Physics with neutrons 1

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Winter semester 2015/16
Exercise sheet 2
Due 2015–Okt–30

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Exercise 2.1

Neutrons from fission ($E \approx 2MeV$) are slowed down to the thermal regime ($E \approx 20meV$) by scattering with the atoms of a moderator material. We assume that the scattering is purely elastic and nonrelativistic. Calculate the energy loss per collision event depending on the mass of the moderator atoms and on the scattering angle. How many collisions are needed to moderate fission neutrons to thermal neutrons in H2O, D2O and graphite?

Solution. For simplicity, we treat moderation as purely elastic, nonrelativistic scattering on a nucleus of mass number A without absorption. Let v be the initial neutron speed in the lab frame, while the nucleus is at rest.
First convert to the center-of-mass frame, moving with speed v_s:

$$m(A+1)v_s = mv + mAv_A.$$

With the nucleus speed $v_A = 0$ we get

$$v_s = \frac{v}{A+1}.$$

The initial speeds of the neutron V and the nucleus V_A in the center-of-mass frame are:

$$V = v - v_s = \frac{A}{A+1}\,v \quad \text{and} \quad V_A = -v_s = -\frac{1}{A+1}\,v.$$

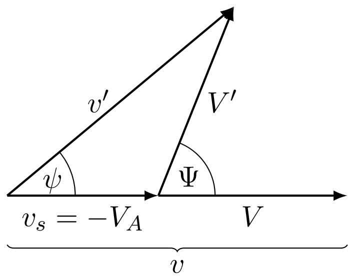
Let V' and V'_A be the center-of-mass speeds of neutron and nucleus after scattering. From energy and momentum conservation we get

$$V + AV_A = V' + AV'_A = 0 \text{ (center of mass!)} \quad \text{and} \quad V^2 + AV_A^2 = V'^2 + AV_A'^2$$

and therefore

$$|V| = |V'| \quad \text{and} \quad |V_A| = |V'_A|.$$

Let Ψ be the scattering angle in the center-of-mass frame (see sketch).



We can calculate the final speed in the lab frame using the cosine theorem:

$$v'^2 = V'^2 + V_A^2 - 2V'V_A\cos(\pi - \Psi) = V'^2 + V_A^2 + 2V'V_A\cos\Psi.$$

Inserting $|V'| = |V| = Av/(A+1)$ and $|V_A'| = |V_A| = V/(A+1)$ and multiplying by $m/2$, we get for the neutron energy

$$E' = E\left(1 - \frac{2A}{(A+1)^2}(1-\cos\Psi)\right),$$

or, with the convenient definition $\alpha = \left(\frac{A-1}{A+1}\right)^2$,

$$E' = \frac{1}{2}E\left((1+\alpha) + (1-\alpha)\cos\Psi\right).$$

The neutron energy loss is therefore

$$\Delta E = E - E' = \frac{1-\alpha}{2}\,E(1-\cos\Psi),$$

which has its maximum at $\Delta E_{\mathrm{max}} = (1-\alpha)E$.
To determine the average energy loss, we have to average over scattering angles Ψ. For isotropic scattering, the probability function for a certain angle, $w(\Psi)$ is given by

$$w(\Psi)d\Psi = \frac{1}{2}\sin\Psi\,d\Psi$$

The rationale for this is: the angle Ψ describes only the scattering angle within the scattering plane; there is another angle Φ defining the scattering plane. The term $\sin\Psi$ accounts for the possible choices of Φ for any given Ψ; for $\Psi = \pi/2$ this is maximal.
Another way to express this $w(\Psi)$ is to transform it to $w(\cos\Psi)$, which happens to be a constant:

$$w(\cos\Psi)d(\cos\Psi) = \frac{1}{2}\,d(\cos\Psi).$$

This means that for the average energy loss we can simply express $\overline{\cos\Psi}$ by the average value of its domain $[-1, 1]$, which is zero:

$$\overline{\Delta E} = \frac{1}{2}(1-\alpha)E.$$

The scattering angle in the lab frame, ψ, depends on the mass of the nucleus:

$$\cos\psi = \frac{A\cos\Psi + 1}{\sqrt{A^2 + 2A\cos\Psi + 1}}.$$

This means that although $\overline{\cos\Psi} = 0$, the average in the lab frame $\overline{\cos\psi} = 2/(3A)$, with the largest values for the smallest nuclei.
For determining n, the average number of collisions needed to thermalize a neutron from a given initial energy E_0 to a given energy E_{th}, we need to average over more than one scattering process. We can write this as

$$E_n = E_0 \prod_{i=1}^{n} \frac{(1+\alpha) + (1-\alpha)\cos\Psi_i}{2},$$

but need to keep in mind that the average of a product is not the product of the average of its factors. Therefore it is useful to define

$$\exp -\xi_i := \frac{(1+\alpha) + (1-\alpha)\cos\Psi_i}{2},$$

with the logarithmic energy decrement ξ, and with this we can transform the product into a sum:

$$\ln\frac{E_n}{E_0} = -\sum_{i=1}^{n} \xi_i,$$

where we can now apply averaging more easily (under the condition that the probability function $w(\cos\Psi)$ is independent of energy):

$$\overline{\ln\frac{E_n}{E_0}} = -n\overline{\xi}.$$

$\overline{\xi}$ can be calculated from the distribution of final energies E' after one collision: from $w(\cos\Psi)$ we can also calculate an energy probability $w(E \to E')dE'$:

$$w(E \to E')dE' = w(\cos\Psi)\frac{d\cos\Psi}{dE'}dE' = \frac{dE'}{(1-\alpha)E}$$

with the limits $\alpha E \le E' \le E$. With this result

$$\overline{\xi} = \int_{\alpha E}^{E} \ln\left(\frac{E}{E'}\right) w(E \to E')dE' = \int_{\alpha E}^{E} \ln\left(\frac{E}{E'}\right) \frac{dE'}{E(1-\alpha)} = 1 + \frac{\alpha\ln\alpha}{1-\alpha} \approx \frac{2}{A + \frac{2}{3}},$$

where the final approximation is good for $A > 2$.
Finally, the average number of collisions from E_0 to E_{th} is:

$$\overline{n} = -\frac{1}{\xi}\ln\frac{E_{th}}{E_0}.$$

With weighted summing over individual nuclei for molecular matter this gives us (for $E_0 = 2\,\mathrm{MeV}$, $E_{th} = 20\,\mathrm{meV}$): $\overline{n(\mathrm{H_2O})} \approx 26$, $\overline{n(\mathrm{D_2O})} \approx 35$ and $\overline{n(\mathrm{C})} \approx 116$. □

Exercise 2.2

From your solid state physics course you should remember the dispersion relation for phonons. Calculate the dispersion of an acoustic phonon of a linear chain of atoms with a lattice constant of $a = 2$ Å. The measured velocity of sound is assumed to be $v_s = 2300 m/s$. Draw the scattering diagram for an inelastic neutron scattering experiment with $kf = 2.57$ Å^{-1} at the boundary of the 2nd Brillouin zone. Consider phonon creation and annihilation.

Solution. The phonon dispersion of a linear chain of equal atoms is:

$$\omega(k) = 2\sqrt{\frac{D}{m}} \left|\sin \frac{ka}{2}\right|,$$

with an effective spring constant D, the atom mass m and the lattice constant a. (If we only take positive k into account, we can omit the absolute value.)
The velocity of sound is defined as the slope around $k = 0$:

$$v_s = \left.\frac{d\omega}{dk}\right|_{k=0} = 2\sqrt{\frac{D}{m}} \frac{a}{2} \cos \left.\frac{ka}{2}\right|_{k=0} = \sqrt{\frac{D}{m}} a,$$

so we can calculate the prefactor of the dispersion for the values given in the exercise:

$$\omega(k) = \frac{2v_s}{a} \sin \frac{ka}{2} = 23\,\mathrm{THz} \cdot \sin(k \cdot 1),$$

or, in terms of energy,

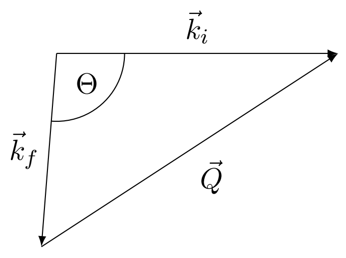
$$E(k) = 15\,\mathrm{meV} \cdot \sin(k \cdot 1).$$

For inelastic scattering, we need to know both q and $\hbar\omega$ of the excitation: the boundary of the second Brillouin zone is defined by $Q = 3\pi/a = 4.71$, and $E(3\pi/a) = 15\,\mathrm{meV}$ as calculated above. The final wavevector is given as $k_f = 2.57$. For calculation of the incident wavevector we use conservation of energy:

$$\frac{\hbar^2 k_i^2}{2m} = \frac{\hbar^2 k_f^2}{2m} \pm \hbar\omega \Longrightarrow k_i = \sqrt{k_f^2 \pm \frac{2m\omega}{\hbar}}.$$

For the "+" sign we get $k_i = 3.73$, while for the "–" sign the radicand is negative. In other words, only phonon creation can be observed with this fixed k_f.
The scattering angle can be calculated from the cosine theorem (see scattering diagram):

$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos\Theta \Longrightarrow \Theta = 94.5°.$$



□

Exercise 2.3

The Maxwell-Boltzmann distribution has been given in the lecture in units of Energy E and particle velocity v. Express the Maxwell-Boltzmann distribution

$$f(v) = \frac{4}{\sqrt{\pi}} \left(\frac{m_n}{2k_b T} \right)^{3/2} v^2 \exp\left(-\frac{\frac{1}{2} m_n v^2}{k_b T} \right)$$

in terms of the particle wavelength λ. Determine $\langle \lambda \rangle, \langle \lambda^2 \rangle$ and λ_{max} (i.e. the λ where $f(\lambda)$ is maximal). On the lecture website will find the data file `hfir_spectrum.xls`. It contains a neutron wavelength spectrum (1st column: wavelength in Å, 2nd column: intensity in arbitrary units) measured at the cold source of the HFIR reactor in Oak Ridge, USA. Use a fitting tool to fit the Maxwell-Boltzmann flux distribution to this data and extract the moderator temperature. Remember that the flux distribution is given by

$$\Psi(v) = v \cdot f(v)$$

Solution. To express the Maxwell-Boltzmann distribution in terms of wavelength, we have to calculate the differential:

$$f(v)\, dv = f(v(\lambda)) \frac{dv}{d\lambda}\, d\lambda.$$

De Broglie's relation helps there:

$$\lambda = \frac{h}{p} \Longrightarrow v = \frac{h}{m_n \lambda} \quad \text{and} \quad dv = -\frac{h}{m_n \lambda^2}\, d\lambda$$

The sign means that we have to exchange integration bounds when integrating over dλ. Now we can express $f(\lambda)\, d\lambda$:

$$f(\lambda)\, d\lambda = \frac{4}{\sqrt{\pi}} \left(\frac{m_n}{2k_b T} \right)^{3/2} \left(\frac{h}{m_n \lambda} \right)^2 \exp\left(-\frac{h^2/2m_n\lambda^2}{k_b T} \right) \frac{h}{m_n \lambda^2}\, d\lambda,$$

which can be simplified using $\lambda_T = h/\sqrt{2m_n k_b T}$, i.e. the wavelength that corresponds to the temperature T:

$$f(\lambda)\, d\lambda = \frac{4}{\sqrt{\pi}} \frac{\lambda_T^3}{\lambda^4} \exp\left(-\frac{\lambda_T^2}{\lambda^2} \right).$$

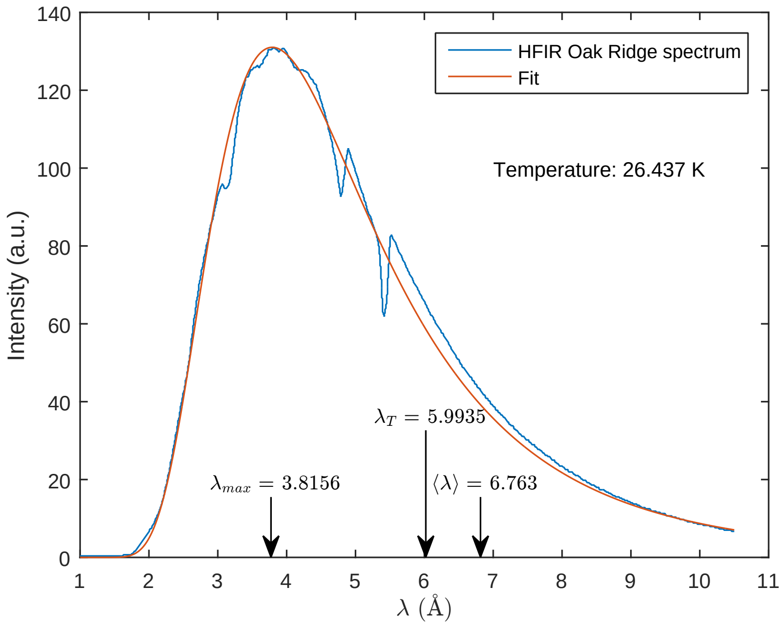
A bit of calculation gives:

$$\langle \lambda \rangle = \frac{2}{\sqrt{\pi}} \lambda_T,\ \langle \lambda^2 \rangle = 2\lambda_T^2,\ \lambda_{\max} = \sqrt{2}\lambda_T = \sqrt{\langle \lambda^2 \rangle}.$$

Compare to $f(v)$:

$$\langle v \rangle = \frac{2}{\sqrt{\pi}} v_T,\ \langle v^2 \rangle = \frac{3}{2} v_T^2,\ v_{\max} = v_T.$$

Plot and fit of the data file:



$$\text{Fitting function: } f(\lambda) = I_0 \cdot \frac{\lambda_T^3}{\lambda^5} \cdot \exp\left(-\frac{\lambda_T^2}{\lambda^2}\right)$$

The prefactor I_0 is arbitrary; the thermal wavelength is $\lambda_T \approx 6\,\text{Å}$.

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