

Appendix A2

A2.1 NEUTRON SCATTERING FROM A COLLECTION OF MOVING NUCLEI—THE SCATTERING LAW

When neutrons are scattered from a rigid array of nuclei the energy of the scattering system cannot change and so, by conservation of energy, the energy of the neutron cannot change either. Such scattering, where the neutron energy does not change, is conventionally referred to as elastic scattering. When we consider scattering from a real system in which the nuclei are able to move, there is a possibility of the scattering system exchanging energy with the scattered neutron. In this section we present the formalism (largely due to Van Hove (1954)) by which this type of scattering is usually discussed.

In Appendix A1 we saw that the elastic scattering was determined by the structure factor, $S(Q)$, which was related to the Fourier transform of the pair distribution function. In this section we will see that the inelastic scattering cross section is related to a function $S(Q, \omega)$ ($\hbar\omega$ is the energy lost by the neutron during the scattering) called the scattering law and given by the Fourier transform of a function $G(r, t)$ which is called the density correlation function and which represents the probability of finding a particle at position r at time t given that there was a particle at the origin ($r = 0$) at time $t = 0$.

We again consider the initial and final states of the neutron to be given by plane waves:

$$\psi_{i,f} = \frac{e^{i\mathbf{k}_{i,f} \cdot \mathbf{r}}}{L^{3/2}} \quad \text{with energies } \epsilon_{i,f} = \frac{\hbar^2 k_{i,f}^2}{2m} \quad (\text{A2.1})$$

where we have now normalized the neutron states to a volume L^3 . We will designate the states of the scattering system by quantum numbers n_i, n_f with energies E_i and E_f . Thus the initial and final states of the entire system (neutron plus scatterer) will be designated

$$|i\rangle = \frac{e^{i\mathbf{k}_i \cdot \mathbf{r}}}{L^{3/2}} |n_i\rangle \quad |f\rangle = \frac{e^{i\mathbf{k}_f \cdot \mathbf{r}}}{L^{3/2}} |n_f\rangle \quad (\text{A2.2})$$

As in (2.28) the interaction is taken as:

$$V(\mathbf{r}, \mathbf{R})$$

We again calculate the cross section per second by the incident neutron as follows

and we will calculate the cross section theory. The standard result (see e.g. 1968), in the case where the scattering is elastic, the case where the neutron energies are different is given by

$$dP = \frac{2\pi}{\hbar} \rho(\epsilon_f) d\epsilon_f$$

where $\rho(\epsilon_f) d\epsilon_f$ is the number of final states per unit energy $d\epsilon_f$ and is given by

for final states whose momentum is \mathbf{k}_f (A2.2), (A2.3) and (A2.5) the cross section per unit solid angle is called the double differential cross section

$$\frac{d^2\sigma}{d\Omega d\epsilon_f} = \frac{k_f}{k_i} \left| \langle n_f | \right.$$

where $\hbar\omega = \epsilon_i - \epsilon_f$ is the energy transferred. This is the cross section for the scattering system makes a transition from the initial state $|i\rangle$ to the final state $|f\rangle$. In the scattering situation the cross section means it will be distributed over all possible final states

where k_B is Boltzmann's constant. The probability of finding the system in the final states of the system is given by $| \langle n_f | \rho | n_i \rangle |^2$. Therefore the actual scattering cross section is over all possible final states

As in (2.28) the interaction between neutron and scattering system will be taken as:

$$V(\mathbf{r}, \mathbf{R}_i) = \frac{2\pi\hbar^2}{m} \sum_i a_i \delta^{(3)}(\mathbf{r} - \mathbf{R}_i). \tag{A2.3}$$

We again calculate the cross section by dividing the transition probability per second by the incident flux. The latter quantity is obtained from (A2.1) as follows

$$\text{incident flux} = \frac{1}{L^3} \cdot \frac{\hbar k_i}{m} \tag{A2.4}$$

and we will calculate the transition rate due to (A2.3) using perturbation theory. The standard result of perturbation theory (Golden Rule—Schiff 1968), in the case where there is a smooth distribution of final states (in our case the neutron energies form a continuum), is that the transition rate is given by

$$dP = \frac{2\pi}{\hbar} |\langle f|V|i \rangle|^2 \rho(\epsilon_f) \delta(E_f + \epsilon_f - E_i - \epsilon_i) \tag{A2.5}$$

where $\rho(\epsilon_f) d\epsilon_f$ is the number of states with final energies between ϵ_f and $\epsilon_f + d\epsilon_f$ and is given by

$$\rho(\epsilon_f) = \frac{mL^3}{8\pi^3\hbar^2} k_f d\Omega_f \tag{A2.6}$$

for final states whose momentum lies in the element of solid angle $d\Omega_f$. Using (A2.2), (A2.3) and (A2.5) and dividing by (A2.4) it is easy to see that the cross section per unit solid angle per unit final neutron energy—which is called the double differential cross section—is given by

$$\frac{d^2\sigma}{d\Omega d\epsilon_f} = \frac{k_f}{k_i} \left| \left\langle n_f \left| \sum_i a_i e^{i\mathbf{Q} \cdot \mathbf{R}_i} \right| n_i \right\rangle \right|^2 \delta(E_f - E_i - \hbar\omega) \tag{A2.7}$$

where $\hbar\omega = \epsilon_i - \epsilon_f$ is the energy lost by the neutron during the scattering. This is the cross section for a scattering process in which the scattering system makes a transition from the state $|n_i\rangle$ to the state $|n_f\rangle$. In an actual scattering situation the system is likely to be in thermal equilibrium which means it will be distributed over a range of initial states. We take

$$P_{n_i} = (1/Z) \exp[-E_i/k_B T]$$

where k_B is Boltzman's constant and Z is a normalizing constant, as the probability of finding the system in a particular initial state $|n_i\rangle$ and the final states of the system will be distributed over a range of states $|n_f\rangle$. Therefore the actual scattering cross section will be given by summing (A2.7) over all possible final states and averaging over the initial states. Thus the

cross section will be (we again divide by N to obtain the cross section per atom).

$$\frac{d^2\sigma}{d\Omega d\epsilon_f} = \frac{1}{N} \cdot \frac{k_f}{k_i} \sum_{n_f, n_i} P_{n_i} \left| \sum_i a_i \langle n_f | e^{i\mathbf{Q} \cdot \mathbf{R}_i} | n_i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega) \quad (\text{A2.8})$$

which we rewrite as

$$\begin{aligned} \frac{d^2\sigma}{d\Omega d\epsilon_f} &= \frac{1}{N} \cdot \frac{k_f}{k_i} \sum_{n_f, n_i} P_{n_i} \sum_{i,j} \overline{a_i^* a_j} \langle n_i | e^{-i\mathbf{Q} \cdot \mathbf{R}_i} | n_f \rangle \\ &\quad \times \langle n_f | e^{i\mathbf{Q} \cdot \mathbf{R}_j} | n_i \rangle \delta(E_f - E_i - \hbar\omega) \end{aligned} \quad (\text{A2.9})$$

where, as in (2.31), the bar refers to averaging over the spin and isotope distribution of the nuclei. Using (2.35) we can separate (A2.9) into a coherent and incoherent part:

$$\frac{d^2\sigma}{d\Omega d\epsilon_f} = \left(\frac{d^2\sigma}{d\Omega d\epsilon_f} \right)_{\text{coh}} + \left(\frac{d^2\sigma}{d\Omega d\epsilon_f} \right)_{\text{inc}} \quad (\text{A2.10})$$

where

$$\begin{aligned} \left(\frac{d^2\sigma}{d\Omega d\omega} \right)_{\text{coh}} &= \frac{\hbar k_f}{N k_i} \sum_{n_f, n_i} P_{n_i} a_{\text{coh}}^2 \left| \sum_i \langle n_f | e^{i\mathbf{Q} \cdot \mathbf{R}_i} | n_i \rangle \right|^2 \delta(E_f - E_i - \hbar\omega) \\ &\equiv a_{\text{coh}}^2 \frac{k_f}{k_i} S_{\text{coh}}(\mathbf{Q}, \omega) \end{aligned} \quad (\text{A2.11})$$

and

$$\begin{aligned} \left(\frac{d^2\sigma}{d\Omega d\omega} \right)_{\text{inc}} &= \frac{\hbar k_f}{N k_i} a_{\text{inc}}^2 \sum_{n_f, n_i} P_{n_i} \sum_i |\langle n_f | e^{i\mathbf{Q} \cdot \mathbf{R}_i} | n_i \rangle|^2 \delta(E_f - E_i - \hbar\omega) \\ &= a_{\text{inc}}^2 \frac{k_f}{k_i} S_{\text{inc}}(\mathbf{Q}, \omega) \end{aligned} \quad (\text{A2.12})$$

where we have written $d\epsilon_f = \hbar d\omega$ (ϵ_i is taken as fixed). We are interested in the Fourier transforms of $S_{\text{coh}}(\mathbf{Q}, \omega)$ and $S_{\text{inc}}(\mathbf{Q}, \omega)$ which we denote by $G(\mathbf{r}, t)$ and $G_s(\mathbf{r}, t)$ respectively.

$$G(\mathbf{r}, t) = \frac{1}{(2\pi)^3} \int \int e^{i(\omega t - \mathbf{Q} \cdot \mathbf{r})} S_{\text{coh}}(\mathbf{Q}, \omega) d^3\mathbf{Q} d\omega \quad (\text{A2.13})$$

which is from (A2.11)

$$\begin{aligned} G(\mathbf{r}, t) &= \frac{1}{(2\pi)^3} \frac{1}{N} \sum_{n_f, n_i} P_{n_i} \int d^3\mathbf{Q} \sum_{i,j} e^{-i\mathbf{Q} \cdot \mathbf{r}} \langle n_i | e^{-i\mathbf{Q} \cdot \mathbf{R}_i} | n_f \rangle \\ &\quad \times \langle n_f | e^{iE_i t} e^{i\mathbf{Q} \cdot \mathbf{R}_j} e^{-iE_i t} | n_i \rangle. \end{aligned} \quad (\text{A2.14})$$

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so we can see that

$$G(\mathbf{r}, t) = \frac{1}{N} \sum_i P_{n_i}$$

$$G_s(\mathbf{r}, t) = \frac{1}{N} \sum_{n_i} P_{n_i}$$

Note that we have carried out the ω -integration by using the properties of the energy conservation δ -function, and omitted a factor of \hbar from the energy exponents.

We recall that we can describe time-dependent situations in quantum mechanics by means of the 'Heisenberg picture' in which the quantum mechanical operators are time-dependent and the quantum states are independent of time. The time-dependent form of an operator \mathbf{R}_j , is given by

$$\mathbf{R}_j(t) = e^{iHt/\hbar} \mathbf{R}_j(0) e^{-iHt/\hbar} \quad (\text{A2.15})$$

where H is the Hamiltonian of the system and $\mathbf{R}_j(0)$ is the operator at $t = 0$. By expanding the exponential $e^{i\mathbf{Q} \cdot \mathbf{R}_j(t)}$ in a power series and applying (A2.15) to each term we obtain

$$e^{i\mathbf{Q} \cdot \mathbf{R}_j(t)} = e^{iHt/\hbar} e^{i\mathbf{Q} \cdot \mathbf{R}_j(0)} e^{-iHt/\hbar} \quad (\text{A2.16})$$

which is the operator in the second matrix element in (A2.14).

Note

$$H |n_{i,f}\rangle = E_{i,f} |n_{i,f}\rangle. \quad (\text{A2.17})$$

Thus

$$G(\mathbf{r}, t) = \frac{1}{(2\pi)^3 N} \sum_{n_i} P_{n_i} \sum_{i,j} \int d^3 Q e^{-i\mathbf{Q} \cdot \mathbf{r}} \langle n_i | e^{-i\mathbf{Q} \cdot \mathbf{R}_i(0)} e^{i\mathbf{Q} \cdot \mathbf{R}_j(t)} | n_i \rangle \quad (\text{A2.18})$$

and by a similar argument:

$$G_s(\mathbf{r}, t) = \frac{1}{(2\pi)^3 N} \sum_{n_i} P_{n_i} \sum_i \int d^3 Q e^{-i\mathbf{Q} \cdot \mathbf{r}} \langle n_i | e^{-i\mathbf{Q} \cdot \mathbf{R}_i(0)} e^{i\mathbf{Q} \cdot \mathbf{R}_i(t)} | n_i \rangle. \quad (\text{A2.19})$$

Now (A2.18) and (A2.19) are the Fourier transforms of a product of two operators. As is well known the Fourier transform of a product of two functions (A and B) is given by the convolution of the Fourier transforms of A and B (Champeney 1973). We also know that, for example

$$\frac{1}{(2\pi)^3} \int d^3 Q e^{-i\mathbf{Q} \cdot \mathbf{r}} e^{-i\mathbf{Q} \cdot \mathbf{R}_i(0)} = \delta^{(3)}(\mathbf{r} + \mathbf{R}_i(0)) \quad (\text{A2.20})$$

so we can see that

$$G(\mathbf{r}, t) = \frac{1}{N} \sum_i P_{n_i} \sum_{i,j} \int d^3 r' \langle n_i | \delta^{(3)}(\mathbf{r} + \mathbf{R}_i(0) - \mathbf{r}') \delta^{(3)}(\mathbf{r}' - \mathbf{R}_j(t)) | n_i \rangle \quad (\text{A2.21})$$

$$G_s(\mathbf{r}, t) = \frac{1}{N} \sum_{n_i} P_{n_i} \sum_i \int d^3 r' \langle n_i | \delta^{(3)}(\mathbf{r} + \mathbf{R}_i(0) - \mathbf{r}') \delta^{(3)}(\mathbf{r}' - \mathbf{R}_i(t)) | n_i \rangle. \quad (\text{A2.22})$$

If the $R_i(t)$ were classical quantities, instead of operators, we could evaluate the integrals to obtain:

$$G(\mathbf{r}, t) = \frac{1}{N} \sum_{n_i} P_{n_i} \sum_{i,j} \langle n_i | \delta^{(3)}(\mathbf{r} + \mathbf{R}_i(0) - \mathbf{R}_j(t)) | n_i \rangle \quad (\text{A2.23})$$

with a similar result for $G_s(\mathbf{r}, t)$.

By the same argument as was given following (A1.4) we see that this is the probability density of finding an atom at position \mathbf{r} at time t given that there was an atom at the origin ($\mathbf{r} = 0$) at time $t = 0$. Similarly $G_s(\mathbf{r}, t)$ is the probability density of finding an atom at time t , given the same atom was at the origin at $t = 0$. The function $G(\mathbf{r}, t)$ is called the space-time pair correlation function while $G_s(\mathbf{r}, t)$ is called the space-time self-correlation function. In quantum mechanics these correlation functions, strictly speaking do not exist, since $R_i(0)$ and $R_i(t)$ do not commute and are not measurable simultaneously. Thus in general it is necessary to work with (A2.21) and (A2.22).

For $t = 0$ all the $R_i(0)$ commute so we can write from (A2.21):

$$G(\mathbf{r}, 0) = \frac{1}{N} \sum_{n_i} P_{n_i} \sum_{i,j} \langle n_i | \delta^{(3)}(\mathbf{r} + \mathbf{R}_i(0) - \mathbf{R}_j(0)) | n_i \rangle \quad (\text{A2.24})$$

and separating into terms with $i = j$ and $i \neq j$ we obtain:

$$\begin{aligned} G(\mathbf{r}, 0) &= \delta^{(3)}(\mathbf{r}) + \frac{1}{N} \sum_{n_i} P_{n_i} \sum_{i \neq j} \delta^{(3)}(\mathbf{r} + \mathbf{R}_i(0) - \mathbf{R}_j(0)) \\ &= \delta^{(3)}(\mathbf{r}) + g(\mathbf{r}) \end{aligned} \quad (\text{A2.25})$$

from (A1.4) and (A1.5). Thus $G(\mathbf{r}, 0)$ is the spatial Fourier transform of the structure factor $S(\mathbf{Q})$.

Since for any function of time the integral of the Fourier transform over all ω is equal to the function evaluated at $t = 0$ it is easy to see that

$$\int S(\mathbf{Q}, \omega) d\omega = S(\mathbf{Q}) \quad (\text{A2.26})$$

a result known as the zero-moment sum rule.

In general it is not possible to calculate $S(\mathbf{Q}, \omega)$ from first principles but its general behaviour can be understood in physical terms and discussion of scattering measurements in terms of $G(\mathbf{r}, t)$ often leads to increased physical insight. If r_0 is the correlation length and τ the correlation time of $G(\mathbf{r}, t)$, i.e. values of r and t for which $G(\mathbf{r}, t)$ shows significant variations, then

since $G(\mathbf{r}, t)$ and $S(\mathbf{Q}, \omega)$ be significant for $Q \sim \dots$

By making use of

we can prove that

if the scattering system is in a state of detailed balance.

$$\epsilon_i e^{-\epsilon_i/k_B T} \sigma(\epsilon_i \rightarrow \epsilon_f, \Omega_f) = \epsilon_f e^{-\epsilon_f/k_B T} \sigma(\epsilon_f \rightarrow \epsilon_i, \Omega_i)$$

where $\sigma(\epsilon_i \rightarrow \epsilon_f, \Omega_f)$ is the cross-section for ϵ_i travelling in the direction Ω_i as a result of the scattering process.

Since the Maxwell-Boltzmann distribution

where Φ_0 is the total number of transitions per second from $\Omega_i \rightarrow \Omega_f$ is exactly the same as the number of transitions from $\epsilon_f \rightarrow \epsilon_i, \Omega_f$ to a moderator at temperature T in equilibrium with the scattering system, the scattering takes place at the same rate.

We will have occasion to discuss the scattering cross-section of UCN.

A2.2 MODELS

A2.2.1 Diffusion

As a simple model for neutron diffusion we use the diffusion equation. This is compared with the scattering measurements at inter-atomic distances.

From (A2.14) we

since $G(\mathbf{r}, t)$ and $S(\mathbf{Q}, \omega)$ form a Fourier transform pair the scattering will be significant for $Q \sim 1/r_0$ and $\omega \sim 1/\tau$.

By making use of the fact that:

$$(A2.23) \quad \langle n_f | e^{i\mathbf{Q} \cdot \mathbf{R}} | n_i \rangle = (\langle n_i | e^{-i\mathbf{Q} \cdot \mathbf{R}} | n_f \rangle)^* \quad (A2.27)$$

we can prove that

$$S(-\mathbf{Q}, -\omega) = e^{-\hbar\omega/k_B T} S(\mathbf{Q}, \omega) \quad (A2.28)$$

if the scattering system is in thermal equilibrium. This is called the principle of detailed balance. From (A2.11) and (A2.28) it follows that

$$\epsilon_i e^{-\epsilon_i/k_B T} \sigma(\epsilon_i \rightarrow \epsilon_f, \Omega_i \rightarrow \Omega_f) = \epsilon_f e^{-\epsilon_f/k_B T} \sigma(\epsilon_f \rightarrow \epsilon_i, \Omega_f \rightarrow \Omega_i) \quad (A2.29)$$

where $\sigma(\epsilon_i \rightarrow \epsilon_f, \Omega_i \rightarrow \Omega_f)$ is the cross section for a neutron with energy ϵ_i travelling in the direction Ω_i finishing up with an energy ϵ_f travelling in the direction Ω_f as a result of the scattering.

Since the Maxwell-Boltzmann flux distribution is given by

$$(A2.24) \quad \Phi(\epsilon) d\epsilon = \Phi_0 \frac{\epsilon}{k_B T} e^{-\epsilon/k_B T} \frac{d\epsilon}{k_B T} \quad (A2.30)$$

where Φ_0 is the total flux, we see the significance of (A2.29). The number of transitions per second made by neutrons from energy $\epsilon_i \rightarrow \epsilon_f$, direction $\Omega_i \rightarrow \Omega_f$ is exactly balanced by the number of neutrons per second going from $\epsilon_f \rightarrow \epsilon_i, \Omega_f \rightarrow \Omega_i$ if the neutrons are in thermal equilibrium in a moderator at temperature T . Thus when the neutrons are in thermal equilibrium with the moderator the balance is 'detailed', i.e. every transition takes place at the same rate as its inverse.

We will have occasion to make use of these properties of $S(\mathbf{Q}, \omega)$ and the scattering cross section in our discussions of the scattering and production of UCN.

A2.2 MODELS OF $G(\mathbf{r}, t)$

A2.2.1 Diffusion

As a simple model we consider a classical liquid whose density obeys the diffusion equation. This should be valid for liquids and gases for times large compared with the collision time and distances large compared with the inter-atomic distance.

From (A2.14) we see that

$$G^*(\mathbf{r}, t) = G(-\mathbf{r}, -t) \quad (A2.31)$$

with a similar expression for $G_s(\mathbf{r}, t)$.

From (A2.13) this is only the condition that $S(\mathbf{Q}, \omega)$ and the scattering cross sections be real. The diffusion equation follows from the equation of continuity (conservation of matter (2.58))

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (\text{A2.32})$$

and the diffusion approximation

$$\mathbf{j} = -D\nabla \rho \quad (\text{A2.33})$$

where D is the diffusion constant. Thus

$$\frac{\partial \rho}{\partial t} - D\nabla^2 \rho = 0. \quad (\text{A2.34})$$

To find the self-correlation function $G_s(\mathbf{r}, t)$ we solve (A2.34) with the initial condition of a particle at the origin at $t = 0$

$$\frac{\partial g_s(\mathbf{r}, t)}{\partial t} - D\nabla^2 g_s(\mathbf{r}, t) = \delta^{(3)}(\mathbf{r}) \delta(t). \quad (\text{A2.35})$$

Putting

$$g_s(\mathbf{r}, t) = \frac{1}{(2\pi)^3} \int d^3 Q e^{i\mathbf{Q} \cdot \mathbf{r}} \gamma(\mathbf{Q}, t) \quad (\text{A2.36})$$

we obtain

$$\frac{\partial \gamma(\mathbf{Q}, t)}{\partial t} + DQ^2 \gamma(\mathbf{Q}, t) = \delta(t) \quad (\text{A2.37})$$

with a solution

$$\gamma(\mathbf{Q}, t) = e^{-DQ^2 t} \Theta(t) \quad (\text{A2.38})$$

where Θ is the unit step function. Substituting in (A2.36) we find

$$g_s(\mathbf{r}, t) = \frac{1}{(4\pi Dt)^{3/2}} e^{-r^2/4Dt} \Theta(t). \quad (\text{A2.39})$$

This is the solution of the problem with the initial condition $g_s(\mathbf{r}, t) = 0$ for $t \leq 0$.

Now $G_s(\mathbf{r}, t)$ must satisfy condition (A2.31) so it is necessary to symmetrize (A2.39) with respect to the time to obtain

$$G_s(\mathbf{r}, t) = \frac{1}{(4\pi D|t|)^{3/2}} e^{-r^2/4|t|D}. \quad (\text{A2.40})$$

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Writing

$$I_s(\mathbf{Q}, t) = \int d^3r e^{i\mathbf{Q} \cdot \mathbf{r}} G_s(\mathbf{r}, t) \tag{A2.41}$$

($I_s(\mathbf{Q}, t)$ is called the intermediate scattering function) we find

$$I_s(\mathbf{Q}, t) = e^{-DQ^2|t|} \tag{A2.42}$$

and

$$S(\mathbf{Q}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{-i\omega t} e^{-DQ^2|t|} \tag{A2.43}$$

$$= \frac{1}{2\pi} 2\mathcal{R}_e \int_0^{\infty} dt e^{-i\omega t} e^{-DQ^2 t} \tag{A2.44}$$

$$S(\mathbf{Q}, \omega) = \frac{1}{\pi} \frac{DQ^2}{(\omega^2 + (DQ^2)^2)} \tag{A2.45}$$

i.e. a Lorentzian in ω with width DQ^2 .

This is a basic result in scattering theory and was first obtained by Vineyard (1958). As we said it should hold for small Q (large distances) and small ω (large times). It serves as the starting point for more accurate treatments.

For example replacing the width of the Gaussian in (A2.40) $4D|t|$ by $2\Gamma(t)$ leads to the 'Gaussian approximation' where more complicated kinds of diffusion can be represented by various forms for $\Gamma(t)$ (Turchin 1965). In liquid Na at 800 K DQ^2 in (A2.45) must be replaced by $DQ^2(1 - aQ)$ with $a = 0.15 \text{ \AA}$ (Morkel *et al* 1987).

A2.2.2 Small motions of large objects

In many large molecules of biological interest there are motions which involve large pieces of a molecule moving over relatively small distances. An example is the motions in the myoglobin molecule which are involved in the opening of a channel allowing an oxygen molecule to be captured or emitted (Parak and Knapp 1984).

In this section we give a simple classical model of the neutron scattering for such a system. As a model we take a spherical shell of radius R , thickness ϵ of density ρ surrounded by an infinite medium of density ρ_0 with $\delta\rho = \rho - \rho_0$. The centre of the shell is located at a position $\mathbf{r} = \mathbf{c}$ and motion of the sphere is represented by taking \mathbf{c} as a function of time.

We start with (2.93) for the static case

$$f(\theta) = a \int d^3r \rho(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} \tag{A2.46}$$

and apply it to this case. We have

$$\begin{aligned} \frac{f(\theta)}{a} &= \int_{\text{shell}} d^3r \rho(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} + \int_{\text{outside shell}} d^3r \rho_0(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} \\ &= \int_{\text{allspace}} d^3r \rho_0(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} + \int_{\text{shell}} d^3r \delta\rho(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}} \\ &= (2\pi)^3 \delta^{(3)}(\mathbf{Q}) + \int_{\text{shell}} d^3r \delta\rho(\mathbf{r}) e^{i\mathbf{Q} \cdot \mathbf{r}}. \end{aligned} \tag{A2.47}$$

Thus we see that in a uniform medium (first term) there is no scattering for $\mathbf{Q} \neq 0$ and the scattering occurs only on inhomogeneities.

We now extend (A2.47) to the time-dependent case

$$f(\mathbf{Q}, \omega) = a \int d^3r \delta\rho(\mathbf{r}, t) e^{i(\mathbf{Q} \cdot \mathbf{r} - \omega t)} dt \tag{A2.48}$$

carrying out the integration over d^3r for the spherical shell centred at $\mathbf{r} = \mathbf{c}(t)$ we have (see equation (A2.52))

$$f(\mathbf{Q}, \omega) = a\delta\rho (4\pi R^2 \epsilon) \int dt e^{-i\omega t} \frac{\sin QR}{QR} e^{i\mathbf{Q} \cdot \mathbf{c}(t)} \tag{A2.49}$$

where we have used the property of Fourier transforms that if $F(\mathbf{Q})$ is the Fourier transform of $f(\mathbf{r})$ then $e^{i\mathbf{Q} \cdot \mathbf{c}} F(\mathbf{Q})$ is the Fourier transform of $f(\mathbf{r} - \mathbf{c})$. Taking $\mathbf{c}(t) = c_0 \cos \omega_0 t$ the time integral in (A2.49) can be evaluated using

$$J_n(z) = \frac{i^{-n}}{2\pi} \int_0^{2\pi} e^{iz \cos \varphi} e^{-in\varphi} d\varphi \tag{A2.50}$$

Champeney (1973), so that the result is

$$\begin{aligned} f(\mathbf{Q}, \omega) &\propto a\delta\rho \frac{R^2 \epsilon}{\omega_0} \left(\frac{\sin QR}{QR} \right) \sum_{n=-\infty}^{\infty} (i)^{-n} J_n(Qc_0 \cos \theta) \delta(\omega - n\omega_0) \\ &\propto a\delta\rho \frac{R^2 \epsilon}{\omega_0} \left(\frac{\sin QR}{QR} \right) \sum_{n=-\infty}^{\infty} \frac{(i)^{-n}}{n!} \left(\frac{Qc_0 \cos \theta}{2} \right)^n \delta(\omega - n\omega_0) \end{aligned} \tag{A2.51}$$

where θ is the angle between \mathbf{Q} and \mathbf{c}_0 and the last step is made under the assumption that $Qc_0 \ll 1$.

$$\left(\text{Note that } J_n(x) = \frac{1}{n!} \left(\frac{x}{2} \right)^n \quad \text{for } x \ll 1. \right)$$

There are two things to note that the scattering is spherically symmetric. First, determined by the size of the scattering motion. Second, remembering that in the cross section we see that the scattering is phonon scattering (A3.1) and an energy-conserving process. The derivation of the phonon cross section

A2.2.3 Scattering from a shell

We proceed as in the previous section. In general the three-dimensional cross section can be calculated as

$$\begin{aligned} F(\mathbf{Q}) &= \int d^3r e^{-i\mathbf{Q} \cdot \mathbf{r}} \\ &= 4\pi \int f(r) r^2 dr \end{aligned}$$

For a spherical region of radius R in a surrounding medium $\delta\rho$

$$\begin{aligned} \frac{f(\theta)}{a} &= \frac{4\pi\delta\rho}{Q} \int_0^R r^2 dr \\ &= 4\pi R^3 a \delta\rho \end{aligned}$$

where $j_1(x)$ is the spherical Bessel function

(see Abramowitz and Stegun (1968) for Bessel functions). Then

$$S(\mathbf{Q}) = \left| \frac{F(\mathbf{Q})}{F(0)} \right|^2$$

Using (A1.5) and (2.109)

$$\sigma_{\text{tot}} = \int d\Omega S(\mathbf{Q})$$

where we took $k_i = k_f = k$

There are two things to note about (A2.51). First the Q dependence is such that the scattering is significant only for $Q \lesssim \pi/R$; that is the Q range is determined by the size of the moving object, not by the amplitude of the motion. Second, remembering we must take $|f(Q, \omega)|^2$ to get a scattering cross section we see that the term for $n = 1$ is very similar to the one for phonon scattering (A3.27) with the cross section proportional to $(Q \cdot \xi)^2$ and an energy-conserving δ -function. Thus we have outlined a semi-classical derivation of the phonon-scattering cross section.

A2.2.3 Scattering from static spherical inhomogeneities

We proceed as in the previous section starting with equation (A2.48). In general the three-dimensional Fourier transform of a function of $r = |\mathbf{r}|$ can be calculated as

$$\begin{aligned}
 F(Q) &= \int d^3r e^{-i\mathbf{Q} \cdot \mathbf{r}} f(r) = 2\pi \int_0^\pi \sin \theta d\theta e^{-iQr \cos \theta} \int r^2 dr f(r) \\
 &= 4\pi \int f(r) \frac{\sin Qr}{Qr} r^2 dr.
 \end{aligned}
 \tag{A2.52}$$

For a spherical region of radius R , and uniform density difference to the surrounding medium $\delta\rho$ we have, from (A2.47) and (A2.52)

$$\begin{aligned}
 \frac{f(\theta)}{a} &= \frac{4\pi\delta\rho}{Q} \int_0^R r \sin Qr dr = 4\pi R^3 a \delta\rho \left(\frac{\sin QR}{(QR)^3} - \frac{\cos QR}{(QR)^2} \right) \\
 &= 4\pi R^3 a \delta\rho \left(\frac{j_1(QR)}{QR} \right)
 \end{aligned}
 \tag{A2.53}$$

where $j_1(x)$ is the spherical Bessel function of order 1

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}
 \tag{A2.54}$$

(see Abramowitz and Stegun (1964) for the properties of spherical Bessel functions). Then

$$S(Q) = \left| \frac{f(\theta)}{a} \right|^2 = (4\pi R^3 \delta\rho)^2 \left(\frac{j_1(QR)}{QR} \right)^2.
 \tag{A2.55}$$

Using (A1.5) and (2.109) we have

$$\sigma_{\text{tot}} = \int d\Omega \left(\frac{d\sigma}{d\Omega} \right) = \frac{2\pi a^2}{k^2} \int S(Q) Q dQ
 \tag{A2.56}$$

where we took $k_i = k_f = k$. Substituting (A2.55) we find

$$\sigma_{\text{tot}} = \frac{2\pi a^2}{k^2} (4\pi R^2 \delta\rho)^2 \int_{k\theta_1}^{2k} \frac{[j_1(QR)]^2}{Q} dQ \quad (\text{A2.57})$$

where the lower limit on Q is determined by the angle subtended by the detector (θ_1)—neutrons scattered through a smaller angle hit the detector and are not counted as scattered in total cross section measurements ('in-scattering'). For large enough k (i.e. $kR \gg 1$) we can take the upper limit as ∞ . Substituting $x = QR$, the integral in (A2.57) is (Lengsfeld 1977)

$$\int \frac{[j_1(x)]^2}{x} dx = -\frac{1}{4} [j_0^2(x) + j_1^2(x)] \quad (\text{A2.58})$$

as can be seen by differentiating the right-hand side using

$$\begin{aligned} \frac{dj_0(x)}{dx} &= -j_1(x) \\ \frac{dj_1(x)}{dx} &= j_0(x) - \frac{2}{x} j_1(x) \end{aligned} \quad (\text{A2.59})$$

(Abramowitz and Stegun 1964). Using (A2.54) and

$$j_0(x) = \frac{\sin x}{x} \quad (\text{A2.60})$$

we have

$$g(x) \equiv j_0^2(x) + j_1^2(x) = \frac{1}{x^2} + \frac{\sin^2 x}{x^4} - \frac{2 \sin x \cos x}{x^3} \quad (\text{A2.61})$$

Thus

$$g(0) = 1 \quad \lim_{x \rightarrow \infty} g(x) = \frac{1}{x^2}$$

so that (A2.57) gives

$$\sigma_{\text{tot}} = \frac{\pi a^2 (4\pi R^2 \delta\rho)^2}{2k^2} \quad (\text{A2.62})$$

i.e. $\propto 1/k^2$ when 'in-scattering' is negligible ($\theta_1 \rightarrow 0$) and

$$\sigma_{\text{tot}} = \frac{\pi a^2}{2k^4 \theta_1^2} (4\pi R \delta\rho)^2 \quad (\text{A2.63})$$

i.e. $\propto 1/k^4$ when k is large so that 'in-scattering' dominates and the detector measures only the scattering which is in the high Q tail. Comparing the asymptotic forms (A2.62) and (A2.63) we see that the intersection of their extrapolation occurs when

$$k_1 = \frac{1}{R\theta_1} \quad (\text{A2.64})$$

and hence can serve as a measure of the size of the scattering objects.

Append

A3.1 PHONON INELASTIC

We will now turn to the problem of neutron scattering from a crystal. Our main goals are to understand the coherent and incoherent scattering. We present some results for simplicity. For simplicity we consider one atom per unit cell as

where ρ_i represent the mass density and $u_i(t)$ represent the displacement. It is a basic assumption that the kinetic energy of the atoms in the

and the potential energy. We take the zero of energy for all i and expand the series in u_i . The

where the $\alpha_{i,j}^{\mu,\nu}$ are the force constants and μ and ν label the