\gamma = 2\theta$):

$$q = |\mathbf{q}| = \frac{4\pi\sin\theta}{\lambda} \tag{12}$$
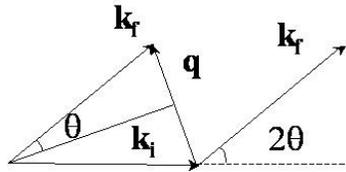
Eq. 12 is illustrated graphically in fig. 2

Figure 2: Scattering triangle for elastic scattering.

The integral

$$\boxed{f(\mathbf{q}) = \int \rho(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}d\mathbf{x}} \tag{13}$$

is known as the **atomic scattering factor or form factor**.

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[1]Throughout this part of the course, we will employ the convention that $\boldsymbol{q}$ is *the change of wavevector of the particle or photon*, so $\boldsymbol{q} = \boldsymbol{k}_f - \boldsymbol{k}_i$. the convention $\boldsymbol{q} = \boldsymbol{k}_i - \boldsymbol{k}_f$ identifies $\boldsymbol{q}$ with the wavevector *transferred to the crystal*, and is widely employed particularly in the context of inelastic scattering — see latter part of the course

We have arrived here at an important result: **the scattering amplitude for many quasi-free electrons is proportional to the Fourier transform of the charge density**. Note that the integral for $\mathbf{q} = 0$ is the **total charge**, which for an atom is the atomic number Z (fig. 3).

A key fact to remember: the *more spread out* the charge is around the atom, the *faster* $f(\mathbf{q})$ will decay at high q.

High q $\equiv$ high scattering angles, short wavelengths.

Eq. 11 can be further simplified in the case of a spherically symmetric charge distribution:

$$f(q) = 4\pi \int_0^\infty dr\, r^2\, \rho(r) \frac{\sin qr}{qr} \tag{14}$$

The cross sections are obtained in the same way as for a single charge — for instance, the unpolarised cross section for an atom is:

$$\left(\frac{d\sigma}{d\Omega} \right)_{atom} = r_0^2 \, |f(\mathbf{q})|^2 \left[\frac{1 + \cos^2 \gamma}{2} \right] \tag{15}$$

which, in forward scattering, becomes:

$$\left(\frac{d\sigma}{d\Omega} \right)_{atom} = r_0^2 \, Z^2 \tag{16}$$

One can find tabulated values for neutral and ionised atoms in the International Tables for Crystallography, volume C [1], p 555 and p 566, respectively.

2.3   X-ray absorption: the photo-electric effect and X-ray fluorescence

When the beam of X-rays impinges at normal incidence on a slab of material of thickness L, it suffers both scattering and absorption, and is therefore ***attenuated*** according to the familiar equation:
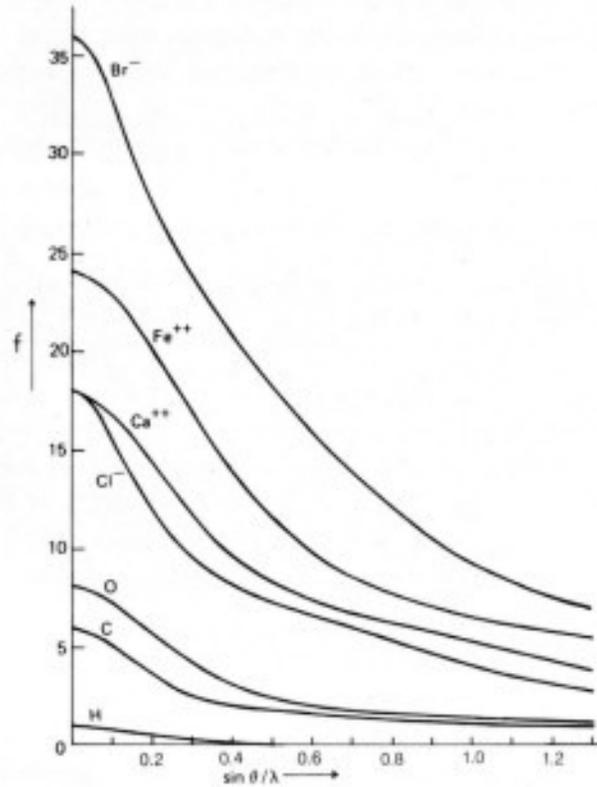
$$I = I_0 e^{-\mu L} \tag{17}$$

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Figure 3: Atomic scattering factors (form factors) for selected neutral atoms and ions. Note that $\sin\theta/\lambda = q/4\pi$.

where μ is the **linear attenuation coefficient**, which is related to the **total cross section** σ_{tot} (scattering plus absorption) by the equation:

$$\mu = \sigma_{tot}\, N_a \tag{18}$$

where N_a is the number of scattering/absorption centres (here atoms) per unit volume. Fig. 4 shows a comparison of the cross sections of different processes leading to X-ray attenuation in materials.

> **At X-ray energies used in typical experiments (5–50 KeV),** *the photo-electric absorption cross section is by far the largest contributor to X-ray attenuation.*
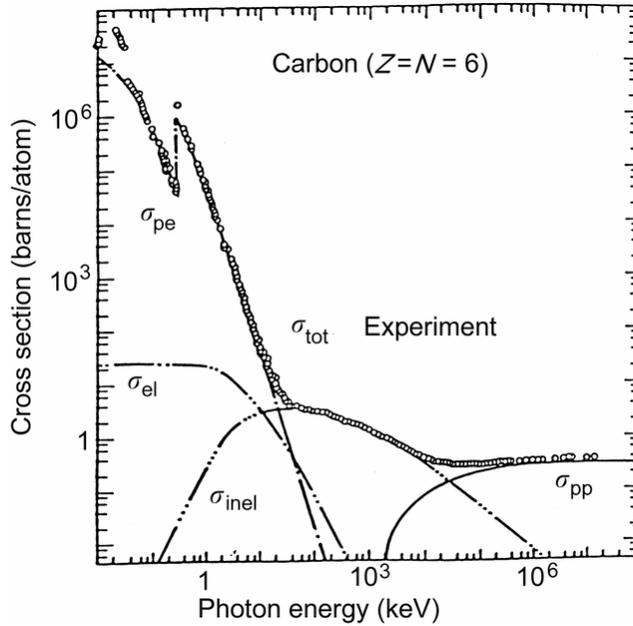
Figure 4: Contributions to the X-ray scattering and absorption cross section for the element carbon (C), from the International Tables for Crystallography, vol. C [1], p 213. In this figure, σ_{el} is the Thomson cross section, σ_{inel} is the Compton inelastic cross section and σ_{pp} is the pair-production cross section, whereby a high-energy photon produces an electron-positron pair. Note the K absorption edge in the photo-electric cross section at 284.2 eV

Key facts about the photoelectric absorption of X-rays

- In the photo-electric absorption process, a photon is completely absorbed and the energy is transferred to a **core electron** (i.e., an electron in the inner atomic shell), which is excited into unoccupied bound states above the Fermi energy or in the continuum.

- The key parameter controlling this effect is, naturally, the **electron binding energy**, which is typical of each shell and atom or ion. **No photoelectric absorption can take place if the photon energy is *lower* than the binding energy of the electron**. This is in complete analogy with the more familiar photo-electric effect in semiconductors. As the photon energy is increased through a binding energy "threshold", **additional absorption can take place**, so absorption increases abruptly. This is known as an **absorption edge** (see fig. 5).

- Binding energy are classified based on the **quantum numbers of the core electron**. **A letter indicates the principal quantum number of the core electron**, so "K" for n=1, "L" for n=2, "M" for n=3 "N" for n=4 and so on. This is followed by a **roman subscript** indicating energy sub-levels. Therefore, the K edge indicates a transition from the $1s$ core state. L_I, L_{II} and L_{III} indicate transitions from the $2s$, $2p_{1/2}$ and $2p_{3/2}$, respectively ($2p_{1/2}$ and $2p_{3/2}$ having distinct values of the *total* angular momentum J).

- An X-ray photo-electric absorption event is followed by a chain of **X-ray emission (or fluorescence) events** whereby the excited atom gradually relaxes to the ground state. The processes of absorption and subsequent re-emission are shown schematically in fig. 6. Strong emission lines are those that follow the **dipole selection rules**, i.e., $\Delta l = \pm 1$ and $\Delta j = 0, \pm 1$. For example, for transition metals, there are 3 strong emission lines: $K_{\alpha 1}$ and $K_{\alpha 2}$ for transitions from $2p_{1/2}$ and $2p_{3/2}$ to $1s$ and K_β for transitions from $3p$ to $1s$. X-ray emission is extensively employed to produce monochromatic X-ray radiation (see below).

- **Far from absorption edges, photo-electric absorption decreases as a function of photon energy**, following the very approximate law:

$$\sigma_{ph} \propto \frac{Z^n}{(\hbar\omega)^3} \tag{19}$$

  where Z is the atomic number and the exponent is a number between 4 and 5.

- A list of characteristic absorption and emission X-ray energies can be found in the International Tables for Crystallography, vol. C [1], starting from p 206.
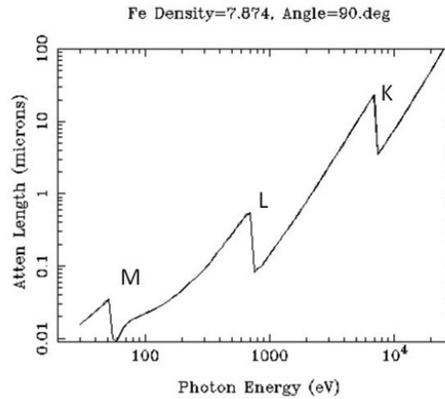

Figure 5: Attenuation length $(1/\mu)$ in microns for elemental iron (Fe), in the energy interval between 30 eV and 25 KeV. The figure was generated using the attenuation calculator in http://henke.lbl.gov/optical_constants/atten2.html. Note the three absorption edges: K at 7.112 KeV, L (actually three edges at 845 eV, 720 eV and 707 eV) and M (edges at 90 eV and 50 eV).

2.4 X-ray scattering beyond the free-electron approximation

Up to now, we have left the issue of "free" electrons somewhat ambiguous. Truly "free' electrons (e.g., conduction electrons in a metal) hardly contribute to the scattering of X-rays, because their probability distribution extends a long way throughout the crystal, and, from eq. 13, the form factor decays very rapidly away from forward scattering (fig. 3). Conversely, the largest contri-
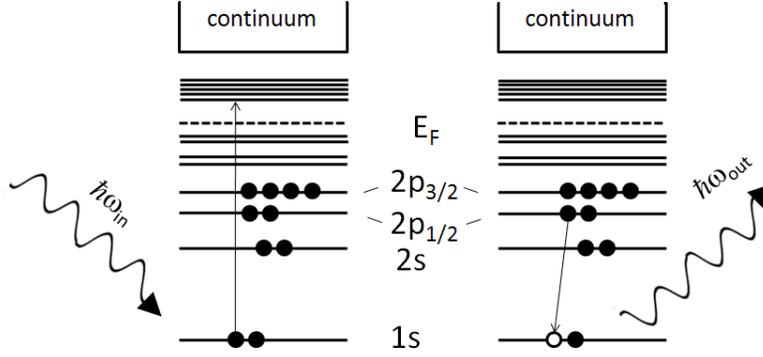
Figure 6: Schematic representation of the absorption and subsequent emission for a K edge event. **Left**: a photon with energy above the K edge is absorbed and an $1s$ electron is ejected above the Fermi energy or into the continuum. **Right**: an electron in the $2p_{1/2}$ shell makes a transition to fill the $1s$ core hole, resulting in the emission of a photon with the characteristic energy $K_{\alpha 2}$.

bution to X-ray scattering from atoms is given by "core" electrons, which are close to the nucleus and have slowly decaying from factors — but these electrons are certainly not free! Indeed, there are large departures from the Thomson scattering formula near *atomic resonances*, where the energy of the photon is just sufficient to eject an electron from a core state into the continuum. Away from resonances, the Thomson formula can be corrected to a very good approximation by replacing the form factor by the *complex* quantity

$$f(\mathbf{q}) = f_{Thom}(\mathbf{q}) + f'(\hbar\omega) + if''(\hbar\omega) \qquad (20)$$

where the so-called *anomalous terms*, f' and f'', away from atomic resonances do not depend on q and are weak functions of the photon energy.

It can be shown, as a consequence of the so-called optical theorem, that *the imaginary part of the scattering factor is proportional to the linear absorption coefficient due to the photoelectric effect*.

$$f''(\hbar\omega) = \frac{\omega}{4\pi r_0 c N_a}\mu \qquad (21)$$

where N_a is the number of atoms per unit volume, and the other symbols have the usual meaning. The quantity μ is the *linear absorption coefficient*, defined in eq. 17.

3 Thermal neutron scattering from atoms and spins

3.1 Introduction

Up to this point, we have carefully examined the case of X-ray scattering from electrons and atoms. One important result we have obtained (for example, see eq. 1) is that

> **The scattering process generates a *spherical wave*, the *squared* amplitude of which is proportional to the cross section.**
> **This result is completely general**, and, within the framework of the approximations we have used, is valid for electron-electron scattering as well as for thermal neutron scattering from nuclei and from magnetic moments. As in the case of photons, we will therefore have to calculate the *scattering amplitudes* from individual scatterers.
> If multiple scattering centres are present, we will **sum up the amplitude from the individual centres with the appropriate phase**.

Naturally, the wave-like nature of particle beams (neutrons and electrons) is *essential* in deriving these results, so, unlike the case of photons, we will have to work within the framework of quantum mechanics.

In the following paragraphs, we will quote the most important results and formulas for the case of *neutrons* and provide a *qualitative* description of the relevant physics.

3.2 Properties of thermal neutrons

- Free neutrons are unstable, with half-life τ = 10.6 min. (β-decay)

- Neutrons bound in nuclei are (generally) stable.

- Mass: $1.67492729(28) \times 10^{-27}$ kg

- Electric dipole moment $D < 10^{-25}$ (e cm)

- Spin: s = $\frac{1}{2}$ — neutrons are *fermions*.

- Magnetic dipole moment: $\mu = -1.9130418 \, \mu_N$, where $\mu_N = \frac{e\hbar}{2m_p} = 5.05078324(13) \times 10^{-27}$ JT^{-1} is the **nuclear magneton**.

Table 2: Neutron wavelenghts and kinetic energies in different "slow" ranges. The thermal energy per particle at room temperature is 25 meV.

	λ (Å)	E (meV)
Cold	3–30	0.1-10
Thermal	1–3	10–100
Hot	0.4–1	100–500
Epithermal	< 0.4	> 500

3.3   Elastic scattering of thermal neutrons

Neutrons are elastically scattered by the condensed matter through two completely different mechanisms, but, as it turns out, yielding comparable scattering lengths.

1. By **nuclear interaction with the atomic nuclei**.

2. By **dipole interaction with the unpaired spin and orbital magnetic moments of the atoms**. This is only present if the atom or ion has a magnetic moment.

A summary of the key result is provided here below.

Neutron-nuclear interaction

- The neutron-nuclear interaction is **isotope and elements specific**, and **depends on the mutual orientation of the neutron and the nuclear spin**.

- As far as neutron crystallography is concerned, **the key parameter is the scattering amplitude *averaged* over the nuclear spin states**, known as the **coherent scattering amplitude**.

- The neutron nuclear coherent scattering amplitude **is independent on q** — it carries **no form factor**, and is therefore expressed by a single number, known as the **Fermi length**.

- **Fermi lengths can be positive or negative, depending on whether the neutron-nuclear interaction is attractive or repulsive**. For typical nuclei, they are of the order of a few fm (10^{-15} m) (see fig 7), which means that they **are comparable to the classical electron radius**. However, atoms have a single nucleus and many electrons, so X-ray scattering cross sections in the *forward* direction are typically much larger than neutron cross sections (X-ray cross sections decay at high q due to the form factor).

- Fermi lengths do not vary in a systematic way across the periodic table (fig 7), which means that **with respect to X-rays, neutrons are uniquely sensitive to some light elements — notably oxygen**. The different scattering lengths of different isotopes is also widely exploited in the so-called **contrast variation techniques.**
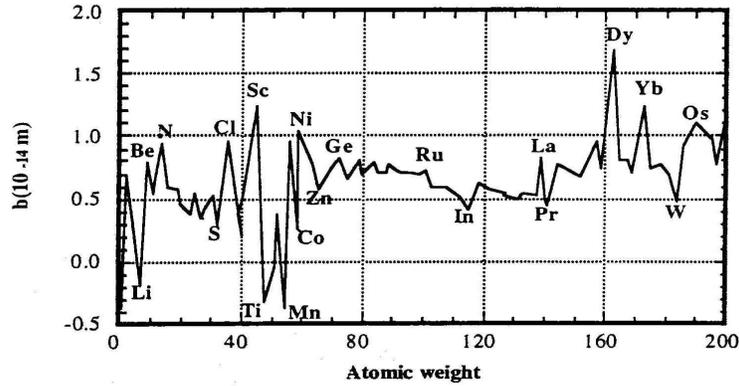

Figure 7: Variation of the Fermi length as a function of atomic weight.

Neutron-magnetic interaction

- When the scatterer carries a magnetic moment, in addition to the normal nuclear interaction, neutron are also scattered by dipole-dipole interaction from the magnetic moment of the atom.

- Magnetic scattering of neutrons is governed by the following **vector** scattering amplitude.

$$A_n = \gamma_N r_0 f_m(q)\mathbf{M}_\perp \tag{22}$$

where γ_N is the neutron gyromagnetic ratio (-1.9130418), r_0 is the familiar **classical electron radius** and $\mathbf{M}_\perp$ is the **projection of the atomic magnetic moment *perpendicular* to the wavevector transfer q**, and is expressed in **Bohr magnetons**.

- The quantity $f_m(q)$ is known as the **neutron magnetic form factor**, and is normalised so that $f_m(0) = 1$. It is similar to the X-ray form factor, except for the fact that it only include the more extended **density of unpaired electrons**. Therefore **magnetic neutron scattering decays very rapidly at high** q.

- From eq. 22 one can obtain a **number of cross sections**, accounting for the different orientations of the neutron spin with respect to the atomic magnetic moment (***neutron polarisation***). The most important cross section is the **unpolarised neutron cross section** (averaged over all the possible neutron polarisations), which, for a *single* atom, is:

$$\frac{d\sigma}{d\Omega} = \gamma_N^2 r_0^2 f_m^2(q)|\mathbf{M}_\perp|^2 = \gamma_N^2 r_0^2 f_m^2(q)M^2 \sin^2\alpha \tag{23}$$

where α is the angle between $\mathbf{M}$ and $\mathbf{q}$. Note that **the cross section is zero if q is parallel to M**.

- Typical magnetic moments for atoms and ions are **a few Bohr magnetons**. Therefore, from eq. 23, one finds that **neutron nuclear and magnetic scattering cross sections are typically comparable in magnitude for magnetic atoms.**

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- Although X-rays are also scattered by magnetic moments, in both resonant and non-resonant conditions, **the magnetic scattering cross section for neutrons is several orders of magnitude greater than that of X-rays. This makes neutrons the technique of choice to study magnetic structures**. X-ray magnetic scattering has some unique advantages, and is steadily gaining in popularity thanks to the advent of powerful synchrotron sources.

Neutron absorption

- Absorption process are those in which there is no neutron in the final state; they can be either **neutron capture** (known as (n, γ)), in which the mass number of the final nucleus is increased by 1 unit, or a **transfer reactions**, in which the mass number of the final nucleus is decreased and an α particle ((n, α)) or a proton ((n, p)) is emitted.

- Thermal neutrons are **weakly absorbed** by most materials, with typical absorption lengths of the order of a cm.

- **Neutrons with longer wavelengths are more strongly absorbed**. For most materials, **absorption cross sections are proportional to the neutron wavelength**, so the absorption lengths are inversely proportional to the wavelength.

4   X-ray sources

X-ray tubes. The most common and ubiquitous source of X-rays is the **high-vacuum tube**, illustrated schematically in fig. 8. Conceptually, the X-ray tube has not changed greatly from the one built by W. Roentgen (Nobel prize 1901). It consists of an **electron gun** — usually a thermoionic cathode —, which produces a well-defined, mono-energetic beam of electrons. It is usually desirable to concentrate the electron beam in a small, intense spot, but other configurations (e.g., "line focus") are possible for particular applications. Typical laboratory devices are completely **sealed tubes**, and run at 40–60 KV (up to over 100 KV for heavy-metal anodes) and 30-40 mA, for a total power up to 3-6 KW.

A typical spectrum from an X-ray tube is shown in fig. 9 and consists of 2 components:

- The **continuous spectrum**, or **"bremsstrahlung"** (="breaking radiation"). This part of the spectrum is produced by the rapid deceleration of the electrons in the anode, due to a variety of processes.

- The **characteristic lines**, or **emission lines**. These are due to atoms in which one of the **core electrons** has been ejected, due to interaction with the incoming electron beam. **The energy of the characteristic lines is the same as that of X-ray emission lines, such as $K_{\alpha 1}$, $K_{\alpha 2}$, K_β etc.** (see section 2.3.)
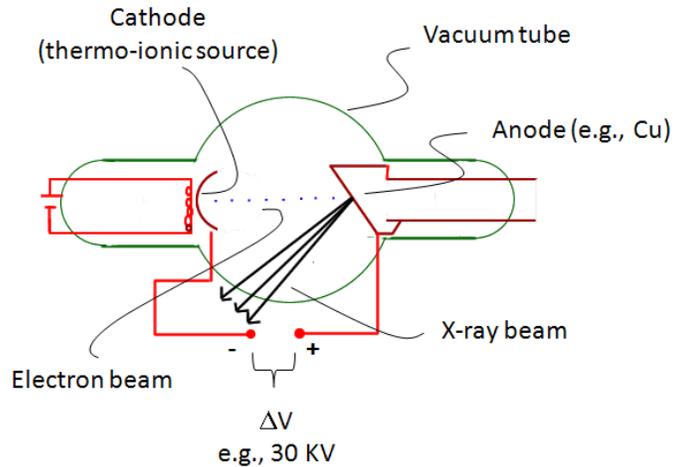
Figure 8: Schematic representation of an X-ray vacuum tube.

- For monochromatic experiments, one generally employs the very intense **characteristic lines**. The bremsstrahlung and some/all the other lines can be removed either by using a monochromator (or analyser, see next lecture) or by a **photon energy discriminator** in the detector.

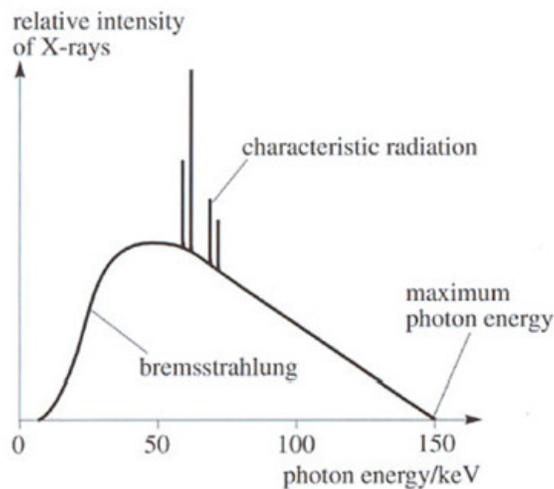- The maximum photon energy is equal to the electron beam energy.

Figure 9: Typical spectrum of an X-ray tube.

Synchrotron sources. As we have seen at the beginning of this lecture, an accelerated charge emits electromagnetic radiation. The characteristic radiation of a **charged particle in circular motion** is known as *synchrotron radiation*. *Parasitic* synchrotron radiation was produced in cyclotrons (since the work of Ernest Lawrence (1929)) and early particle accelerators , but it was not until the late seventies that the first synchrotrons *dedicated to producing synchrotron radiation* were conceived. The first synchrotron of this kind with the Synchrotron Radiation Source in Daresbury, in Cheshire. **All modern synchrotrons accelerate either electrons or**

positrons. A concise description is contained in the international Tables for Crystallography vol. C [1], p 195. A complete derivation of the relativistic case is given in [5], p 654f.
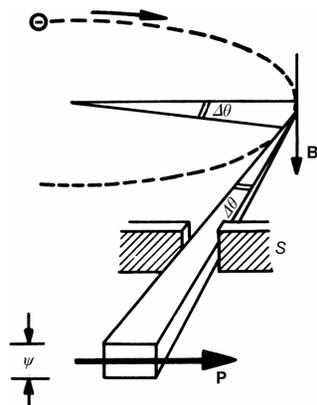

Figure 10: Radiation emitted by a synchrotron in the relativistic limit. The angle ψ is given by $\psi = mc^2/E$. The direction of polarisation is also shown. $\boldsymbol{B}$ is the magnetic field *perpendicular* to the electron orbit, as generated by the bending magnet. The horizontal divergence is limited by means of slits.
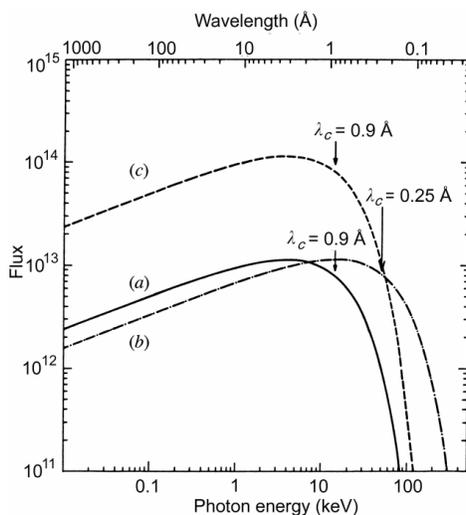
Figure 11: Photon energy spectra for (a) a bending magnet (b) two types of "wigglers" (insertion devices). Note how the flux decays rapidly above the characteristic energy corresponding to λ_c.

5   Neutron sources

Radioactive sources of neutrons. The sources originally employed by Bothe and Becker and Chadwick exploited a fusion reaction between α particles (emitted by polonium or radium and light nuclei such as Li, Be or B). For instance

$$^{4}He + {}^{9}Be \rightarrow {}^{1}2C + n + 5.7\,\text{MeV} \tag{24}$$

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Modern sealed sources, which are commercially available, usually employ ^{241}Am, ^{238}Pu or ^{239}Pu as sources of α particles. Another type of isotope-based source contains elements that undergo spontaneous fission, such as ^{252}Cf. These types of sources can produce 10^7-10^9 neutrons per second, and are mainly used to calibrate neutron detectors.

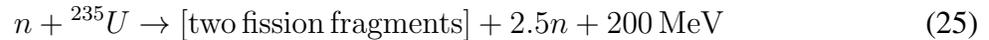**Reactor sources** Nuclear reactors exploit the **fission** reaction

$$n + {}^{235}U \rightarrow [\text{two fission fragments}] + 2.5n + 200\,\text{MeV} \tag{25}$$

which produces, on 2.5 (on average) neutrons per fission event (fig 12). Of these, 1 is requires to maintain the chain reaction, 0.5 are absorbed and 1 escapes the core and is available for use. The **nuclear cross section** for the reaction in eq. 25 is about ~ 1 **barn for the fast neutrons** emerging from the fission event, but is **1000 barns for slow thermal neutrons** (thermal energies in the tens of meV range). Therefore, in most reactor designs, neutrons are slowed down (**thermalised**) by means of a **moderator** — typically **graphite** (as in the Chicago pile CP-1, December 2, 1942), **water** or **heavy water**.
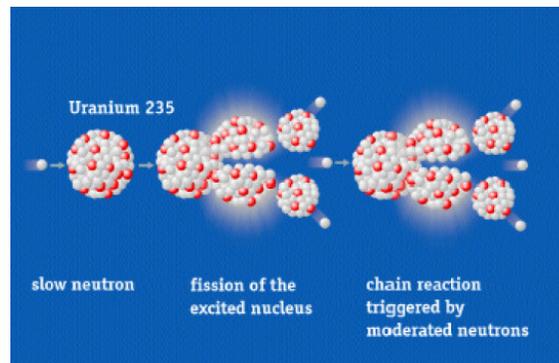

Figure 12: A schematic representation of the fission nuclear reaction.

The most powerful reactor source in the world is the ILL. It generates fluxes of 1.5×10^{15} neutrons per second per cm^2 at the exit of the beam tubes, with a thermal power of 58.3 MW.

Spallation sources. When a fast particle, such as a high-energy proton, bombards a heavy atomic nucleus (such as lead, tungsten or tantalum), some neutrons are "spalled," or knocked out, in a nuclear reaction called spallation. Other neutrons are "boiled off" as the bombarded nucleus heats up, while the fast neutron produce secondary spallation reactions with other nuclei (fig 13). These reactions are much more efficient than fission at producing neutrons (20-30 neutrons are produced for each spallation event), but, of course, one has to accelerate the protons in the first place to energies of the order of to 0.5-2 GeV, using a linear accelerator (LINAC), a synchrotron or a combination thereof.

The neutrons leaving the heavy-metal target are highly energetic, and need to be moderated before they can be employed for scattering experiments. This is done in a series of **moderators**

Figure 13: Schematic representation of some of the nuclear processes involved in "spallation" neutron production. Heavy-element nuclei are fragmented ("spalled") either by the incident protons (**top**) or by secondary neutrons (**bottom left**). Other nuclei are left in a highly excited state and "boil off" additional neutrons (**bottom right**).

that surround the **target assembly** (which usually includes a series of beryllium neutron reflectors as well). As for the case of reactor sources, **moderators can be held at different temperatures** to produce characteristic spectral distributions. A modern pulsed spallation source, such as the ISIS facility in Chilton, Oxfordshire is shown diagrammatically in fig. 14.

Figure 14: Schematic representation of the ISIS pulsed spallation neutron source, located in Chilton, Oxfordshire (near Harwell). One can recognise the **LINAC** (topmost), the **synchrotron** (top right) and the two **target stations** (left and bottom), surrounded by a series of **beamlines**.

6 Bibliography

The International Tables for Crystallography vol C [1] contains an excellent compendium of most X-ray, neutron and electron diffraction techniques.

Warren, "X-ray diffraction" [2] is a rather old book with a very dated notation, but somehow

I always find myself going back to it. Some of the explanations are very clear.

G.L. Squires "Introduction to thermal neutron scattering" [3] is a classic introductory book, and has all the basic derivations of nuclear and magnetic cross sections.

J.D. Jackson, "Classical Electrodynamics" [5]. This book provides detailed derivation of the classical X-ray scattering cross section. It is a very complete compendium of electrodynamics, although not always easy to digest...

A.S. Davydov, "Quantum Mechanics" [6]. I tend to use this rather old quantum mechanics textbook (mainly for sentimental reasons) for the calculation of the cross sections in the so-called "first Born approximation".

References

[1] T. Hahn, ed., *International tables for crystallography*, vol. C (Kluver Academic Publisher, Do- drecht: Holland/Boston: USA/ London: UK, 2002), 5th ed.

[2] B.E. Warren, *X-ray diffraction* (Dover Publications, Inc., New York) 2nd Ed. 1990.

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[4] Stephen W. Lovesey, "Theory of neutron scattering from condensed matter", Oxford Science Publications, Clarendon Press, Oxford (1984) — Volume 2.

[5] John D. Jackson, "Classical Electrodynamics", John Wiley & sons, New York, Chichister, Brisbane, Toronto, Singapore, (1975)

[6] A.S. Davydov, "Quantum Mechanics", Pergamon/Addison-Wesley, (1965).

7 Useful constants

$$\epsilon_0 = 8.854187 \times 10^{-12} \text{ F m}^{-1} \text{ — vacuum permittivity}$$

$$\mu_0 = 4\pi \times 10^{-7} \text{ N } A^{-2} \text{ — vacuum permeability (exact)}$$

$$c = 2.99792458 \times 10^{8} \text{ m } s^{-1} \text{ — speed of light in vacuum}$$

$$e = 1.602176487(40) \times 10^{-19} \text{ C — unit charge}$$

$$m_e = 9.10938215(45) \times 10^{-31} \text{ Kg — electron rest mass}$$

$$m_p = 1.672621637(83) \times 10^{-27} \text{ Kg — proton rest mass}$$

$$m_n = 1.674927729(28) \times 10^{-27} \text{ Kg — neutron rest mass}$$

$$r_0 = \frac{e^2}{4\pi\epsilon_0 m c^2} = 2.82 \times 10^{-15} \text{ m — classical electron radius}$$

$$\mu_N = \frac{e\hbar}{2m_p} = 5.05078324(13) \times 10^{-27} \text{ JT}^{-1} \text{ — nuclear magneton}$$

$$\gamma_N = -1.9130418 \text{ — neutron gyromagnetic ratio}$$

$$\mu_B = \frac{e\hbar}{2m_e} = 9.27400915(23) \times 10^{-24} \text{ JT}^{-1} \text{ — Bohr magneton}$$