Physics with neutrons 1

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Exercise sheet 10
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Exercise 10.1

Calculate $\langle \zeta^2 \rangle_T$ and f_{DWF}^2 for lead ($\theta_D = 88\,\mathrm{K}$), copper ($\theta_D = 315\,\mathrm{K}$), and diamond ($\theta_D = 1860\,\mathrm{K}$) at $T = 10\,\mathrm{K}$ and $T = 1000\,\mathrm{K}$ with the low and high temperature approximations. Which material is most useful as a monochromator? What can be done to improve the reflectivity of copper monochromators?

Solution. The DWF form-factor contribution is given by

$$f_{DWF}^2 = e^{-2W(Q)} = e^{-\frac{1}{6}Q^2\langle\zeta^2\rangle}$$

with the mean square atomic displacement $\langle\zeta^2\rangle$, which of course depends on the temperature of the material, and can be approximated with different models.
One model is the Debye model, assuming a spectrum of excitation frequencies for N atoms given by

$$Z(\omega) = \frac{9N\omega^2}{\omega_{max}^3},$$

where the cutoff frequency is expressed in terms of the Debye temperature Θ_D:

$$\omega_{max} = \frac{k_b\Theta_D}{\hbar}.$$

For this model we get a mean square displacement of (Exercise 9)

$$\langle\zeta^2\rangle = \frac{9\hbar^2}{2k_b\Theta_D M}P(T) = \frac{9k_b\Theta_D}{2M\omega_{max}^2}P(T),$$

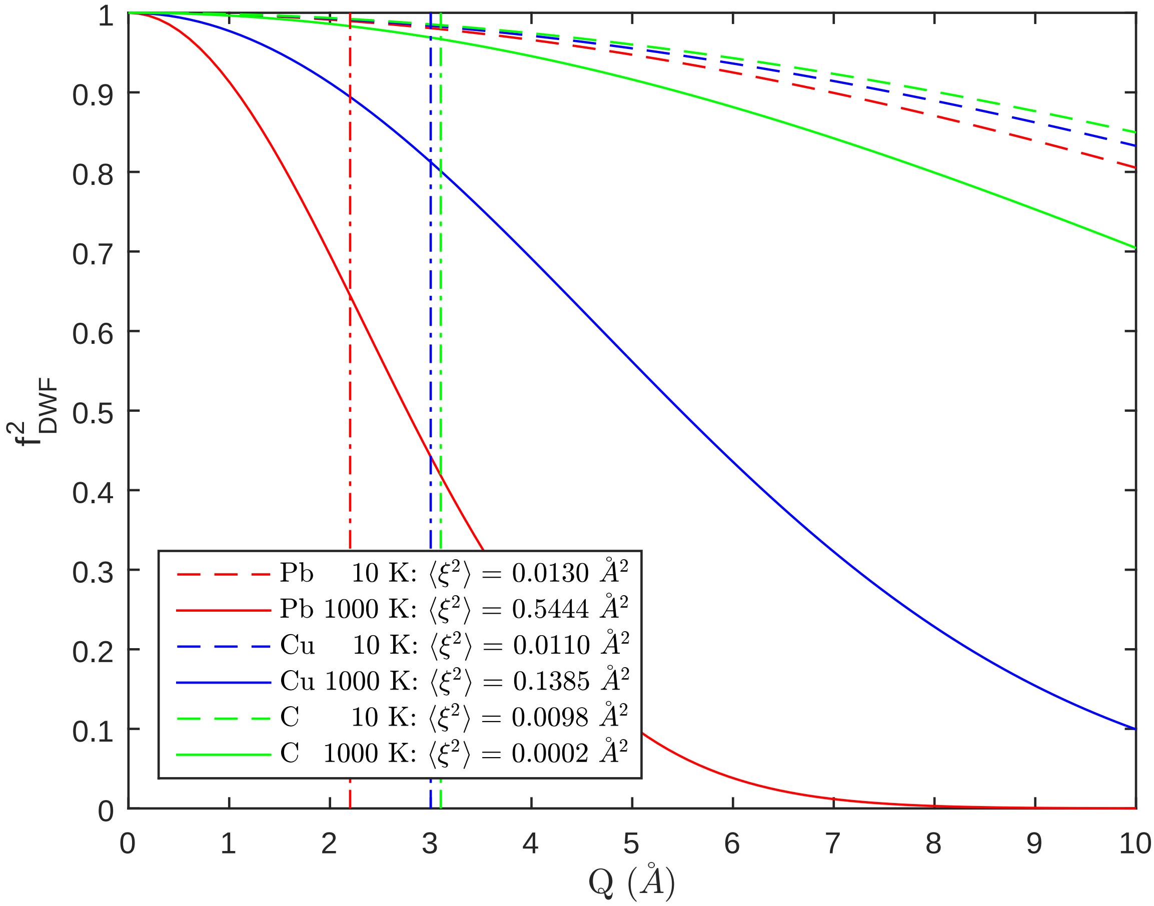
with a function $P(T)$ that depends on the temperature relative to Θ_D.
In the high-temperature regime, $T \gg \Theta_D$, it is simply given by

$$P(T) = 4\frac{T}{\Theta_D} \Longrightarrow \langle\zeta^2\rangle = \frac{18\hbar^2 k_b T}{k_b^2\Theta_D^2 M}.$$

In the low-temperature regime, $T \ll \Theta_D$, we get

$$P(T) = 1 + 4\frac{\pi^2}{6}\left(\frac{T}{\Theta_D}\right)^2 \Longrightarrow \langle\zeta^2\rangle = \frac{9\hbar^2}{2k_b\Theta_D M} + \frac{3\pi^2\hbar^2 k_b^2 T^2}{k_b^3\Theta_D^3 M}.$$

The figure shows the DWF for the given materials and temperatures:



The vertical lines indicate the first allowed Bragg reflexion, which can be used for monochromatizing neutrons. The most useful monochromator material obviously would be diamond. Lead, on the other hand, is quite unsuitable. The reflectivity of copper, which is a commonly used monochromator because it is easy to produce large good quality single crystals, benefits strongly from cooling it down. □

Exercise 10.2

Derive the representation

$$G(\mathbf{r},t) = \frac{1}{N}\sum_{j,j'}\int\langle\delta\Big(\mathbf{R}-\mathbf{r}_{j'}(0)\Big)\delta\Big(\mathbf{R}+\mathbf{r}-\mathbf{r}_j(t)\Big)\rangle dR$$

from the expression for the intermediate scattering function

$$I(\mathbf{Q},t) = \frac{1}{N}\sum_{j,j'}\langle e^{-i\mathbf{Q}\cdot\mathbf{r}_{j'}(0)}e^{i\mathbf{Q}\cdot\mathbf{r}_j(t)}\rangle_T$$

using the substitution

$$e^{-i\mathbf{Q}\cdot\mathbf{r}_{j'}(0)} = \int e^{-i\mathbf{Q}\cdot\mathbf{r}'}\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)d\mathbf{r}'.$$

Solution. $G(\mathbf{r},t)$ is the so called space-time pair correlation function, transforming the reciprocal spatial space coordinates $\mathbf{Q}$ to real space $\mathbf{r}$. With this ansatz we calculate

$$\begin{aligned}G(\mathbf{r},t) &= \frac{1}{(2\pi)^3}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}} I(\mathbf{Q},t) = \frac{1}{(2\pi)^3}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}} \frac{1}{N}\sum_{j,j'}\langle e^{-i\mathbf{Q}\cdot\mathbf{r}_{j'}(0)} e^{i\mathbf{Q}\cdot\mathbf{r}_j(t)}\rangle_T \\ &= \frac{1}{N}\sum_{j,j'}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}}\left\langle \frac{1}{(2\pi)^3}\int d\mathbf{r}' e^{-i\mathbf{Q}\cdot\mathbf{r}'}\,\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)\, e^{i\mathbf{Q}\cdot\mathbf{r}_j(t)}\right\rangle_T \\ &= \frac{1}{N}\sum_{j,j'}\int d\mathbf{r}'\,\left\langle \frac{1}{(2\pi)^3}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot(\mathbf{r}+\mathbf{r}'-r_j(t))}\,\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)\right\rangle_T \\ &= \frac{1}{N}\sum_{j,j'}\int d\mathbf{r}'\,\left\langle \delta\left(\mathbf{r}'+\mathbf{r}-\mathbf{r}_j(t)\right)\,\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)\right\rangle_T,\end{aligned}$$

where we used

$$\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}} = (2\pi)^3\delta(\mathbf{r})$$

in the last step. $G(\mathbf{r},t)$ describes the correlation between the atom j' at time $t=0$ at position $\mathbf{r}'$ and the atom j at a later time t at another position $\mathbf{r}'+\mathbf{r}$, i.e. the probability of having two atoms j and j' in a well defined spatial and temporal correlation. $G(\mathbf{r},t)$ may therefore be considered as the most general description of the statics and dynamics of condensed matter on an atomic scale. □

Exercise 10.3

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 an excitation, i.e. inelastic scattering. Discuss (a) the classical limit (high temperatures, $k_BT \gg E$) and (b) the quantum limit ($T\to 0$).
Note: Quasi-elastic scattering is represented by a Gaussian of the form $e^{-\frac{\omega^2}{2\sigma^2}}$, $\sigma = 1\,\mathrm{meV}$. Inelastic scattering is represented by a Gaussian of the form $e^{-\frac{(\omega\pm\omega_0)^2}{2\sigma^2}}$, $\sigma = 0.1\,\mathrm{meV}$, $\omega_0 = 1\,\mathrm{meV}$.

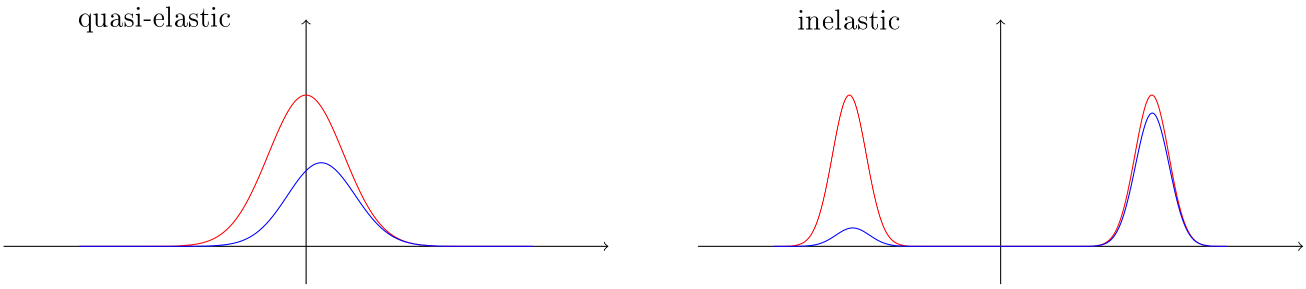
Solution. The occupation factors are

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

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

□