Physics with neutrons 2

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Exercise sheet 1
To be discussed 2017-05-09, room C.3203

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Exercise 1.1

Calculate and draw the coherent and incoherent differential scattering cross section from scattering at two nuclei with scattering lengths b_1 and b_2 and a distance of R.
How does the coherent cross section evolve with an increasing number of nuclei with equal distances placed along a line?

Solution. The differential cross section for nuclei is given by

$$\frac{d\sigma}{d\Omega} = N(\langle b^2\rangle - \langle b\rangle^2) + \langle b\rangle^2 \left| \sum_{j=1}^{N} e^{i\vec{Q}\cdot\vec{R}_j} \right|^2.$$

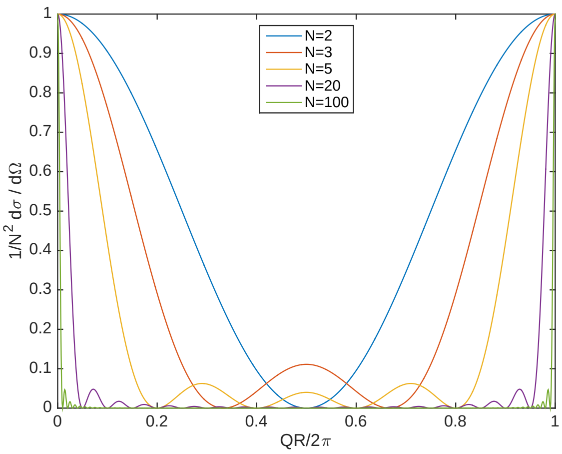
The incoherent scattering doesn't depend on the nucleus positions. It is given by the first part of the cross section:

$$\frac{1}{N}\frac{d\sigma}{d\Omega}\bigg|_{\text{inc}} = \langle b^2\rangle - \langle b\rangle^2 = \frac{b_1^2+b_2^2}{2} + \frac{(b_1+b_2)^2}{4} = \frac{(b_1-b_2)^2}{4}.$$

Let the first nucleus be placed at the origin and the second at $\vec{R}$. Then the coherent part per nucleus can be written as:

$$\frac{1}{N}\frac{d\sigma}{d\Omega}\bigg|_{\text{coh}} = \frac{\langle b\rangle^2}{2}\left|1+e^{i\vec{Q}\cdot\vec{R}}\right|^2 = \frac{\langle b\rangle^2}{2}\left(1+e^{i\vec{Q}\cdot\vec{R}}\right)\left(1+e^{-i\vec{Q}\cdot\vec{R}}\right) = \langle b\rangle^2\left(1+\cos(\vec{Q}\cdot\vec{R})\right).$$

With more than two nuclei placed in the scattering arrangement with equal distance $\vec{R}$, the coherent cross section forms sharper peaks at $\vec{Q}\cdot\vec{R}=0$ and $\vec{Q}\cdot\vec{R}=2\pi$, which become two delta peaks in the limit $N\to\infty$. The following plot shows this (for $\langle b\rangle^2 = 1$).



Note that the y axis is normalized by N^2 to have the curve shapes better comparable. Since the total cross section per nucleus must stay the same, the peak intensity scales with N in order to keep the integrated intensity constant.

□

EXERCISE 1.2

1. In equation (C.1.12) the scattering field ψ_s is given for a general scattering length density distribution $\rho(r)$. As neutrons scatter from unpaired electrons and therefore an extended potential, show how the magnetic form factor results from the generalised distribution.

2. Calculate the form factor for an unpaired electron in a spherical shell of radius R_0.

3. What is the form factor for an unpaired electron inside a solid sphere of radius R_0?

Solution.

$$\psi \mathbf{r}, t = -\frac{e^{i(\mathbf{k}_f \cdot \mathbf{r} - \omega t)}}{|\mathbf{r}|} \int \mathrm{d}\mathbf{r}' \rho(\mathbf{r}') e^{i\mathbf{Q}\mathbf{r}'} \propto \int \mathrm{d}\mathbf{r}' \sum_j \rho_j(\mathbf{r}') e^{i\mathbf{Q}(\mathbf{r}'+\mathbf{R}_j)}$$

with $\rho_j(\mathbf{r}')$ as the spin density at atom site $\mathbf{R}_j$. As the spin density is the same for all lattice sites, one can write

$$= \int \mathrm{d}\mathbf{r}' \sum_j \rho(\mathbf{r}') e^{i\mathbf{Q}\cdot\mathbf{r}'} e^{i\mathbf{Q}\cdot\mathbf{R}_j} = \underbrace{\int \mathrm{d}\mathbf{r}' \rho(\mathbf{r}') e^{i\mathbf{Q}\cdot\mathbf{r}'}}_{mag. formfactor} \sum_j e^{i\mathbf{Q}\cdot\mathbf{R}_j}$$

The form factor is defined as

$$f(\mathbf{Q}) = \int \mathrm{d}^3 r \rho(\mathbf{r}) e^{i\mathbf{Q}\mathbf{r}}.$$

In spherical coordinates

$$\begin{aligned}
f(Q) &= 2\pi \int \mathrm{d}r r^2 \int \mathrm{d}\cos(\theta) \rho(r) e^{iQr\cos(\theta)} \\
&= 2\pi \int \mathrm{d}r r^2 \rho(r) \left[-\frac{i}{Qr} e^{iQr\cos\theta} \right]_{-1}^{1} \\
&= 2\pi \int \mathrm{d}r r^2 \rho(r) \left[\frac{i}{Qr} e^{-iQr\cos\theta} - \frac{i}{Qr} e^{-iQr\cos\theta} \right] \\
&= 4\pi \int \mathrm{d}r \frac{r}{Q} \sin(Qr) \cdot \rho(r) \qquad \text{using } \sin x = \frac{i}{2}\left(e^{-x} - e^{x}\right)
\end{aligned}$$

Shell of radius R_0, using delta function:

$$\begin{aligned}
f(Q) &= r\pi \int \mathrm{d}r \frac{r}{Q} \sin(Qr) \cdot \frac{\delta(R_0 - r)}{4\pi R_0^2} \\
&= \frac{1}{QR_0} \sin(QR_0)
\end{aligned}$$

Sphere of radius R_0, using Heaviside step function:

$$\begin{aligned} f(Q) &= 4\pi \int \mathrm{d}r \frac{r}{Q} \sin(Qr) \cdot \frac{\theta(R_0 - r)}{\frac{4}{3}\pi R_0^3} \\ &= 3 \cdot \int_0^{R_0} \mathrm{d}r \frac{r}{Q} sin(Qr) \frac{1}{R_0^3} \\ &= \frac{3\sin(QR_0)}{(QR_0)^3} - \frac{3\cos(QR_0)}{(QR_0^3)} \end{aligned}$$

□

EXERCISE 1.3

Proof that $\mathbf{G}_{n'}\mathbf{r}_n = 2\pi m$ for all n and n' with $\mathbf{G}_{n'} = n_1\mathbf{g}_1 + n_2\mathbf{g}_2 + n_3\mathbf{g}_3$ given in (C.1.16) and $\mathbf{r}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ describing the Bravais lattice.

Solution. Assuming a Bravais lattice

$$\mathbf{R}_n = n_1 \cdot \mathbf{a}_1 + n_2 \cdot \mathbf{a}_2 + n_3 \cdot \mathbf{a}_3 \qquad \text{with } n_1, n_2, n_3 \in \mathbb{Z}.$$

The position of the atoms in the lattice can be written as a periodic function

$$f(\mathbf{r}) = f(\mathbf{R_n} + \mathbf{r})$$

As the function is periodic, we rewrite it in a Fourier expansion

$$f(\mathbf{R_n} + \mathbf{r}) = \sum_{\mathbf{m}} f_{\mathbf{m}} e^{i\mathbf{G_m}\cdot\mathbf{r}} e^{i\mathbf{G_m}\cdot\mathbf{R_n}}$$

Due to the periodicicty $f(\mathbf{R_n} + \mathbf{r}) = f(\mathbf{R_k} + \mathbf{r})$ for any $\mathbf{n}, \mathbf{k} \in \mathbb{Z}$ the last formula is also true for the particular case $\mathbf{R_0} = \mathbf{0}$.

$$\sum_{\mathbf{m}} f_{\mathbf{m}} e^{i\mathbf{G_m}\cdot\mathbf{r}} e^{i\mathbf{G_m}\cdot\mathbf{R_n}} = \sum_{\mathbf{m}} f_{\mathbf{m}} e^{i\mathbf{G_m}\cdot\mathbf{r}} e^{i\mathbf{G_m}\cdot\mathbf{0}} = \sum_{\mathbf{m}} f_{\mathbf{m}} e^{i\mathbf{G_m}\cdot\mathbf{r}} \cdot 1$$

Therefore, $e^{i\mathbf{G_m}\cdot\mathbf{R_n}} = 1$ and it follows

$$\mathbf{G_m} \cdot \mathbf{R_n} = 2\pi N \qquad \text{with} N \in \mathbb{Z}.$$

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