🏠 / **4th_Year** / **Product_Characterisation** / **3**

# 3. Scattering

Introduction to Scattering

Scattering has been holding paramount importance in the realm of physics, as it serves as the foundation for one of the most pervasive tools in the field. Countless breakthroughs in nuclear and atomic physics have been achieved through the meticulous examination of scattering experiments. Iconic discoveries, including Rutherford's remarkable identification of the atomic nucleus and the subsequent revelation of sub-atomic particles like quarks, owe their existence to the insights gleaned from scattering phenomena. In the domain of low energy physics, scattering phenomena continue to serve as the gold standard for investigating solid-state systems. Techniques such as neutron, electron, and X-ray scattering play a vital role in probing and comprehending the intricacies of such systems.

In scattering experiments, radiation, such as photons, electrons, or neutrons, is directed towards a sample or target material. As the radiation interacts with the atoms, molecules, or particles in the material, it undergoes scattering, resulting in a change in its direction, energy, or phase. Fundamentally, the scattering process itself is a manifestation of the interaction between radiation and matter, and thus the scattered radiation carries information about the nature, arrangement, and characteristics of the scattering material.

Interaction Between Radiation and Matter

When radiation interacts with matter, several outcomes are possible: reflection, transmission, absorption, and scattering.

Reflection occurs when radiation encounters a surface and bounces back, changing its direction. The angle of reflection is equal to the angle of incidence, obeying the law of reflection.
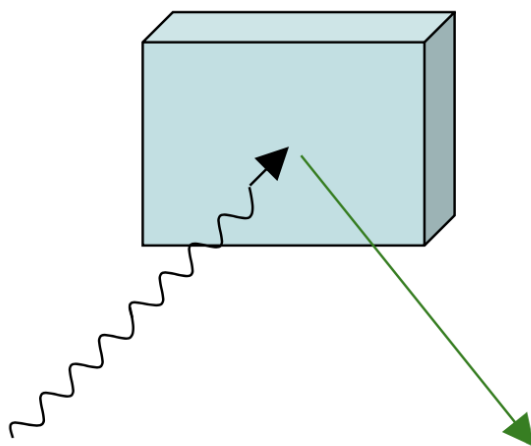
Transmission refers to the passage of radiation through a material without significant interaction or loss of energy.
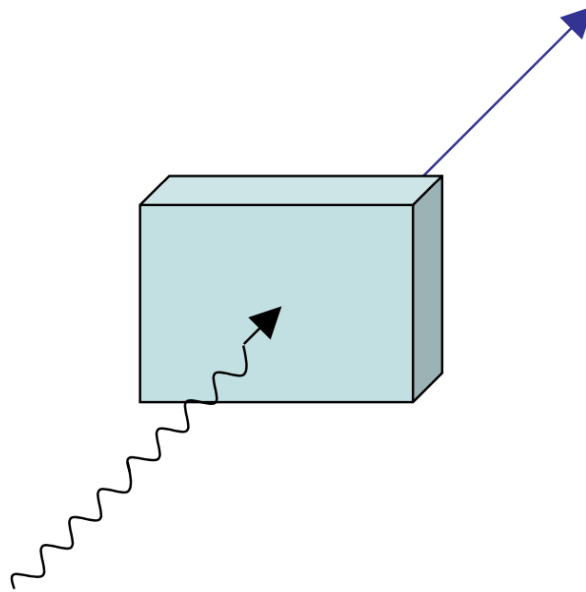

Refraction is a common mechanism of transmission that occurs when the properties of the two media, such as their optical densities, differ. When radiation encounters the interface between two media, it experiences a change in speed and direction due to the variation in the refractive index of the media. The refractive index n_i is a property of a material i that quantifies how much the light speed c is reduced when it travels through that material with speed v_i.

$$n_i \equiv \frac{c}{v_i}$$

Snell's Law mathematically describes the relationship between the angles of incidence and refraction:

$$n_i \sin(\theta_i) = n_r \sin(\theta_r)$$
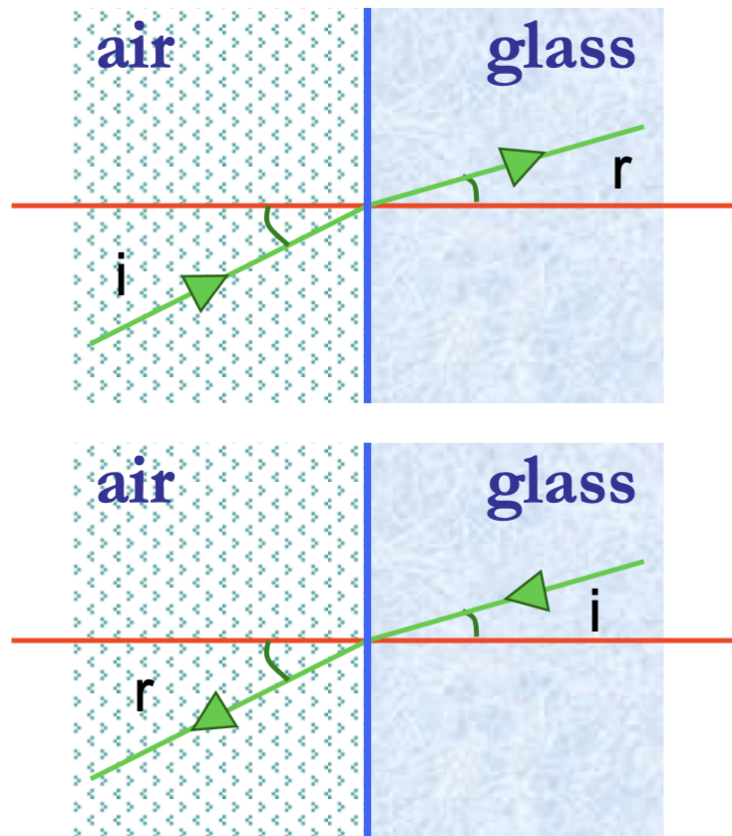
where i and r represents the incident and refracted ray, respectively.

Absorption takes place when radiation transfers its energy to the atoms or molecules of the material, leading to excitation or ionisation. This process can result in the heating of the material or the initiation of chemical reactions.
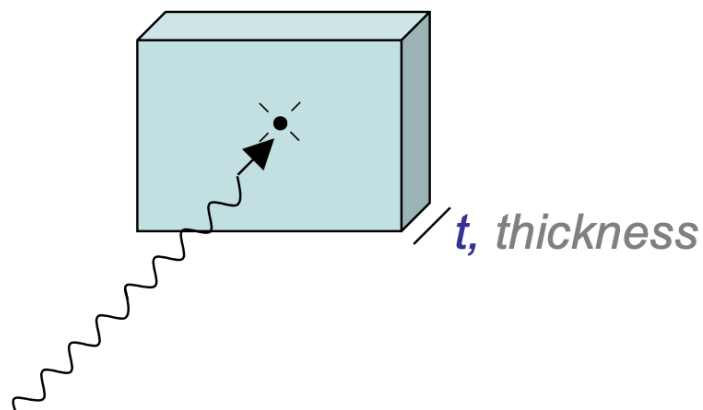

The Beer-Lambert Law is a fundamental relationship that quantitatively describes the absorption of light by a homogeneous medium, which describes the decay in intensity of light as it passes through an absorbing medium:

$$I(x) = I(0) \exp(-\mu x)$$

where $I(x)$ is the transmitted light intensity, $I(0)$ is the incident light intensity, μ is the attenuation coefficient that characterises the absorption capability of the material at a specific wavelength and x is the path length.

Finally, scattering occurs when radiation interacts with the atoms or molecules of the material and changes its direction. This can happen through elastic scattering, where the radiation retains its energy but changes its path, or inelastic scattering, where the radiation transfers some of its energy to the material during the interaction.
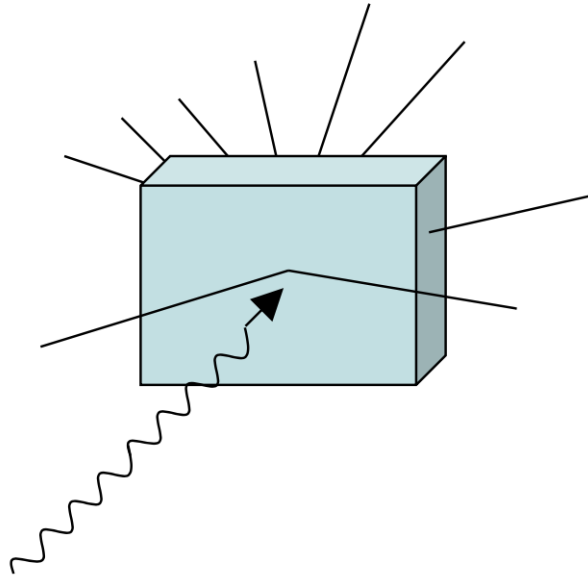
Diffraction is a specific type of scattering when radiations encounter an obstacle or an aperture that is comparable in size to their wavelength. which is the bending and spreading of waves as they pass through or around an object. It involves the bending and spreading of waves as they pass through or around the object, resulting in changes in direction and intensity. For instance, when a beam of X-ray encounters a regular crystalline lattice,
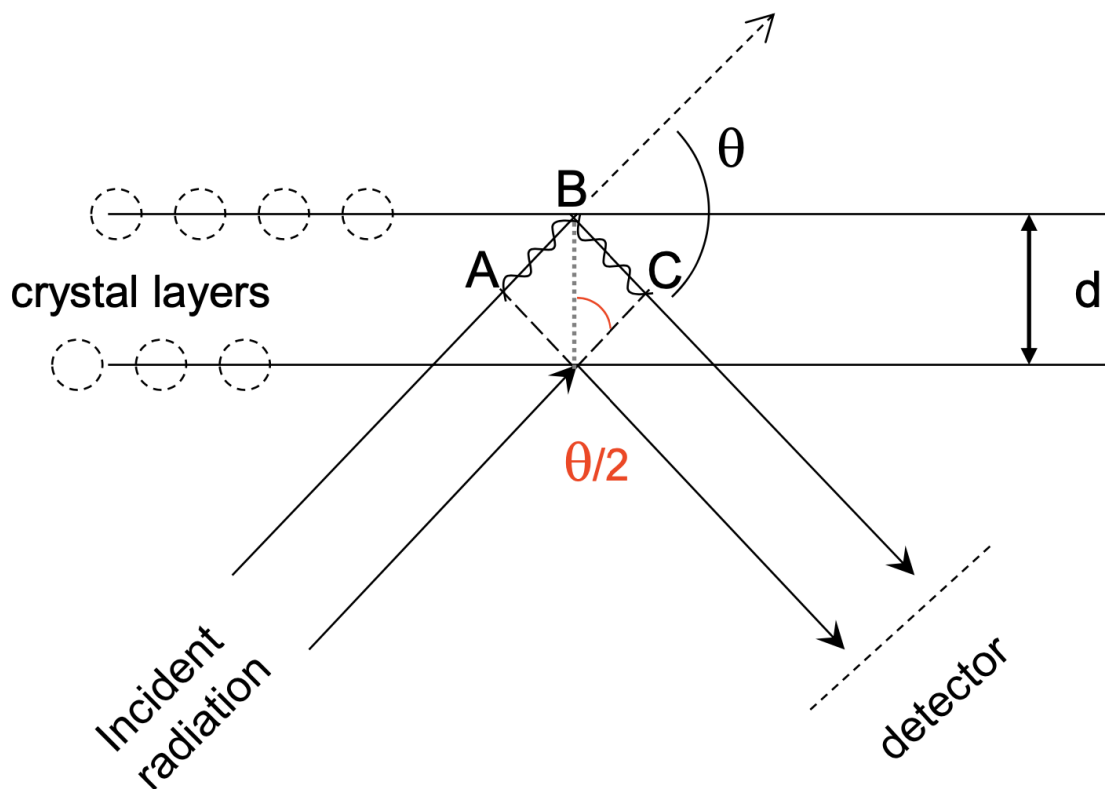
the incident waves encounter the lattice and are diffracted. The diffracted waves interfere with each other, creating a pattern of bright and dark spots known as a diffraction pattern. Constructive interference occurs when the diffracted waves that have taken different paths within the crystal lattice recombine and reinforce each other. This reinforcement results in regions of increased wave intensity in the diffraction pattern, corresponding to bright spots.
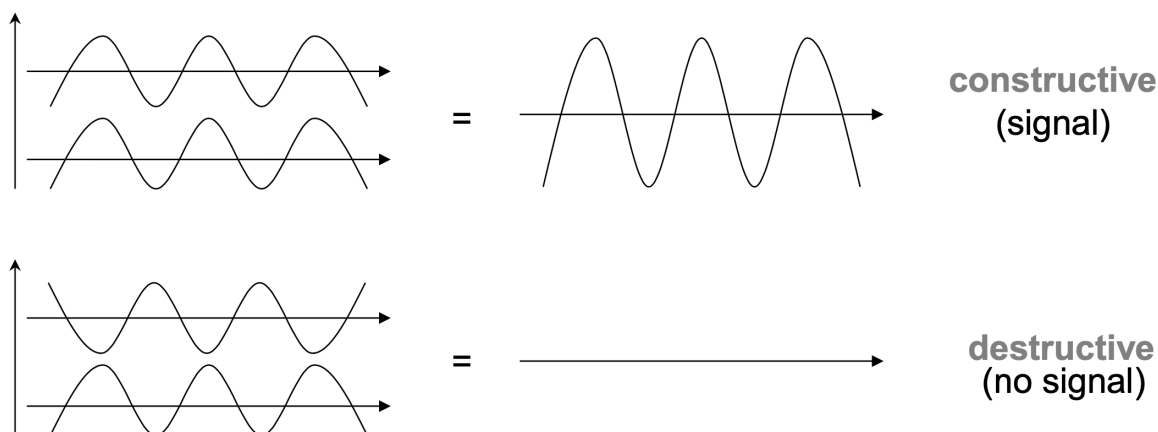
The length of the additional path taken is $AB + BC = 2d\sin\left(\frac{\theta}{2}\right)$, where d is the spacing between the crystal layers and θ is the scattering angle. As constructive interference occurs when the waves are in phase with each other, i.e., when the phase difference between the waves is a multiple of the wavelength λ. Therefore, the condition for constructive interference in a crystal lattice is:

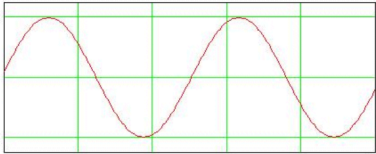$$2d\sin\left(\frac{\theta}{2}\right) = n\lambda$$

where n is an integer representing the order of diffraction. This is the Bragg's law for conditions for constructive interference in crystal lattice diffraction.

Finally, it is worth noting that the Fourier transform is a crucial and powerful mathematical tool for analysing and interpreting scattering patterns. It allows us to examine the spatial frequency components present in the scattered waves and extract valuable information about the scattering object or structure.

$$H(f) = \int_{-\infty}^{\infty} h(t)\, e^{2\pi i f t}\, dt$$

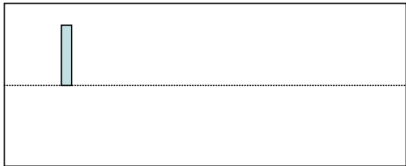$$h(t) = \int_{-\infty}^{\infty} H(t)\, e^{-2\pi i f t}\, df$$

Fourier transform:

$$\Phi(H(f), t) = h(t)$$
$$\Phi^{-1}(h(t), f) = H(f)$$


$$h(t) = A e^{i(t + \phi)}$$

$$H(f) = \int_{-\infty}^{\infty} h(t)\, e^{2\pi i f t}\, dt$$

$$H(f) = 0 \qquad \text{if } (ft \neq 1)$$

$$H(f) = A\, e^{i\phi} \qquad \text{if } (ft = 1)$$

For example, scattering patterns, such as those observed in X-ray scattering or electron diffraction, consist of a series of bright and dark spots or fringes. These patterns contain information about the spatial frequencies and amplitudes of the scattered waves. By applying the Fourier transform to the scattering pattern, the spatial frequency spectrum can be obtained, which reveals the specific spatial components that contribute to the scattering process. This helps in determining the size, shape, and arrangement of particles or structures responsible for scattering the waves.

In addition, the Fourier transform enables the mapping of the scattering information from the real space (where the object is located) to the reciprocal space, also known as Fourier space. Reciprocal space provides a convenient representation of the scattering phenomena, where each point in reciprocal space corresponds to a specific spatial frequency or scattering vector.
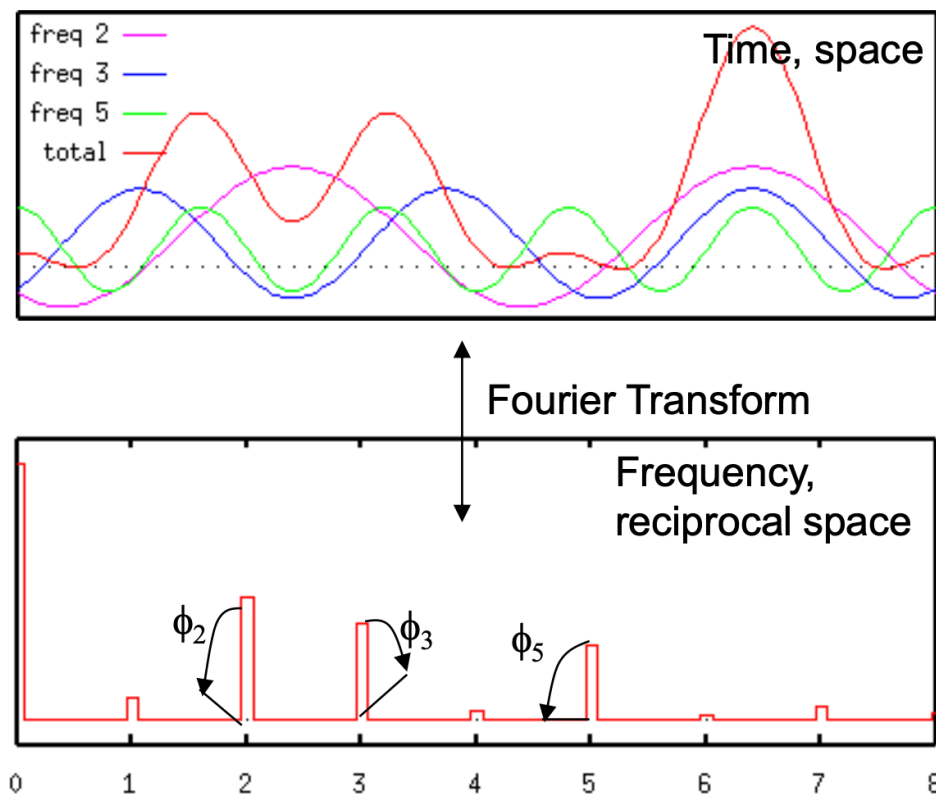
Small-angle Scattering

Small-angle scattering (SAS) is a scattering technique used to study the structures and properties of materials at the nanoscale. It involves the interaction of waves, such as light, X-rays, neutrons, or electrons, with particles or structures in a sample, resulting in the scattering of these waves at small angles relative to the incident beam. Consider the following SAS experiment:
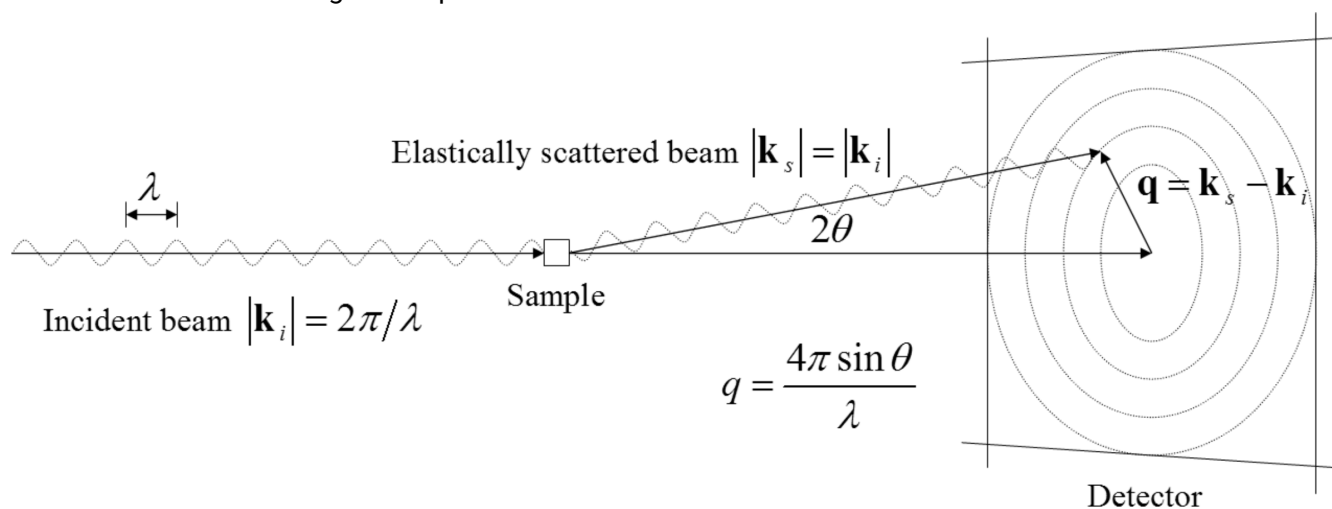
In terms of the experiment and theory, the fundamental principles remain the same for light, X-rays, and neutrons. The key difference lies in the physics of how each type of radiation interacts with matter:

- ‣ Light sources: light-based SAS techniques often employ visible or ultraviolet (UV) light sources, which are convenient and readily accessible, making them suitable for a wide range of samples. Light-based SAS techniques include small-angle light scattering (SALS) and dynamic light scattering (DLS). These techniques are particularly useful for studying dilute solutions, macromolecules, colloids, and nanoparticle suspensions.

- ‣ X-ray sources: X-ray-based SAS techniques, such as small-angle X-ray scattering (SAXS), utilise high-energy X-rays produced by synchrotron radiation sources or X-ray generators. X-rays have shorter wavelengths than visible light, allowing for higher resolution and the ability to probe smaller sample features. SAXS is commonly employed to study materials with larger nanostructures, such as nanoparticles, polymers, complex fluids, and biomolecular assemblies.

- ‣ Neutron sources: neutron-based SAS techniques, such as small-angle neutron scattering (SANS), use beams of neutrons produced by nuclear reactors or spallation sources. Neutrons are neutral particles with unique interaction properties, allowing them to penetrate deeply into samples and provide information about the internal structure of materials. SANS is particularly useful for studying materials with hydrogen-rich components, such as biological macromolecules, polymers, and magnetic materials.

The measurement in scattering experiments focuses on the coherent scattering from the sample. This is where the scattered waves maintain a fixed phase relationship with each other, and coherent scattering provides information about the structure and properties of the sample. In the SAS experiment, $\mathbf{q}$ is the scattering vector, representing the momentum transfer between the incident and scattered particles or waves. It provides information about the spatial arrangement and distribution of scattering centres within a sample. Mathematically, $\mathbf{q}$ is defined as the difference between the wave vector of the scattered radiation ($\mathbf{k_s}$) and the wave vector of the incident radiation ($\mathbf{k_i}$):

$$\mathbf{q} = \mathbf{k_s} - \mathbf{k_i}$$

The magnitude of the scattering vector, $|\mathbf{q}|$, is related to the scattering angle and the wavelength of the incident radiation:

$$|\mathbf{q}| = \frac{4\pi \sin\theta}{\lambda}$$

which determines the spatial resolution of the scattering experiment and provides information about the characteristic length scales of the scattering structures within the sample. In simple terms, $\mathbf{q}$ can be thought of as a measure of how far the scattered waves deviate from the direction of the incident waves. A larger $|\mathbf{q}|$ corresponds to a larger deviation or larger momentum transfer between the incident and scattered particles. For the sake of simplicity, we will represent $|\mathbf{q}|$ as q.

Moreover, the characteristic length scale d, which represents "interparticle spacing" or "interplanar spacing" depending on the context, is:

$$d = \frac{2\pi}{q}$$

The value of d provides insights into the size of sample features detectable. As d is proportional to λ, radiation of small wavelength λ is capable of capturing smaller sample features. This is, in fact, in agreement

with the phenomenon of diffraction. According to the Bragg's law, smaller wavelength radiation can interact with smaller features and yield a smaller diffraction angle. Consequently, using radiation with a smaller wavelength enables smaller angles of scattering to be probed, allowing for the detection of finer structural details in the sample.

However, the above finding is subject to one condition: provided there is sufficient contrast. Light, X-ray and neutron scattering probe different length scales of materials and have different sources of contrast, deriving from their different wavelength and interaction with a sample. While the wavelength defines what length scales are observable, contrast between constituents of a sample is needed for their structure to be visible.
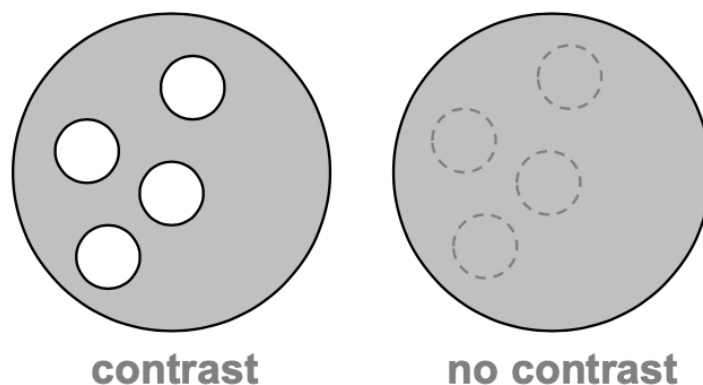
Seeing objects requires a difference in refractive index between the object and its surroundings. For instance, glass beads ($n \approx 1.5$) nearly disappears in toluene ($n \approx 1.49$) but is visible in air ($n \approx 1$). Any radiation can be used in the same way as light to "see". The requirement is a difference between the way the radiation interacts with the atoms and molecules in the object and its surroundings, i.e., contrast.

Back to SAS. Furthermore, the assumption of elastic scattering is usually made to simplify the models. In elastic scattering, the incident radiation interacts with the sample, and the scattered radiation retains the same energy as the incident radiation. However, the direction of the scattered radiation can be different from the incident direction, leading to a non-zero scattering vector. Scattering experiments are often conducted using high-energy radiations, and these high-energy particles can induce significant changes in the sample, such as heating or chemical reactions, if energy transfer occurs. However, extensive research has demonstrated that inelastic scattering contribution to SAS is negligible.

For an ensemble of identical, randomly oriented particles, the intensity of coherently, elastically scattered radiation is dependant only upon q:

$$I(q) = N(\Delta\bar{\rho}V)^2 P(q)S(q)$$

where $I(q)$ represents the intensity of the scattered radiation. N represents the number of molecules per unit volume (number density). $\Delta\bar{\rho} = \langle\rho(\mathbf{r})\rangle - \bar{\rho}_s$ represents the contrast, which is the difference in scattering density between the scattering particle and the surrounding solvent. V represents the molecular volume, which is the volume occupied by a single molecule.

$P(q)$ represents the form factor, which refers to a mathematical function that describes the scattering intensity distribution of a particle or a structure. It provides information about the shape, size, and internal structure of the scattering object. The form factor is obtained by calculating the Fourier transform of the spatial distribution of electron or nuclear densities within the scattering object. Different types of form factors

are used depending on the nature of the scattering object. For example, in X-ray and neutron scattering, common form factors include the Guinier form factor, the Debye form factor, and the Porod form factor. The form factor of a spherical particle can be described by the Debye formula, which is given by:

$$P(q) = \frac{3(\sin(qR) - (qR)\cos(qR))}{(qR)^3}$$

where R is the radius of the sphere.

Form factor *P*

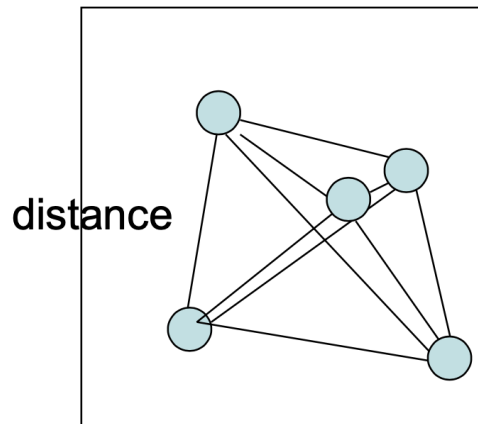'sample'
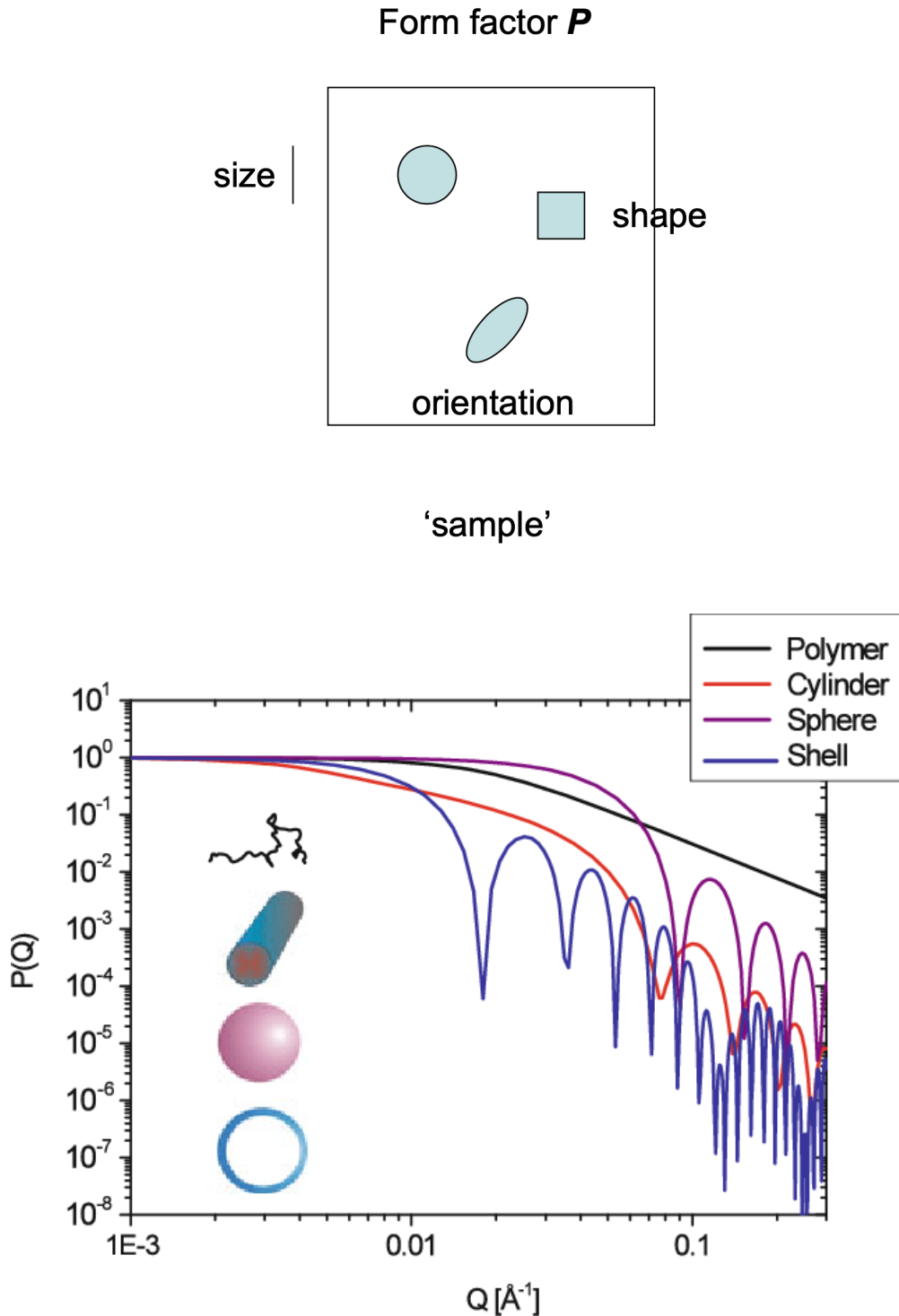
$S(q)$ represents the structure factor, which takes into account the inter-particle correlation distances and describes the collective scattering behaviour of all the particles in the ensemble, such as their periodicity, packing arrangements, and the presence of any correlations or ordering. The structure factor is the Fourier

transform of the correlation function, which describes the spatial distribution of scattering objects in the sample. It characterises how the scattered waves from individual scattering objects interfere with each other. In other words, it quantifies the constructive and destructive interference of scattered waves due to the relative positions and orientations of the scattering objects.

Structure factor *S*

'sample'
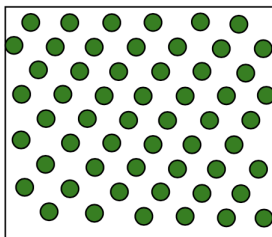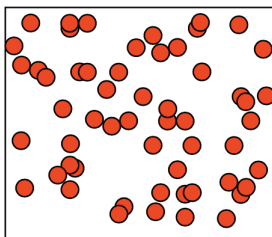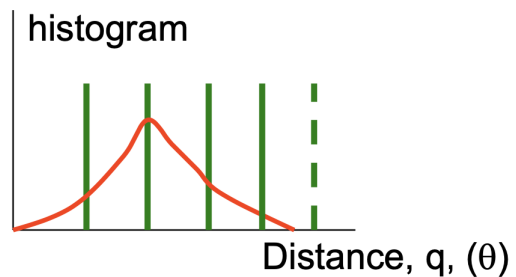
Light Scattering

Low Angle Light Scattering

Two important types of light scattering are Rayleigh scattering and Mie scattering.

Rayleigh scattering specifically refers to the elastic scattering of light by particles or molecules that are much smaller in size compared to the wavelength of the incident light. This type of scattering occurs when the particles are smaller than approximately 1/10 of the wavelength of the light. Rayleigh scattering intensity is strongly dependent on the size of the particles and inversely proportional to the fourth power of the

wavelength of light. The intensity I of light scattered by a single small particle from a beam of unpolarised light of wavelength λ and intensity I_0 is given by:

$$I = I_0 \frac{1 + \cos^2 \theta}{2R^2} \left(\frac{2\pi}{\lambda} \right)^4 \left(\frac{n^2 - 1}{n^2 + 2} \right)^2 \left(\frac{d}{2} \right)^6$$

where R is the distance between the particle and the observer, θ is the scattering angle, n is the refractive index of the particle, and d is the diameter of the particle. As a result of this, shorter wavelengths of light (such as violet and blue) are scattered more strongly than longer wavelengths (towards the red end of the visible spectrum). This phenomenon is why the sky appears blue during the day, as the shorter blue wavelengths are scattered by the molecules in the Earth's atmosphere. During sunrise and sunset, the path length of sunlight through the atmosphere is longer, resulting in greater scattering of shorter wavelengths and giving rise to the orange colours observed.

It is important to note that Rayleigh scattering only applies to particles that are smaller than approximately 1/10 of the wavelength of light. This limitation means that microemulsions, nanoparticles, and polymers can be sized using Rayleigh scattering. However, due to the strong dependence on particle size d, experiments utilising Rayleigh scattering can be significantly affected by even very small amounts of dust or impurities.

Mie scattering is another type of light scattering that occurs when the size of the scattering particles is comparable to or larger than the wavelength of the incident light. The Mie Theory takes into account the optical properties of the particles, such as the refractive index, to model the scattering behaviour. Unlike Rayleigh scattering, which is limited to particles much smaller than the wavelength, Mie scattering can accurately describe the scattering of light by particles of various sizes. For instance, clouds are composed of water droplets or ice crystals suspended in the air, whose sizes are comparable to the wavelength of visible light. When sunlight passes through the cloud, the water droplets or ice crystals scatter the light in all directions. Mie scattering is the primary mechanism responsible for this scattering process, resulting in the diffusion of light and the appearance of a diffuse, white light from the cloud. Similarly, raindrops act as individual scattering particles in Mie scattering. When sunlight enters a raindrop, it undergoes refraction, internal reflection, and multiple reflections within the drop. Mie scattering within the raindrop causes the incident sunlight to disperse into its constituent colours. Each colour is refracted at a slightly different angle, leading to the separation of colours within the raindrop. When the dispersed light exits the raindrop, it undergoes another refraction, leading to further separation of colours. The separated colours then reach the observer's eye, forming a circular arc of colours in the sky known as a rainbow.

For particles larger than the wavelength of light, the light scatters from the edges of the particles. The Mie equation reduces to the Fraunhofer equation and the Fraunhofer diffraction theory can be applied to analyse the scattering pattern. Note that, if the particles approach or become smaller than the wavelength of light, the scattering behaviour changes. More of the light intensity is scattered to higher angles and back-scattered. In such cases, the Mie scattering theory is required to accurately describe the scattering phenomenon.

With these, a single algorithm to be used to analyse the scattering data across the entire size range. This is the low angle light scattering (LALS) technique, which is typically used to determine the size distribution of particles or molecules in a sample. The angles at which the light is scattered depend on the size of the particles. Larger particles scatter light at relatively smaller angles, while smaller particles scatter light at larger angles. By measuring the intensity of scattered light at different angles, information about the relative amounts of particles of different sizes can be obtained. The intensity distribution provides insights into the size distribution of the particles in the sample. A light diffraction technique involves the following components:

‣ Laser: as a source of coherent and intense light with a fixed wavelength. The laser emits a narrow beam of light that is directed towards the sample being analysed.

‣ Sample presentation system: ensures that the material being tested passes through the laser beam in a homogeneous stream of particles that are uniformly dispersed. This system helps create a controlled and reproducible state of dispersion for accurate measurements. The sample may be in the form of a liquid suspension, dry powder, or aerosol, depending on the nature of the material being analysed.

‣ Detectors: positioned at various angles around the sample, which measure the light pattern produced by the interaction of the laser beam with the particles in the sample at different angles, covering a wide range of scattering angles.

Dynamic Light Scattering

Currently, available techniques cover particle sizes ranging from greater than 1 μm to less than 50 nm. For particles falling within this intermediate size range, dynamic light scattering is utilised.

Dynamic light scattering (DLS), also known as quasi-elastic light scattering (QELS) or photon correlation spectroscopy (PCS), is a technique used to analyse the properties of macromolecules or particles in solution. When macromolecules or particles are in solution, they experience random motion due to the collisions with solvent molecules. (Brownian motion, a result of being buffeted by the surrounding solvent molecules). As light interacts with the moving macromolecules or particles, their motion imparts randomness to the phase of the scattered light. When the scattered light from multiple particles is combined, the changing phases can lead to constructive or destructive interference, resulting in time-dependent fluctuations in the intensity of the scattered light. In a DLS measurement, a fast photon counter is used to measure the time-dependent fluctuations in the intensity of the scattered light. These fluctuations are directly related to the rate of diffusion of the molecules or particles through the solvent. By analysing the characteristics of these fluctuations, such as their magnitude and frequency, it is possible to determine a hydrodynamic radius for the sample, which represents an effective size of the molecule or particle in solution. It takes into account not only the physical size of the molecule but also its interactions with the surrounding solvent molecules, and provides information about the size and behaviour of the particles, such as their aggregation state or interactions with other molecules.
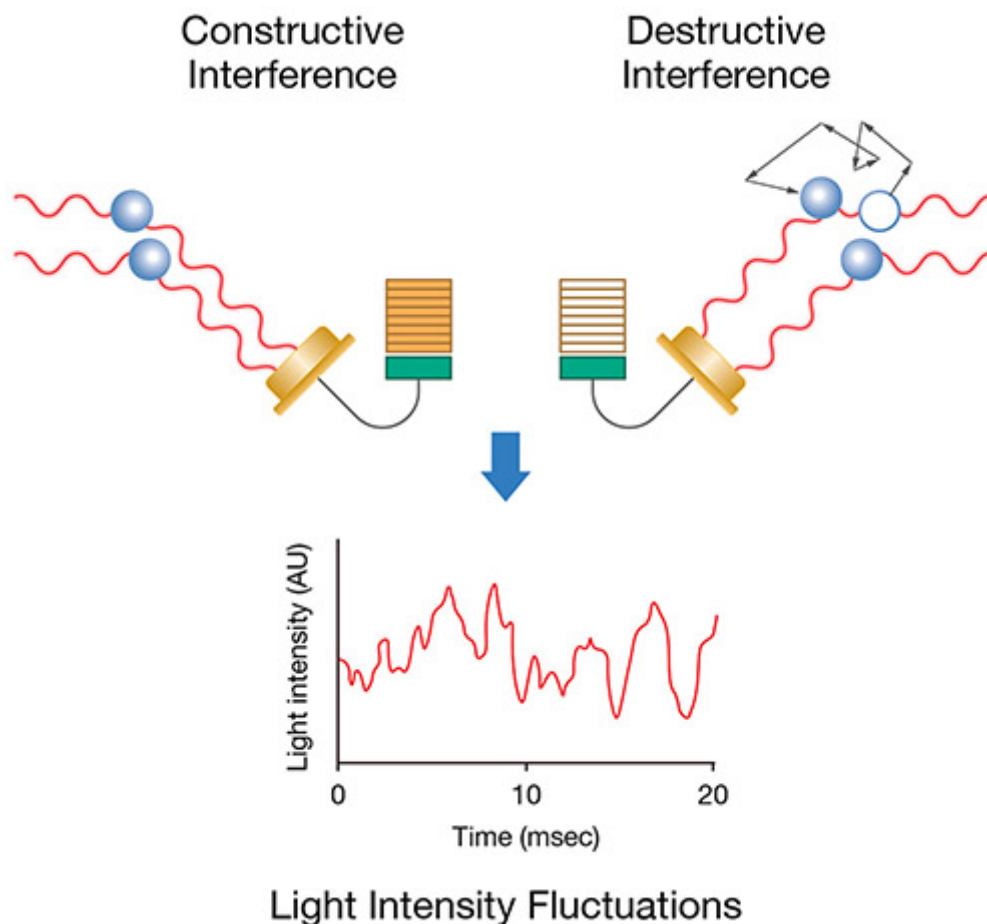
Light Intensity Fluctuations

Moreover, particles in an intermediate size range may be prone to aggregation or flocculation, especially when there are variations in environmental conditions such as temperature or pH. DLS can monitor changes in the size distribution over time, helping to assess the stability of the particles and provide insights into these interactions by measuring changes in the diffusion behaviour and hydrodynamic radius of the particles.

The second-order autocorrelation function, also known as the intensity autocorrelation function, is used to analyse the fluctuations in scattered light intensity over time. This is denoted as $g^2(t)$ and is defined as the normalised autocovariance function of the scattered intensity $I(t)$ at a given time delay t. Mathematically:

$$g^2(\tau) = \frac{\langle I(t) \cdot I(t+\tau)\rangle}{\langle I(t)\rangle^2} = B + \beta \exp(-2\Gamma\tau)$$

where τ is the time delay. $I(0)$ refers to the scattered intensity at zero-time delay, the average intensity of the scattered light from the particles in the sample without any time delay or correlation. $<>$ denotes the ensemble average. This is a statistical operation that calculates the average value over a set of measurements or a distribution of particles. In the context of DLS, the ensemble average is used to obtain an average value of a property or variable by considering multiple measurements or multiple particles in the sample. B is the baseline of the correlation function at infinite delay, β is the correlation function amplitude at zero delay, and Γ is the decay rate.

This function describes the decay of correlations in the intensity fluctuations over different time scales. A nonlinear least squares fitting algorithm is used to fit the measured correlation function to the above equation to retrieve the correlation function decay rate Γ. Γ can be converted to the diffusion constant D for the particle via the relation:

$$D = \frac{\Gamma}{q^2}$$

Here, q is the magnitude of the scattering vector, and is given by

$$q = \frac{4\pi n_0}{\lambda}\sin\left(\frac{\theta}{2}\right)$$

where n_0 is the solvent refractive index, λ is the wavelength of the incident light, and θ is the scattering angle. The diffusion constant can be interpreted as the hydrodynamic radius r_h of a diffusing sphere via the Stokes-Einstein equation:

$$r_h = \frac{kT}{6\pi\eta D}$$

where k is Boltzmann's constant, T is the temperature in K, and η is the solvent viscosity.

Limitations

Finally, the limitations with light scattering include:

- Light scattering techniques are primarily effective for studying the scattering of light by individual particles. When multiple particles are present in a sample and interact with each other, the scattering patterns become more complex, making it challenging to interpret the results accurately. As a result, light scattering methods are typically suitable for analysing very dilute suspensions where particle interactions are minimal.

- Light scattering techniques, excluding DLS, are generally limited to the analysis of relatively large particles. These methods provide information about the size of the particles but do not offer insights into their chemical composition, shape, or internal structure. Therefore, when using conventional light scattering approaches, it is not possible to obtain detailed information about the nature or properties of the particles being studied.

When the particles or features of interest are smaller in size, or when more detailed information about their structures is desired, light scattering techniques using visible light may not be sufficient. Instead, other types of radiation with shorter wavelengths, such as X-rays or neutrons, are employed.

Neutron Scattering

Neutrons are subatomic particles that have zero electric charge and negligible electric dipole moment. This means they do not experience electromagnetic interactions like charged particles do (such as interacting with electric fields), but instead interact primarily through nuclear forces. Due to the short range of nuclear forces and the small size of nuclei compared to the distances between them, neutrons can travel relatively long distances in a material without being scattered or absorbed. This characteristic makes them highly penetrating

particles, capable of penetrating to depths of 0.1-0.01 m. Neutrons also have different interactions with matter compared to other types of radiation. Low-energy neutrons are attenuated (weakened) by materials like aluminium (Al) at a rate of about 1% per mm of travel. In contrast, X-rays are attenuated by more than 99% per mm. This demonstrates the relatively lower interaction of neutrons with matter compared to X-rays.

Wave-particle duality suggests that neutrons also exhibit properties of plane waves. They can be scattered elastically or inelastically when interacting with atomic nuclei. Again, the elastic, coherent scattering of neutrons, where they change direction but not magnitude, gives rise to a small-angle scattering (SAS). The neutron scattering power of an atom is denoted as b and is measured in units of length. It represents the radius of the nucleus as seen by the neutron, hence the strength of the interaction between neutrons and the nucleus of the atom:

$$s = 4\pi b^2$$

where s is the scattering cross section of an atom. The cross section gives a measure of the probability of a neutron being scattered by the nucleus of an atom. Thus, the larger the value of b, the stronger the neutron-nucleus interaction.

The value of b for certain nuclei can depend on the energy of the incident neutrons. This is because the scattering process can form compound nuclei with energies close to excited nuclear states. As a result, the neutron-nucleus interaction strength can vary with the energy of the incident neutrons. Such energy dependence of b can give rise to a resonance phenomenon. This means that certain energies of incident neutrons can lead to enhanced scattering or absorption of neutrons by the nucleus. In these cases, b can have both real and imaginary components. The real part corresponds to the scattering process, while the imaginary part corresponds to neutron absorption. Moreover, the value of b for each nucleus cannot be reliably calculated from fundamental constants. It needs to be determined experimentally through neutron scattering experiments and measurements. Experimental techniques are used to determine the interaction strength between neutrons and the nucleus for different isotopes.

As aforementioned, in terms of the experiment and theory, the fundamental principles for SAS remain the same for light, X-rays, and neutrons. The key difference lies in the physics of how each type of radiation interacts with matter. Therefore, the basic scattering equation

$$I(q) = N(\Delta\bar{\rho}V)^2 P(q)S(q)$$

holds for neutron scattering. The average scattering length density for a particle is simply the sum of the scattering lengths b multiplied by the number density. Inter-particle distance correlations between charged molecules gives a non-unity structure factor $S(q)$ term that is concentration dependent.

From a semi-classical point of view, the incoming (or initial) neutron can be described as a (complex) plane wave:

$$\psi_i(\mathbf{r}) = \frac{1}{\sqrt{Y}}\exp(i\mathbf{k}_i \cdot \mathbf{r})$$

where $Y = L^3$ is a normalisation constant, implying that the density of the incoming neutron wave is $|\psi_i|^2 = 1/Y$, and can be identified as the (large) normalisation volume for the state which is assumed

enclosed in a cubic box with a side length L. By the de-Broglie relationship, the velocity of a neutron described by a plane wave is

$$v = \frac{\hbar k_i}{m_\mathrm{n}}$$

where k_i is the wavenumber, $m_\mathrm{n} = 1.675 \cdot 10^{-27}$ kg is the mass of the neutron. The corresponding incoming neutron flux is:

$$\Psi_\mathrm{i} = |\psi_\mathrm{i}|^2 v = \frac{1}{Y}\frac{\hbar k_\mathrm{i}}{m_\mathrm{n}}$$

If we consider the idealised situation where a neutron with a well-defined velocity is scattered by a single nucleus, labelled j, which is (somehow) fixed in position. The scattered neutron can be described as a spherical wave leaving the nucleus, which is centred at $\mathbf{r}_j$:
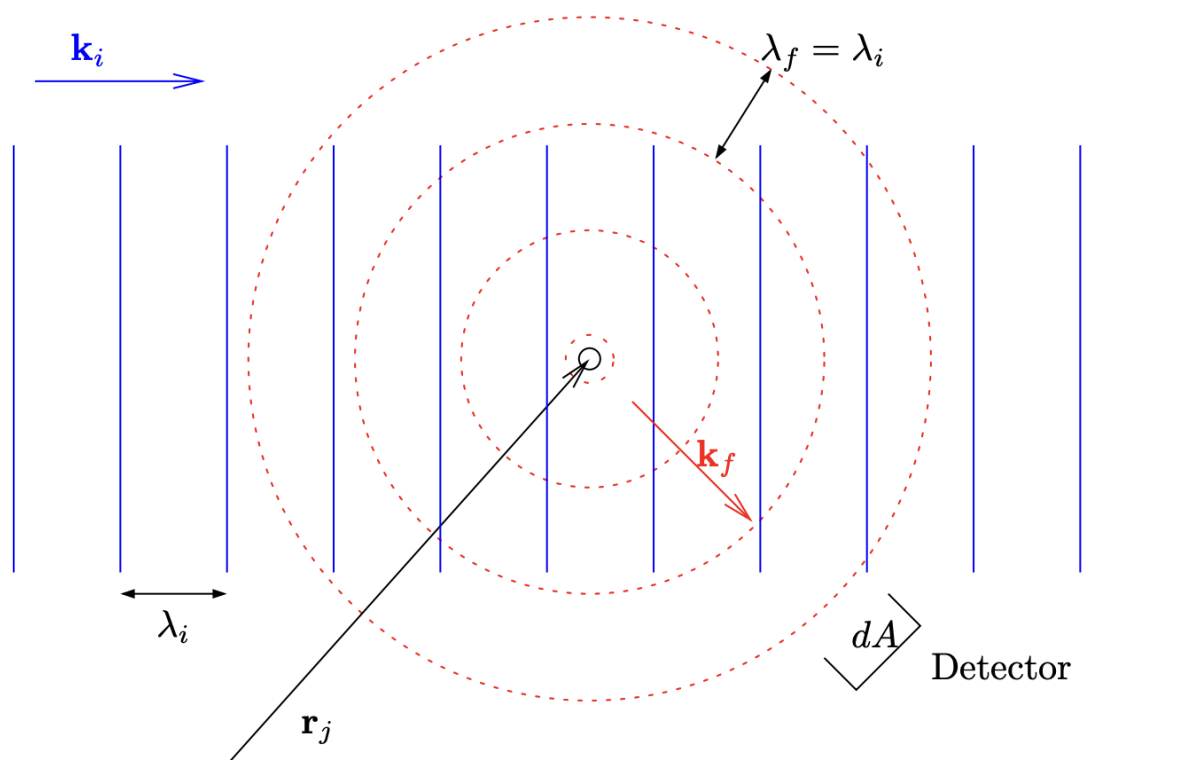

Figure 2.1: An illustration of the initial wave, ψ_i, of wavelength λ_i, and the final wave, ψ_f, of wavelength λ_f, describing a neutron scattering off a single nucleus with positive scattering length (meaning a phase shift of π). The area, dA, for measuring the flux of the outgoing neutrons is the detector area as sketched.

The scattered, or final, wave function is:

$$\psi_\mathrm{f}(\mathbf{r}) = \psi_\mathrm{i}(\mathbf{r}_j)\frac{-b_j}{|\mathbf{r} - \mathbf{r}_j|}\exp(ik_\mathrm{f}|\mathbf{r} - \mathbf{r}_j|)$$

This above equation is valid only "far" from the nucleus, i.e. for $|\mathbf{r} - \mathbf{r}_j| \gg b$, The minus sign is a convention chosen so that most nuclei will have a positive value of b_j. In experiments, r is typically of the order 1 m. In addition, we choose to place origo close to the centre of the "relevant" part of the sample. Hence, the nuclear coordinate, r_j, is typically of the order $1\ \mathrm{mm}$ or less, and the density of outgoing neutrons can be approximated by $|\psi_\mathrm{f}|^2 \approx b_j^2 / \left(Y r^2\right)$, omitting $\mathbf{r}_j$ in the denominator. The number of neutrons per second intersecting a small surface, dA, is $v|\psi_\mathrm{f}|^2 dA = v b_j^2 / \left(Y r^2\right) dA$. Using $v = \frac{\hbar k_\mathrm{i}}{m_\mathrm{n}}$ and the expression for solid angle $d\Omega = dA/r^2$, we reach

$$\text{number of neutrons per second in } d\Omega = \frac{1}{Y} \frac{b_j^2 \hbar k_\mathrm{f}}{m_\mathrm{n}} d\Omega$$

Since the scattering nucleus is fixed, energy conservation requires that the energy of the neutron is unchanged. In this elastic scattering, we therefore have $k_\mathrm{i} = k_\mathrm{f}$. Using the definition of the scattering cross section:

$$\frac{d\sigma}{d\Omega} = \frac{1}{\Psi} \frac{\text{number of neutrons scattered per second into solid angle } d\Omega}{d\Omega}$$

and the previously derived expression for the incoming neutron flux

$$\Psi_\mathrm{i} = |\psi_\mathrm{i}|^2 v = \frac{1}{Y} \frac{\hbar k_\mathrm{i}}{m_\mathrm{n}}$$

leads to the simple expression for the differential cross section for one nucleus:

$$\frac{d\sigma}{d\Omega} = b_j^2$$

giving the total scattering cross section of

$$\sigma = 4\pi b_j^2$$

Note that this same expression can also be obtained from a quantum mechanics point of view. The interaction responsible for the scattering can be described by an operator denoted $\hat{V}$. The scattering process itself is described by the Fermi Golden Rule [18]. This gives the rate of change between the neutron in the single incoming state, $|\psi_\mathrm{i}\rangle$ and a final state, $|\psi_\mathrm{f}\rangle$, where $|\psi_\mathrm{f}\rangle$ resides in a continuum of possible states.

$$W_{\mathrm{i}\to\mathrm{f}} = \frac{2\pi}{\hbar} \frac{dn}{dE_\mathrm{f}} \left| \left\langle \psi_\mathrm{i} | \hat{V} | \psi_\mathrm{f} \right\rangle \right|^2$$

The interaction between the neutron and the nuclei is expressed by the Fermi pseudopotential:

$$\hat{V}_j(\mathbf{r}) = \frac{2\pi\hbar^2}{m_\mathrm{n}} b_j \delta\left(\mathbf{r} - \mathbf{r}_j\right)$$

Thus,

$$
\begin{aligned}
\left\langle \psi_\mathrm{f} \left| \hat{V}_j \right| \psi_\mathrm{i} \right\rangle &= \frac{2\pi\hbar^2}{m_\mathrm{n}} b_j \int \exp(-i\mathbf{k}_\mathrm{f} \cdot \mathbf{r}) \delta\left(\mathbf{r} - \mathbf{r}_j\right) \exp(i\mathbf{k}_\mathrm{i} \cdot \mathbf{r}) d^3\mathbf{r} \\
&= \frac{2\pi\hbar^2}{m_\mathrm{n}} b_j \exp(i\mathbf{q} \cdot \mathbf{r}_j)
\end{aligned}
$$

More information about the underlying principles and mechanics of neutron scattering can be found [here](#) ☐ .

For a single particle in solution, $S(q) = 1$. Again, $\Delta\bar{\rho} = \langle \rho(\mathbf{r}) \rangle - \bar{\rho}_s$, which highlights the importance of contrast and the technique of contract matching, which is also known as solvent matching. This is a technique used to selectively study specific components of a complex system by manipulating the contrast between different parts of the system. By adjusting the scattering length density of a component of interest to match that of the surrounding solvent, contrast matching can be achieved. This means that the component of interest becomes "invisible" to the neutrons, as its scattering contribution is effectively cancelled out by that of the solvent. The scattering length density of the component of interest is typically adjusted by either selectively deuterating (replacing hydrogen with deuterium) or protonating (replacing deuterium with hydrogen) specific parts of the molecule. Deuterium and hydrogen have different scattering lengths, allowing for control over the contrast between the component and the solvent.

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