Neutron Scattering Theory
— *an elementary guide*

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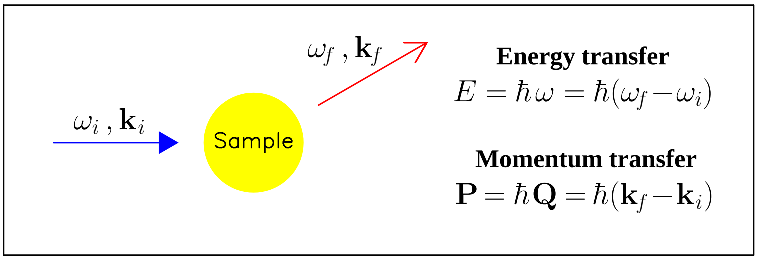
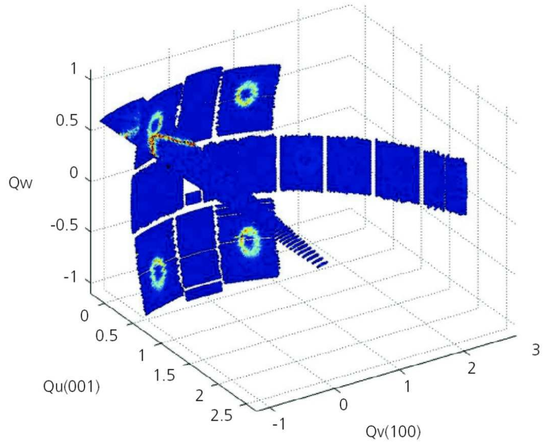
Basic Picture



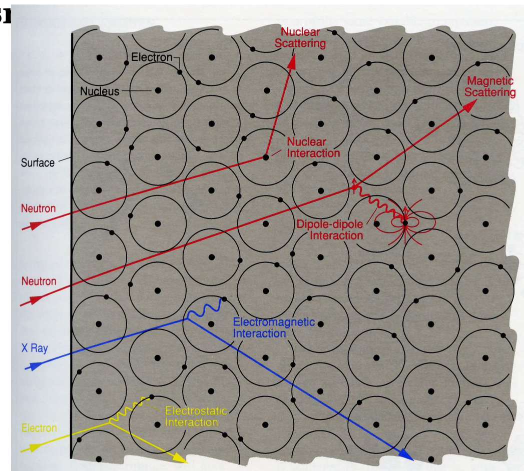
- Scattering function, $\mathrm{S}(\mathbf{Q},\omega)$, is 4-dimensional
  - $\mathrm{S_{el}}(\mathbf{Q}) = \mathrm{S}(\mathbf{Q},0)$
  - $\mathrm{S_{tot}}(\mathbf{Q}) = \int_{-\infty}^{\infty} \mathrm{S}(\mathbf{Q},\omega)\,\mathrm{d}\omega$

Scattering Function



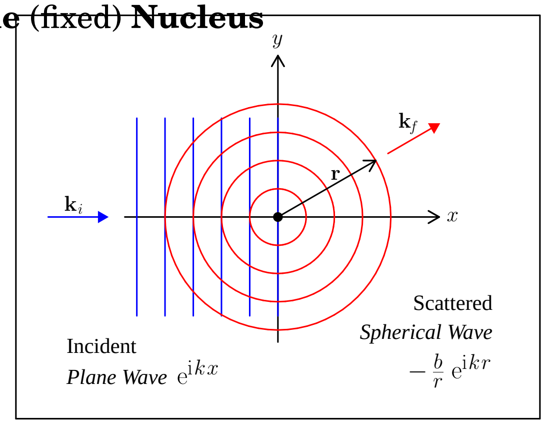
Kinematics: $\mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i$ and $\omega = \frac{\hbar}{2m}\left(k_f^2 - k_i^2\right)$

Interaction Mechanism



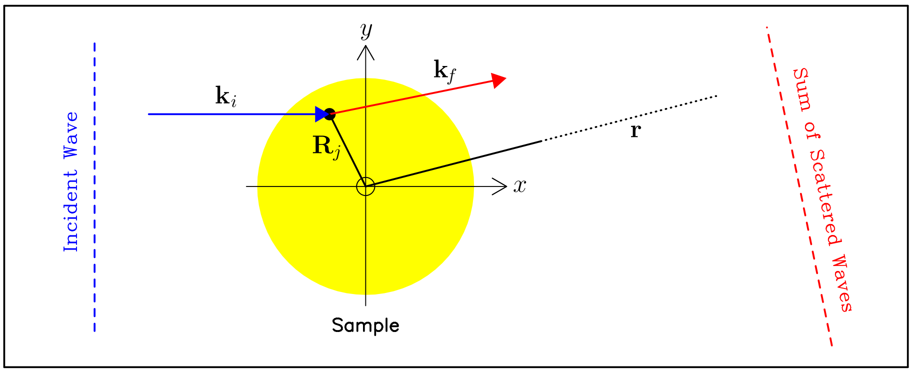
- Neutrons interact with
  - atomic nuclei via the short-range (fm) strong force;
  - unpaired orbital electrons via a magnetic dipole interaction.

Scattering by a Single (fixed) Nucleus



- Elastic scattering ($\omega = 0$): $\omega = 0 \;\Rightarrow\; |\mathbf{k}_i| = |\mathbf{k}_f| = k = \frac{2\pi}{\lambda}$
- b is called the neutron scattering length.
  - TWO values for nuclei with non-zero spin.
  - Cross-section $\sigma = 4\pi b^2$.

Scattering from Many Nuclei



Relative to the origin, the contribution of the scattered wave from atom j is

$$-\frac{b_j}{|\mathbf{r}-\mathbf{R}_j|}\,e^{i\mathbf{k}_f\bullet(\mathbf{r}-\mathbf{R}_j)}\;e^{i\mathbf{k}_i\bullet\mathbf{R}_j}$$

Neutron Scattering and Fourier Transforms

Since the sample is much smaller than the flight-path to the detectors,

$$\Psi_{\text{scat}} = -\frac{\mathrm{e}^{\mathrm{i}\mathbf{k}_f \bullet \mathbf{r}}}{r} \sum_j b_j\, \mathrm{e}^{-\mathrm{i}\mathbf{Q}\bullet\mathbf{R}_j} \quad \text{where } \mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i \text{ and } r \gg R_j$$

The probability of being scattered into a detector of small area $\mathrm{d}A$ is proportional to

$$\underbrace{\left|\Psi_{\text{scat}}\right|^2 \mathrm{d}A}_{\mathrm{d}\sigma} = \underbrace{\frac{\mathrm{d}A}{r^2}}_{\mathrm{d}\Omega} \left| \sum_j b_j\, \mathrm{e}^{-\mathrm{i}\mathbf{Q}\bullet\mathbf{R}_j} \right|^2$$

In the continuum limit of scatterers, the differential cross-section becomes

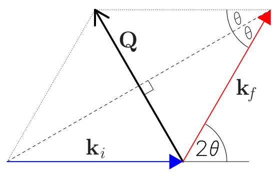
$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left| \iiint \beta(\mathbf{R})\, \mathrm{e}^{-\mathrm{i}\mathbf{Q}\bullet\mathbf{R}}\, \mathrm{d}^3\mathbf{R} \right|^2 \propto S(\mathbf{Q})$$

Some Fourier Consequences

- Bragg's law – scattering from a periodic lattice

d-spacing in $\mathbf{R} \Longleftrightarrow \frac{2\pi}{d}$-spacing in $\mathbf{Q}$

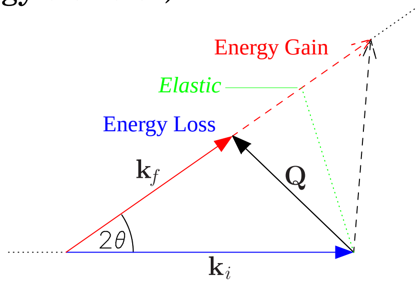
$(n\lambda = 2\,d\sin\theta)$



$$Q = 2\,k\sin\theta = \frac{4\pi\sin\theta}{\lambda}$$

- Debye-Waller and magnetic form factors – scattering from diffuse objects
  - *Convolution theorem* $\Rightarrow$ fall-off in scattered intensity with high-Q!

Inelastic scattering
(non-zero energy transfer)



$\omega \neq 0 \;\Rightarrow\; |\mathbf{k}_i| \neq |\mathbf{k}_f|$

$$Q^2 = k_i^2 + k_f^2 - 2\,k_i\,k_f\cos 2\theta$$

"Cosine Rule"

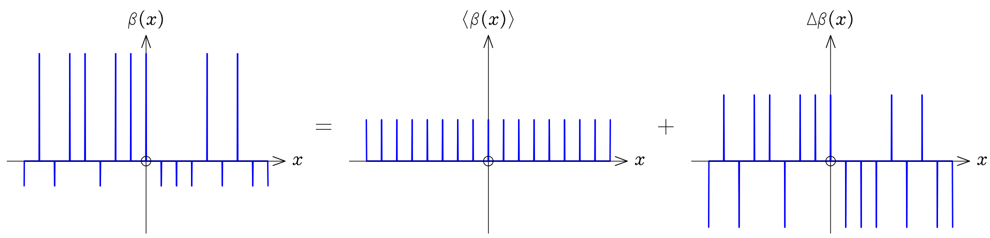
Time-dependence yields the partial differential cross-section

$$\frac{k_i}{k_f} \times \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E} = \left| \iiiint \beta(\mathbf{R},t)\,\mathrm{e}^{-\mathrm{i}(\mathbf{Q}\bullet\mathbf{R}-\omega t)}\,\mathrm{d}^3\mathbf{R}\,\mathrm{d}t \right|^2 \propto S(\mathbf{Q},\omega)$$

- Elastic scattering gives information on time-averaged structure.
- Inelastic scattering tells us about the dynamical behaviour of the sample.
- Total scattering is related to the instantaneous correlations.

Coherent and Incoherent Elastic Scattering

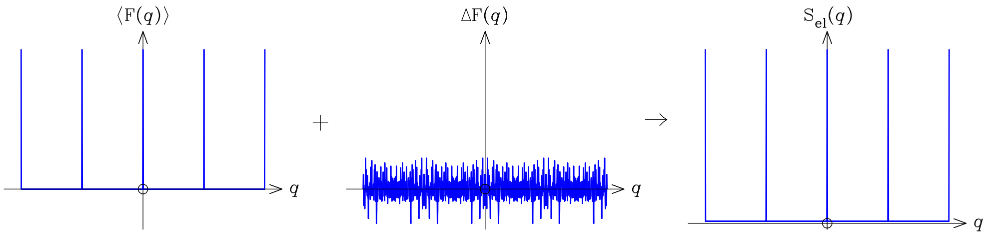
Since atoms of the same element are not "indentical", because of isotope and spin effects, it is useful to split the scattering into two parts:



- Coherent, or scattering from the average — $b_{coh} = \langle b \rangle$
- Incoherent, or scattering from fluctuations — $b_{inc}^2 = \langle b^2 \rangle - \langle b \rangle^2$

Coherent and Incoherent Scattering

- For elastic scattering, the incoherent contribution is background-like.



- For inelastic scattering, a model or polarisation analysis is required.
  - Coherent → correlated motion of atoms. (e.g. phonons and magnons)
  - Incoherent → self-correlations, or local dynamics. (e.g. diffusion)