Physics with neutrons 2

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Exercise sheet 7
To be discussed 2017-06-20, room C.3203

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Exercise 7.1

Discuss and draw qualitatively the thermal occupation factors of $\langle n \rangle$ and $\langle n+1 \rangle$ for a diffusion process leading to quasi-elastic scattering and a excitation, i.e. inelastic scattering. Discuss (a) the classical limit (high temperatures, $k_B T \gg E$) and (b) the quantum limit ($T \to 0$).

Note: Quasi-elastic scattering is represented by a Gaussian of the form $e^{-\frac{\omega^2}{2\sigma^2}}$, $\sigma = 1\,\text{meV}$. Inelastic scattering is represented by a Gaussian of the form $e^{-\frac{(\omega\pm\omega_0)^2}{2\sigma^2}}$, $\sigma = 0.1\,\text{meV}$, $\omega_0 = 1\,\text{meV}$.

Solution. The occupation factors are

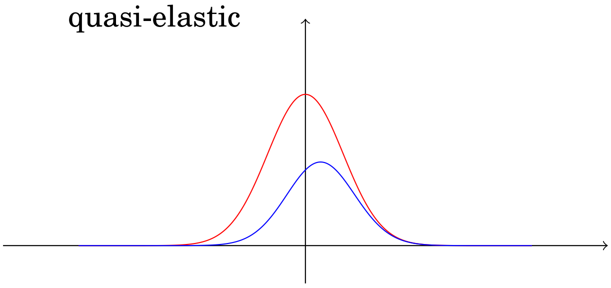
$$\langle n \rangle = \frac{1}{e^{\hbar\omega/kT} - 1} \quad \text{and} \quad \langle n+1 \rangle = 1 + \frac{1}{e^{\hbar\omega/kT} - 1} = \frac{e^{\hbar\omega/kT}}{e^{\hbar\omega/kT} - 1}.$$

The ratio of the factors, and therefore of the scattering functions, for neutron energy gain and neutron energy loss is given by

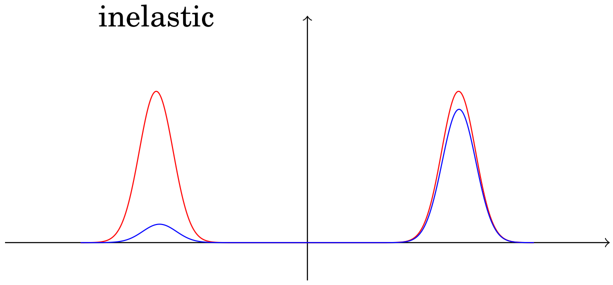
$$S(-\mathbf{Q}, -\omega) = \mathbf{e}^{-\hbar\omega/\mathbf{kT}}\mathbf{S}(\mathbf{Q}, \omega)$$

(cf. Furrer, page 14).
For the "classical" limit, $T \gg E$, where E is the characteristic energy scale of the problem (σ in the quasi-elastic, ω_0 in the inelastic case), we get that $\hbar\omega \ll kT$ and therefore $\langle n \rangle \approx \langle n+1 \rangle$, i.e. a symmetric cross section for Stokes- and anti-Stokes processes.
For the "quantum-mechanical" limit, $T \to 0$, which makes the exponential very big. In this limit $\langle n \rangle \to 0$, while $\langle n+1 \rangle \to 1$.
The effect on the two scattering processes can thus be plotted (red = high temperature limit, symmetric; blue = low temperature limit, asymmetric):

quasi-elastic



inelastic



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EXERCISE 7.2

Derive the intermediate scattering function, pair correlation function, and the scattering law $S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t} I(\mathbf{Q},t)$ for a single atom that oscillates harmonically in one dimension with a frequency ω_0. When you perform the Fourier transform, assume that the amplitude of the oscillation is very small.

Solution. We start with the intermediate scattering function in one dimension:

$$I(Q,t) = \frac{1}{N}\sum_{j,j'} \langle e^{-iQr_{j'}(0)} e^{iQr_j(t)} \rangle$$

For a single atom, we have $N = 1$ and therefore

$$I(Q,t) = \langle e^{-iQr_j(0)} e^{iQr_j(t)} \rangle = \langle e^{-iQ(r_j(0)-r_j(t))} \rangle.$$

Set $\rho(t) = r(t) - r(0)$. For a harmonic oscillation $\rho(t) = \rho_0 \cos(\omega_0 t)$. Since the cosine is an even function, $r(t) - r(0) = r(0) - r(t)$. This gives us

$$I(Q,t) = \langle e^{-iQ\rho_0 \cos(\omega_0 t)} \rangle$$

As given in the exercise, the amplitude ρ_0 is very small, so we can Taylor-expand the exponential:

$$I(Q,t) = \langle 1 - iQ\rho_0 \cos(\omega_0 t) - \frac{1}{2}Q^2\rho_0^2 \cos^2(\omega_0 t) + \frac{i}{6}Q^3\rho_0^3 \cos^3(\omega_0 t) \pm ... \rangle.$$

All terms with odd powsers of the cosine vanish and therefore we are left with

$$I(Q,t) = 1 - \frac{1}{6}Q^2\rho_0^2, \qquad \text{using } \langle \cos^2 x \rangle = \frac{1}{3}.$$

Taking all terms into account, we arrive at

$$I(Q,t) = e^{-\frac{1}{6}Q^2\rho_0^2}$$

(which is analogous to the derviation of the Debye-Waller factor).
The pair correlation function is

$$G(r,t) = \frac{1}{2\pi}\int dQ\, e^{-iQr} I(Q,t) = \frac{1}{2\pi}\int dQ\, e^{-iQr} e^{-\frac{1}{6}Q^2\rho_0^2} = \sqrt{\frac{3}{2\pi}}\frac{1}{\rho_0}\exp\left(-\frac{3r^2}{2\rho_0^2}\right).$$

The scattering law is

$$S(Q,\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t} I(Q,t) = \frac{1}{2\pi\hbar}\int dQ\, e^{-i\omega t} e^{-\frac{1}{6}Q^2\rho_0^2} = \exp\left(-\frac{1}{6}Q^2\rho_0^2\right)\delta(\hbar\omega).$$

EXERCISE 7.3

Estimate the energy scale of the magnetic interaction for

- two electrons,

- an electron and a neutron,
- an electron and a nucleus (for example Cu), and
- a neutron and a nucleus (for example In).

The respective particles are supposed to have a distance of 1 Å.

Solution. The magnetic interaction energy is given by

$$\hat{U}_m(\mathbf{R}) = -\hat{\mu} \cdot \mathbf{B}(\mathbf{R}),$$

where $\hat{\mu}$ is the magnetic moment operator. We use the expression for the field $\mathbf{B}(\mathbf{R})$ of an electron for a spin-only system and get:

$$U_m(\mathbf{R}) = -\mu_1 \cdot \frac{\mu_0}{4\pi}\left(\nabla \times \frac{\mu_2 \times \mathbf{R}}{R^3}\right) = -\mu_1 \cdot \frac{\mu_0}{4\pi}\left(\frac{3\mathbf{R}(\mu_2 \cdot \mathbf{R})}{R^5} - \frac{\mu_2}{R^3}\right).$$

Assuming both moments to be collinear, and perpendicular to $\mathbf{R}$, we get

$$U_m(R) = \frac{\mu_0}{4\pi}\frac{\mu_1\mu_2}{R^3}.$$

The magnetic moments of the given particles and atoms are:

Particle	Magnetic moment
Neutron	$-1.91\,\mu_N$
Electron	$-1.001\,\mu_B$
^{63}Cu	$2.22\,\mu_N$
^{65}Cu	$2.38\,\mu_N$
^{113}In	$5.53\,\mu_N$

(μ_B is the Bohr magneton, $e\hbar/2m_e = 9.274 \times 10^{-24}$ J/T. μ_N is the nuclear magneton, $e\hbar/2m_p = 5.051 \times 10^{-27}$ J/T. The nuclear moments of isotopes can readily be found on the web, e.g. on webelements.com.)

Now we can calculate the magnetic interaction of the given systems:

System	μ_1 (10^{-27} J/T)	μ_2 (10^{-27} J/T)	U_m (µeV)
e-e	−9285	−9285	53.8
e-n	−9285	−9.66	0.056
e-^{63}Cu	−9285	12.3	−0.065
e-^{65}Cu	−9285	12.8	−0.070
n-^{113}In	−9.66	27.9	-1.68×10^{-4}

As one can see, the interaction between neutrons and the nuclear spins is about 1000 times weaker than between neutrons and free electrons. It still plays a role in spin-incoherent scattering though. □