Physics with neutrons 1

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Exercise sheet 4
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Exercise 4.1

Calculate the magnetic interaction potential for a typical rare earth magnet, $\mu \approx 10\,\mu_B$ (Tb^{3+}, Dy^{3+}, Ho^{3+}), and of a Cu spin in a high-T_c superconductor, $\mu \approx 1\,\mu_B$, in a field of 1 T.

Solution. The magnetic interaction potential is given as

$$V = \mu \cdot B.$$

The Bohr magneton is $\mu_B = \frac{e\hbar}{2m_e} = 5.79 \cdot 10^{-5}\,\mathrm{eV/T}$. From this:

$$V(10\mu_B) = 5.79 \cdot 10^{-4}\,\mathrm{eV}; \quad V(1\mu_B) = 5.79 \cdot 10^{-5}\,\mathrm{eV}.$$

□

Exercise 4.2

The potential

$$U(r, \vartheta, \varphi) = -U_0\,\Theta(R - r)$$

is called a hard sphere potential with radius R. ($\Theta(x)$ is the Heaviside step function, which is defined to be zero for $x < 0$ and unity for $x \geq 0$.)

1. Calculate the differential and the total cross section of scattering from this potential.
2. Using small-angle neutron scattering, a biologist would like to measure the diameter of spherical micelles (aggregated "clusters" of molecules in a solvent). What is the form factor $F(QR)$ (i.e. the Q-dependent part of the differential scattering cross section) of one such micelle under the assumption that it can be approximated by a homogeneous sphere with a radius of 200 nm?
3. For small values of QR, the form factor can be Taylor-expanded. What is the resulting behavior?
4. Plot the form factor (versus QR) on a log-log scale. For large values of QR, what is the behavior of $F(QR)$ when one averages over the oscillations?
5. What happens (qualitatively) when the sphere is placed in a solvent? What happens when there are multiple spheres present?

Solution. The scattering amplitude is given by

$$f(\vec{Q}) = -\frac{m}{2\pi\hbar^2}\int d^3r\, U(\vec{r})\, \exp(-i\vec{Q}\cdot\vec{r}),$$

or, in spherical coordinates,

$$f(Q) = -\frac{m}{2\pi\hbar^2}\int dr\, d(\cos\vartheta)\, d\varphi\, r^2\, U(r)\, \exp(-iQr\cos\vartheta).$$

Since the potential is spherically symmetric, we can use ϑ as the angle between $\vec{Q}$ and $\vec{r}$ in the exponential because we can select the coordinate system freely, so that $\vec{Q}$ is along the z axis.
Inserting our given potential and doing the trivial φ integration we get

$$f(Q) = -\frac{m}{2\pi\hbar^2}(-2\pi U_0)\int_0^\infty dr\, r^2\Theta(R-r)\int_{-1}^{1} d(\cos\vartheta)\, \exp(-iQr\cos\vartheta).$$

The integration over $\cos\vartheta$ is also easy:

$$f(Q) = \frac{mU_0}{\hbar^2}\int_0^\infty dr\, r^2\Theta(R-r)\frac{1}{-iQr}\left(\exp(-iQr) - \exp(iQr)\right).$$

Now we replace the exponential representation of the sine and resolve the Θ function by adjusting the integration limits:

$$f(Q) = \frac{2mU_0}{\hbar^2}\frac{1}{Q}\int_0^R dr\, r\sin(Qr).$$

$$f(Q) = \frac{2mU_0}{\hbar^2}\frac{1}{Q}\left[\frac{\sin Qr}{Q^2} - \frac{r\cos Qr}{Q}\right]_0^R = \frac{2mU_0}{\hbar^2}\frac{\sin QR - QR\cos QR}{Q^3}.$$

The final step is to rewrite this a bit:

$$f(Q) = \frac{mU_0}{2\pi\hbar^2}\frac{4\pi R^3}{3}\frac{3(\sin QR - QR\cos QR)}{(QR)^3} = \rho\cdot V_s\cdot 3\frac{\sin QR - QR\cos QR}{(QR)^3},$$

where $\rho = mU_0/2\pi\hbar^2$ is the "scattering length density" (SLD) and V_s the volume of the sphere. Note that the SLD definition matches well with the Fermi pseudopotential used for scattering at single nuclei: the singular $b\delta(r)$ is replaced by an $\rho(r)$ extended over the sphere. This is sensible because in small angle scattering, we are looking at very large structures and so cannot resolve individual scattering centers inside the spheres any more.
The differential cross section $d\sigma/d\Omega$ is simply given by $|f(Q)|^2$.
The total cross section is obtained by integrating over all solid angle. For this, we need to express $d\Omega$ in terms of Q:

$$Q = 2k\sin\frac{\theta}{2} \Longrightarrow \frac{dQ}{d\theta} = k\cos\frac{\theta}{2}$$

$$\Longrightarrow d\Omega = 2\pi d\theta\sin\theta = 2\pi\frac{dQ}{k\cos\frac{\theta}{2}}\sin\theta = 2\pi dQ\frac{2\sin\frac{\theta}{2}}{k} = 2\pi\frac{Q}{k^2}dQ.$$

The integration now gives

$$\sigma = \int_\Omega d\Omega\frac{d\sigma}{d\Omega} = \int_0^{2k} dQ\frac{2\pi Q}{k^2}|f(Q)|^2;$$

note that we integrate in Q from o to $2k$, which is the maximum momentum transfer (a backscattering process). Inserting $f(Q)$ gives

$$\sigma = \int_0^{2k} dQ\frac{2\pi Q}{k^2}9\rho^2V^2\frac{(\sin QR - QR\cos QR)^2}{(QR)^6} = \frac{18\pi\rho^2V^2}{(kR)^2}\int_0^{2kR} du\frac{\sin^2 u - 2u\sin u\cos u + u^2\cos^2 u}{u^5}$$

with the substitution $u = kR$, and solving the integral we have

$$\sigma = \frac{9\pi\rho^2V^2}{2(kR)^2}\left[1 - \frac{1}{(2kR)^2} + \frac{\sin 4kR}{(2kR)^3} - \frac{\sin^2 2kR}{(2kR)^4}\right]$$

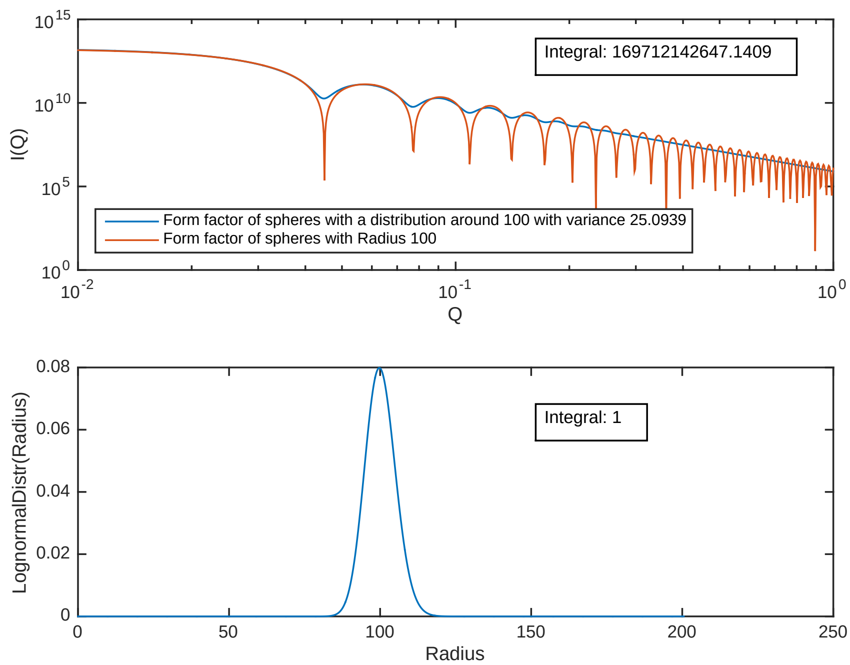
as the total scattering cross section.
The form factor for the micelle is the Q-dependent part of the differential cross section for the hard sphere potential with $R = 200\,\mathrm{nm}$:

$$F(QR) = \rho^2 \cdot V_s^2 \cdot 9\frac{\sin^2 QR - 2QR\sin QR\cos QR + Q^2R^2\cos^2 QR}{(QR)^6}.$$

For small values of QR, the Taylor expansion of the form factor reads

$$F(QR) \approx 1 - \frac{(QR)^2}{5},$$

This is called the "Guinier approximation", and it gives information about the micelle size.
A plot of the form factor:



The behavior for large QR, when averaging over oscillations, is $\propto (QR)^{-4}$.
With the sphere placed in a solvent, the scattering length density ρ is replaced by the SLD contrast between sphere and solvent $\rho_{\mathrm{sphere}} - \rho_{\mathrm{solvent}}$. By appropriate "contrast matching" with different solvents (e.g. different mixtures of D_2O and H_2O), one can accurately determine ρ_{sphere}. For N spheres, the form of $d\sigma/d\Omega$ stays the same (with a factor of N) only if the spheres are noninteracting. In reality, they are interacting (e.g. certain sphere–sphere distances are preferred), which leads to an additional factor in $d\sigma/d\Omega$ called the "structure factor". □

Exercise 4.3

Electrons are the origin of the magnetism in magnetic materials. Assume that the probability density of finding an electron at $\vec{r} = (r, \vartheta, \varphi)$ is given by a Gaussian profile

$$\rho(r) = \rho_0 \exp\left[-\frac{r^2}{2\sigma^2}\right]$$

with a half-width at half maximum of $a = 2\,\text{Å}$ (what is the relation between σ and a?). From this profile, calculate the magnetic form factor of an unpaired electron.

Solution. From setting $\rho(a) = \frac{1}{2}$, you can find out the relationship between standard deviation σ and HWHM a:

$$a = \sigma\sqrt{2\ln 2}.$$

Consider the scattering amplitude as in exercise 8:

$$f(Q) = -\frac{m}{2\pi\hbar^2}\int d^3r\,\rho_0 \exp\left[-\frac{r^2}{2\sigma^2}\right]\exp\left[-i\vec{Q}\cdot\vec{r}\right] = -\frac{m\rho_0}{\hbar^2}\int_{-1}^{1} d\cos\vartheta \int_0^\infty dr\, r^2 e^{-iQr\cos\vartheta} e^{-r^2/2\sigma^2}$$

$$= -\frac{m\rho_0}{Q\hbar^2}\int_0^\infty dr\, r\sin(Qr)e^{-r^2/2\sigma^2} = -\frac{m\rho_0\sqrt{\pi}a^3}{4\hbar^2\sqrt{\ln 2}^3}\exp\left[-\frac{Q^2a^2}{4\ln 2}\right]$$

□