Physics with neutrons 1

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EXERCISE 5.1

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:

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

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:

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

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 5.2

A 2-dimensional hexagonal lattice with lattice constant a is given in the normal space. Draw the corresponding lattice in reciprocal space. How are the reciprocal lattice vectors determined? What does the first Brillouin zone look like?

Solution. The hexagonal lattice is determined by the two unit vectors

$$\vec{a}_1 = (a_{11}, a_{12}) = \frac{a}{2}(1, \sqrt{3})$$
 and $\vec{a}_2 = (a_{21}, a_{22}) = a(1, 0).$

Between real-space unit vectors \vec{a}_i and reciprocal unit vectors $vecb_j$, the following relation must hold, just as for 3-dimensional lattices:

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$$

From this, we can formulate a system of equations that needs to be satisfied:

$$(a_{ij})^T \cdot (b_{ij}) = 2\pi I,$$

where (a_{ij}) and (b_{ij}) are the matrices formed by the components of the base vectors, and I is the identity matrix in two dimensions. Writing $A = (a_{ij})^T$, we can solve this system by multiplying with A^{-1} :

$$(b_{ij}) = 2\pi A^{-1},$$

and A^{-1} is easily found as

$$A^{-1} = \frac{1}{\det A} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}.$$

This means that we have found our reciprocal unit vectors:

$$\vec{b}_1 = \frac{4\pi}{a\sqrt{3}}(0,1)$$
 and $\vec{b}_2 = \frac{2\pi}{a\sqrt{3}}(\sqrt{3},-1),$

which again form a hexagonal lattice. The first Brillouin zone therefore is a regular hexagon. The following sketch shows real and reciprocal unit cells:



EXERCISE 5.3

Calculate the total coherent and incoherent scattering cross sections of SiO₂. Hint: You can look up neutron scattering lengths and cross sections at http://www.ncnr.nist.gov/resources/n-lengths/.

 ${\it Solution}.$ From the NCNR scattering length database, we get

$$\langle b \rangle_{\rm Si} = 4.149 \,\mathrm{fm}$$
 and $\langle b \rangle_{\rm O} = 5.803 \,\mathrm{fm}$,

and

$$\langle b^2 \rangle_{\rm Si} = 17.239 \, {\rm fm}^2 \quad {\rm and} \quad \langle b^2 \rangle_{\rm O} = 33.676 \, {\rm fm}^2,$$

which are then combined:

$$\sigma_{\rm coh,SiO_2} = 4\pi \left(\frac{1}{3} \langle b \rangle_{\rm Si} + \frac{2}{3} \langle b \rangle_{\rm O}\right)^2 = 346.6 \,\mathrm{fm}^2 = 3.466 \,\mathrm{b}$$

$$\sigma_{\rm inc,SiO_2} = 4\pi \left(\frac{1}{3} \langle b^2 \rangle_{\rm Si} + \frac{2}{3} \langle b^2 \rangle_{\rm O}\right) - \sigma_{\rm coh,SiO_2} = 7.7 \,\mathrm{fm}^2 = 0.077 \,\mathrm{b}$$

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