Physics with Neutrons I

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Exercise sheet 11 https://wiki.mlz-garching.de/n-lecture06:index

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Solutions

1. Specular reflectivity

Assume a single planar interface between vacuum and a material with refractive index n. Derive the reflectivity of a neutron beam in the case of specular reflection and compute it for neutrons with wavelength $\lambda = 4\,\text{Å}$and $n = 1 \pm 10^{-5}$. All neutron beams can be assumed as planar waves and the boundary conditions at the interface are the continuity of the wave function and its derivative. Use, that the wave vector changes due to the refractive index and that all components parallel to the surface stay constant at the interface.
What happens for $n < 1$ mathematically and what is the physical interpretation?

The reflectivity can also be derived starting from a scattering point of view. The crucial steps are to start from the differential scattering cross section and evaluate this for $Q_x = Q_y = 0$ and a scattering length density which only depends on z. Still, this has to be integrated over a small solid angle which represents the inherent uncertainty of Q. The result is the following approximation:

$$R(Q) \approx \frac{16\pi^2}{Q^2} \Big| \int_{-\inf}^{\inf} \Delta\rho_b(z) e^{-i\,Q_z\,z} dz \Big|^2$$

This formula has a problem for 'infinitely thick' materials, because the integral will not converge. This is caused by the unphysical assumption that we neglect absorption. The problem can be solved by simply dropping the integration terms evaluated at $z = \pm\inf$.
Use this approximation to calculate the reflectivity of the same interfaces as given above. Where is the approximation valid and which important effect is not taken into account?

Compared to the optical approach, it is easier to calculate the effect of multiple interfaces with the scattering approximation. How does the reflectivity change, if the sample has finite thickness (e.g. $10\,\mu$m)? What is the physical interpretation?

Solution

Three plane waves have to be considered, the incident, transmitted and reflected wave. In specular reflections ony the z component (normal to the surface) changes and has to be considered.

$$\psi_i(z) = \psi_0 e^{-i\,z\,k_i\,\sin(\theta_i)}$$
$$\psi_r(z) = \psi_r e^{i\,z\,k_i\,\sin(\theta_i)}$$
$$\psi_t(z) = \psi_t e^{-i\,z\,k_t\,\sin(\theta_t)}$$

The unknown quantities k_t and θ_t can be replaced by the definition of the refractive index:

$$k_t = n\,k_i$$

and the specular condition:

$$k_{t,x} = k_{i,x}$$

$$k_t\,\cos(\theta_t) = k_i\,\cos(\theta_i) = \frac{k_t}{n}\,\cos(\theta_i)$$

$$1 - \sin^2(\theta_t) = \frac{1}{n^2}\left(1 - \sin^2(\theta_i)\right)$$

$$\sin(\theta_t) = \sqrt{1 - \frac{1 - \sin^2(\theta_i)}{n^2}}$$

The usual boundary conditions for waves at an interface apply. Continuity of the waves at $z = 0$ gives:

$$\psi_i(z=0) + \psi_r(z=0) = \psi_t(z=0)$$

$$\psi_0 + \psi_r = \psi_t$$

Continuity of the derivative yields:

$$\frac{d\psi_i}{dz}(z=0) + \frac{d\psi_r}{dz}(z=0) = \frac{d\psi_t}{dz}(z=0)$$

$$(\psi_0 - \psi_r)\,k_i\,\sin(\theta_i) = \psi_t\,k_t\,\sin(\theta_t)$$

Inserted into each other we get expressions for ψ_r and ψ_t:

$$\psi_r = \psi_0 \frac{k_i\,\sin(\theta_i) - k_t\,\sin(\theta_t)}{k_i\,\sin(\theta_i) + k_t\,\sin(\theta_t)}$$

$$\psi_t = 2\psi_0 \frac{k_i\,\sin(\theta_i)}{k_i\,\sin(\theta_i) + k_t\,\sin(\theta_t)}$$

both can be rewritten with the abbreviation α:

$$\alpha = \frac{k_t\,\sin(\theta_t)}{k_i\,\sin(\theta_i)} = \frac{n}{\sin(\theta_i)}\sqrt{1 - \frac{1 - \sin^2(\theta_i)}{n^2}}$$

Note, that α can become imaginary for $n < 1$. The expressions are now only depending on n and the incident beam:

$$\psi_r = \psi_0 \frac{1-\alpha}{1+\alpha}$$

$$\psi_t = \psi_0 \frac{2}{1+\alpha}$$

The Reflection is the calculated as relative intensity (absolute square of the amplitude ψ) between incoming and reflected waves:

$$R = \left|\frac{\psi_r}{\psi_0}\right|^2 = \left|\frac{1-\alpha}{1+\alpha}\right|^2 = \frac{1 - 2Re(\alpha) + |\alpha|^2}{1 + 2Re(\alpha) + |\alpha|^2}$$

Total reflectivity ($R = 1$) is only possible if α has no real part. This is the case if the square root in alpha is zero or below:

$$1 - \frac{1 - \sin^2(\theta_i)}{n^2} \leq 0$$

$$n^2 \leq \cos^2(\theta_i)$$

Note, that while $R = 1$ (and $T = 1 - R = 0$) the transmitted amplitude $\psi_t \neq 0$!

In order to compare the scattering based approximation to the optical calculations, we need to replace some quantities:

$$k_i = \frac{2\pi}{\lambda}$$
$$Q = k_r - k_i = k_{r,z} - k_{i,z} = (-)2k_i\,\sin(\theta_i)$$
$$n = \sqrt{1 - \frac{\lambda^2\,\rho_b}{\pi}}$$

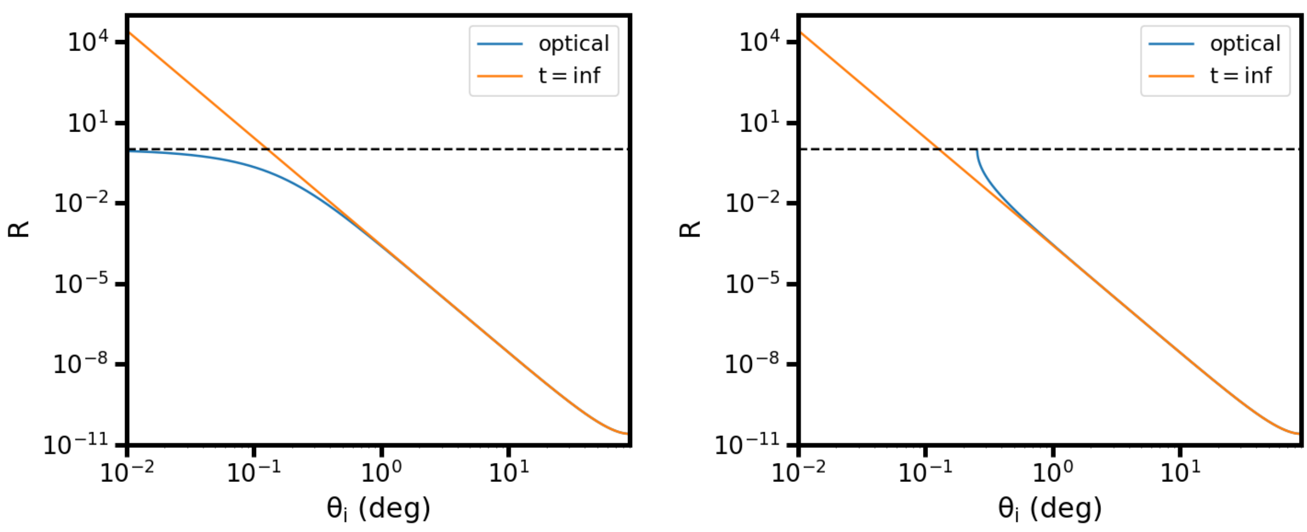
For a single interface (infinitely thick substrate in the half space $-\inf < z < 0$) we get:

$$R(Q) \approx \frac{16\pi^2}{Q^2}\Big|\int_{-t}^{0} \rho_b(z) e^{-i\,Q\,z} dz\Big|^2$$
$$= \frac{16\pi^2}{Q^2}\Big|\frac{\rho_b}{-i\,Q}e^{-i\,Q\,0} - \frac{\rho_b}{-i\,Q}e^{i\,Q\,\inf}\Big|^2$$

At this point we simply drop the term containing the exponential with $z = \inf$. The physical justification is, that for reflection and transmission only the interface between materials is important, not the bulk of a material. So we identify the term with $z = 0$ as the interface we are interested in. The second term is only of interest in thin samples or multylayers, where multiple reflections ca happen. As most materials are not infinitely thick, but only very thick compared to the neutron wave length, we need a criterion for when we are allowed to drop a term at large z. This is the case, if the sample is thicker than the neutron coherence length. In that case, waves reflected from different interfaces can no longer interfere which means the interfaces can be evaluated independent from each other. With this justification we arrive at the expression:

$$R(Q) = \frac{16\pi^2\rho_b^2}{Q^4} = \frac{(1-n^2)^2}{16\,\sin^4(\theta_i)}$$

The following images show the results for the correct optical calculation (blue) and the scattering approximation (orange) for the cases of $n = 1 + 10^{-5}$ (left) and $n = 1 - 10^{-5}$ (right). The approximation holds true for most of the angular range and only deviates below $\approx 0.5°$. However, at low angles the approximation cannot distinguish between the two cases of $n < 1$ and $n > 1$ and does not include total reflectivity at all.



Now we repeat the derivation for a thin layer of finite thickness, where we keep the second term of the integral:

$$R(Q) \approx \frac{16\pi^2}{Q^2}\Big|\int_{-\inf}^{0} \rho_b(z) e^{-i\,Q\,z} dz\Big|^2$$
$$= \frac{16\pi^2}{Q^2}\Big|\frac{\rho_b}{-i\,Q}e^{-i\,Q\,0} - \frac{\rho_b}{-i\,Q}e^{i\,Q\,t}\Big|^2$$
$$= \frac{16\pi^2\rho_b^2}{Q^4}\Big|1-e^{i\,Q\,t}\Big|^2 = \frac{16\pi^2\rho_b^2}{Q^4}(2-2\cos(Q\,t))$$
$$= \frac{(1-n^2)^2}{16\,\sin^4(\theta_i)}(2-2\cos(\frac{4\,\pi\,t}{\lambda}\,\sin(\theta_i)))$$

Again, this approximation is not valid for low θ or Q. However, it is much easier to calculate arbitrary structures, like multylayers or gradual changes in the scattering length density, which makes it a powerful and simple tool if you are interested in the high angle regime. The following image shows the result for a 10 nm thick layer with $n = 1 + 10^{-5}$ (without substrate) alongside the results for a single interface from before. The general trend at high angles is the same, but overlaid with an oscillation which stems from the interference of back reflected waves at the second layer. (This is very analogous to a double slit). The intensity can be higher than for the single interface because part of the transmitted beam is reflected back.