Dynamic Structure Factor

Masaru Okada (岡田 大)

2025 年 10 月 24 日

These are notes on the dynamic structure factor. The discussion is set in the context of neutron scattering.

On the Interaction Between Neutrons and the Lattice

Consider a neutron with momentum $\vec{p}$ being scattered by a crystal, emerging with momentum $\vec{p'}$. Before the scattering, the lattice is assumed to be in an eigenstate of the crystal Hamiltonian with energy E_{i}, and after scattering, it is in an eigenstate with energy E_{f}. The states of the combined neutron-lattice system are, respectively:

Wave function and eigenenergy before scattering:

$$\Psi_{\mathrm{i}} = \psi_{\vec{p}}(\vec{r})\Phi_{\mathrm{i}} \tag{1}$$

$$\varepsilon_{\mathrm{i}} = E_{\mathrm{i}} + \frac{p^2}{2M_n} \tag{2}$$

Wave function and eigenenergy after scattering:

$$\Psi_{\mathrm{f}} = \psi_{\vec{p'}}(\vec{r})\Phi_{\mathrm{f}} \tag{3}$$

$$\varepsilon_{\mathrm{f}} = E_{\mathrm{f}} + \frac{p'^2}{2M_n} \tag{4}$$

Here, M_n is the neutron mass, and V is the volume of the system, used as a normalization constant. The function $\psi_{\vec{p}}(\vec{r})$ is a plane wave $\psi_{\vec{p}}(\vec{r}) = \dfrac{1}{\sqrt{V}}e^{i\vec{p}\cdot\vec{r}}$. The energy gain and momentum change of the lattice are:

$$\hbar\omega = \frac{p'^2}{2M_n} - \frac{p^2}{2M_n} \tag{5}$$

$$\hbar\vec{q} = \vec{p'} - \vec{p} \tag{6}$$

Letting $\vec{R}$ be a lattice point and $\vec{r}(\vec{R})$ be the position of the ion belonging to $\vec{R}$, which fluctuates due to heat etc., the neutron-lattice interaction is:

$$U(\vec{r}) = \sum_{\vec{R}} u\big[\vec{r} - \vec{r}(\vec{R})\big] \;=\; \frac{1}{V}\sum_{\vec{k},\vec{R}} u_{\vec{k}} e^{i\vec{k}\cdot[\vec{r}-\vec{r}(\vec{R})]} \tag{7}$$

The range of the interaction $u\big[\vec{r} - \vec{r}(\vec{R})\big]$ is at most the size of the nucleus, i.e., about 10^{-13} cm. Its Fourier component $u_{\vec{k}}$ is thought to vary on the scale of $k \sim 10^{13}$ cm^{-1}. The important scale for the phonon spectrum is a wave vector of about 10^8 cm^{-1}, and compared to this, the variation of k is sufficiently slow (by a factor of 10^5). Therefore, the Fourier component of the interaction $u_{\vec{k}}$ can be regarded as independent of the wave vector, and we will write this constant as u_0.

Suppose the total scattering cross-section for a single lattice point is given by $4\pi a^2$. Using the averaged length a that characterizes this scattering,

$$u_0 = 4\pi a^2 \times \frac{\hbar^2}{2M_n}\frac{1}{a} \tag{8}$$

we have,

$$U(\vec{r}) = \frac{2\pi\hbar^2 a}{M_n V}\sum_{\vec{k},\vec{R}} e^{i\vec{k}\cdot[\vec{r}-\vec{r}(\vec{R})]} \tag{9}$$

Note that performing the $\vec{k}$ integration yields,

$$\begin{aligned} U(\vec{r}) &= \frac{2\pi\hbar^2 a}{M_n}\sum_{\vec{R}}\int \frac{d^3\vec{k}}{(2\pi)^3} e^{i\vec{k}\cdot[\vec{r}-\vec{r}(\vec{R})]} \\ &= \frac{2\pi\hbar^2 a}{M_n}\sum_{\vec{R}} \delta[\vec{r}-\vec{r}(\vec{R})] \end{aligned} \tag{10}$$

This naturally shows that the assumptions we have made are, in fact, equivalent to assuming that the interaction is a point-contact type that acts only on the lattice points.

Fermi's Golden Rule and the Scattering Cross-Section

The probability P per unit time of scattering from $\vec{p}$ to $\vec{p'}$ can be calculated to the lowest order of perturbation theory using the formula known as Fermi's Golden Rule. Writing the inner product of functions $f = f(x)$ and $g = g(x)$ as

$$\int dx \big[f(x)\big]^* g(x) = \big(f, g\big) \tag{11}$$

we can calculate P as:

$$
\begin{aligned}
P &= \frac{2\pi}{\hbar}\sum_{\mathrm{f}}\delta(\varepsilon_{\mathrm{f}}-\varepsilon_{\mathrm{i}})\Big|\big(\Psi_{\mathrm{f}},U\Psi_{\mathrm{i}}\big)\Big|^2 \\
&= \frac{2\pi}{\hbar}\sum_{\mathrm{f}}\delta(E_{\mathrm{f}}-E_{\mathrm{i}}+\hbar\omega)\bigg|\frac{1}{V}\int d^3\vec{r}\; e^{i\vec{q}\cdot\vec{r}}\big(\Phi_{\mathrm{f}},U(\vec{r})\Phi_{\mathrm{i}}\big)\bigg|^2 \\
&= \frac{2\pi}{\hbar}\frac{1}{V^2}\Big(\frac{2\pi\hbar^2 a}{M_n V}\Big)^2\sum_{\mathrm{f}}\delta(E_{\mathrm{f}}-E_{\mathrm{i}}+\hbar\omega)\bigg|\sum_{\vec{k},\vec{R}}\int d^3\vec{r}\; e^{i(\vec{k}+\vec{q})\cdot\vec{r}}\big(\Phi_{\mathrm{f}},e^{-i\vec{k}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\bigg|^2 \\
&= \frac{(2\pi\hbar)^3}{V^2(M_nV)^2}a^2\sum_{\mathrm{f}}\delta(E_{\mathrm{f}}-E_{\mathrm{i}}+\hbar\omega)\bigg|\sum_{\vec{k},\vec{R}}(2\pi\hbar)^3\delta(\vec{k}+\vec{q})\big(\Phi_{\mathrm{f}},e^{-i\vec{k}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\bigg|^2 \\
&= \frac{(2\pi\hbar)^3}{V^2(M_nV)^2}a^2\sum_{\mathrm{f}}\delta(E_{\mathrm{f}}-E_{\mathrm{i}}+\hbar\omega)\bigg|\sum_{\vec{R}}(2\pi\hbar)^3\frac{V}{(2\pi\hbar)^3}\int d^3\vec{k}\;\delta(\vec{k}+\vec{q})\big(\Phi_{\mathrm{f}},e^{-i\vec{k}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\bigg|^2 \\
&= \frac{(2\pi\hbar)^3}{(M_nV)^2}a^2\sum_{\mathrm{f}}\delta(E_{\mathrm{f}}-E_{\mathrm{i}}+\hbar\omega)\bigg|\sum_{\vec{R}}\big(\Phi_{\mathrm{f}},e^{i\vec{q}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\bigg|^2 \qquad (12)
\end{aligned}
$$

The scattering probability P is related to the measurable quantity, the differential scattering cross-section $\dfrac{d^3\sigma}{d^2\Omega dE}$. The incident neutron flux is

$$
j = \frac{p}{M_n}\big|\psi_{\vec{p}}\big|^2 \;=\; \frac{1}{V}\frac{p}{M_n} \qquad (13)
$$

From the conservation of flux,

'(Integral of differential scattering cross-section over all solid angles and energies) = (Sum of probability P over all states)'

Therefore, the following holds:

$$
\int j\frac{d^3\sigma}{d^2\Omega dE}d^2\Omega dE = \int P\frac{V}{(2\pi\hbar)^3}\; d^3\vec{p'} \qquad (14)
$$

The left-hand side is,

$$
\int j\frac{d^3\sigma}{d^2\Omega dE}\; d^2\Omega dE = \int\frac{1}{V}\frac{p}{M_n}\frac{d^3\sigma}{d^2\Omega dE}\; d^2\Omega dE \qquad (15)
$$

On the other hand, the right-hand side is

$$
\begin{aligned}
\int P\frac{V}{(2\pi\hbar)^3}\; d^3\vec{p'} &= \int P\frac{V}{(2\pi\hbar)^3}p'^2\; dp'd^2\Omega \\
&= \int P\frac{V}{(2\pi\hbar)^3}M_np'\; dEd^2\Omega \qquad (16)
\end{aligned}
$$

Comparing both sides,

$$
\frac{1}{V}\frac{p}{M_n}\frac{d^3\sigma}{d^2\Omega dE} = P\frac{V}{(2\pi\hbar)^3}M_np' \qquad (17)
$$

That is,

$$
\begin{aligned}
\frac{d^3\sigma}{d^2\Omega dE} &= \frac{p'}{p}\frac{(M_nV)^2}{(2\pi\hbar)^3}P \\
&= \frac{p'}{p}\frac{(M_nV)^2}{(2\pi\hbar)^3}\cdot\frac{(2\pi\hbar)^3}{(M_nV)^2}a^2\sum_{\mathrm{f}}\delta(E_{\mathrm{f}}-E_{\mathrm{i}}+\hbar\omega)\bigg|\sum_{\vec{R}}\big(\Phi_{\mathrm{f}}, e^{i\vec{q}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\bigg|^2 \\
&= \frac{p'}{p}\frac{Na^2}{\hbar}S_{\mathrm{i}}(\vec{q},\omega) \qquad (18)
\end{aligned}
$$

This $S_{\mathrm{i}}(\vec{q},\omega)$ is defined as follows.

$$
S_{\mathrm{i}}(\vec{q},\omega) = \frac{1}{N}\sum_{\mathrm{f}}\delta\Big(\frac{E_{\mathrm{f}}-E_{\mathrm{i}}}{\hbar}+\omega\Big)\bigg|\sum_{\vec{R}}\big(\Phi_{\mathrm{f}}, e^{i\vec{q}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\bigg|^2 \qquad (19)
$$

Here, N is the number of lattice sites in the system. Now, the following identity holds for the Heisenberg operator $A(t) = e^{iHt/\hbar}Ae^{-iHt/\hbar}$:

$$
\begin{aligned}
\big(\Phi_{\mathrm{f}}, A(t)\Phi_{\mathrm{i}}\big) &= \big(\Phi_{\mathrm{f}}, e^{iHt/\hbar}Ae^{-iHt/\hbar}\Phi_{\mathrm{i}}\big) \\
&= \big(\Phi_{\mathrm{f}}, e^{iE_{\mathrm{f}}t/\hbar}Ae^{-iE_{\mathrm{i}}t/\hbar}\Phi_{\mathrm{i}}\big) \\
&= e^{i(E_{\mathrm{f}}-E_{\mathrm{i}})t/\hbar}\big(\Phi_{\mathrm{f}}, A\Phi_{\mathrm{i}}\big) \qquad (20)
\end{aligned}
$$

By expanding the delta function (Fourier transform) and using this,

$$
\begin{aligned}
S_{\mathrm{i}}(\vec{q},\omega) &= \frac{1}{N}\int\frac{dt}{2\pi}e^{i\omega t}\sum_{\mathrm{f}}e^{i(E_{\mathrm{f}}-E_{\mathrm{i}})t/\hbar}\bigg|\sum_{\vec{R}}\big(\Phi_{\mathrm{f}}, e^{i\vec{q}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\bigg|^2 \\
&= \frac{1}{N}\int\frac{dt}{2\pi}e^{i\omega t}\sum_{\mathrm{f}}e^{i(E_{\mathrm{f}}-E_{\mathrm{i}})t/\hbar}\sum_{\vec{R}}\big(\Phi_{\mathrm{f}}, e^{i\vec{q}\cdot\vec{r}(\vec{R})}\Phi_{\mathrm{i}}\big)\sum_{\vec{R}'}\big(\Phi_{\mathrm{i}}, e^{-i\vec{q}\cdot\vec{r}(\vec{R}')}\Phi_{\mathrm{f}}\big) \\
&= \frac{1}{N}\int\frac{dt}{2\pi}e^{i\omega t}\sum_{\mathrm{f}}\sum_{\vec{R},\vec{R}'}\big(\Phi_{\mathrm{i}}, e^{-i\vec{q}\cdot\vec{r}(\vec{R}')}\Phi_{\mathrm{f}}\big)\big(\Phi_{\mathrm{f}}, e^{i\vec{q}\cdot\vec{r}(\vec{R},t)}\Phi_{\mathrm{i}}\big) \qquad (21)
\end{aligned}
$$

Furthermore, since Φ_{f} forms a complete set, for operators A and B,

$$
\sum_{\mathrm{f}}\big(\Phi_{\mathrm{i}}, A\Phi_{\mathrm{f}}\big)\big(\Phi_{\mathrm{f}}, B\Phi_{\mathrm{i}}\big) = \big(\Phi_{\mathrm{i}}, AB\Phi_{\mathrm{i}}\big) \qquad (22)
$$

also holds. Letting $\delta\vec{R}$ $(=\vec{r}(\vec{R})-\vec{R})$ be the displacement of the ion from the lattice point due to thermal motion,

$$S_{\mathrm{i}}(\vec{q},\omega) = \frac{1}{N}\int \frac{dt}{2\pi} e^{i\omega t} \sum_{\mathrm{f}} \sum_{\vec{R},\vec{R}'} \big(\Phi_{\mathrm{i}}, e^{-i\vec{q}\cdot[\delta\vec{R}'+\vec{R}']}\Phi_{\mathrm{f}}\big)\big(\Phi_{\mathrm{f}}, e^{i\vec{q}\cdot[\delta\vec{R}(t)+\vec{R}]}\Phi_{\mathrm{i}}\big)$$

$$= \frac{1}{N}\int \frac{dt}{2\pi} e^{i\omega t} \sum_{\mathrm{f}} \sum_{\vec{R},\vec{R}'} e^{i\vec{q}\cdot(\vec{R}-\vec{R}')} \big(\Phi_{\mathrm{i}}, e^{-i\vec{q}\cdot\delta\vec{R}'}\Phi_{\mathrm{f}}\big)\big(\Phi_{\mathrm{f}}, e^{i\vec{q}\cdot\delta\vec{R}(t)}\Phi_{\mathrm{i}}\big)$$

$$= \frac{1}{N}\int \frac{dt}{2\pi} e^{i\omega t} \sum_{\vec{R},\vec{R}'} e^{i\vec{q}\cdot(\vec{R}-\vec{R}')} \big(\Phi_{\mathrm{i}}, e^{-i\vec{q}\cdot\delta\vec{R}'} e^{i\vec{q}\cdot\delta\vec{R}(t)}\Phi_{\mathrm{i}}\big) \tag{23}$$

In general, the crystal in the initial state is in thermal equilibrium. To find the scattering cross-section, we should take a statistical average over all initial states. If we write the statistical average of an operator A as

$$\langle A\rangle = \sum_{\mathrm{i}} \frac{e^{-E_{\mathrm{i}}/k_{\mathrm{B}}T}\big(\Phi_{\mathrm{i}}, A\Phi_{\mathrm{i}}\big)}{e^{-E_{\mathrm{i}}/k_{\mathrm{B}}T}} \tag{24}$$

the statistical average of $S_{\mathrm{i}}(\vec{q},\omega)$ is:

$$S(\vec{q},\omega) = \frac{1}{N}\int \frac{dt}{2\pi} e^{i\omega t} \sum_{\vec{R},\vec{R}'} e^{i\vec{q}\cdot(\vec{R}-\vec{R}')} \big\langle e^{-i\vec{q}\cdot\delta\vec{R}'} e^{i\vec{q}\cdot\delta\vec{R}(t)}\big\rangle \tag{25}$$

This quantity is called the **dynamic structure factor**, and it is related to the differential scattering cross-section as follows.

$$\frac{d^3\sigma}{d^2\Omega dE} = \frac{p'}{p}\frac{Na^2}{\hbar} S(\vec{q},\omega) \tag{26}$$

The dynamic structure factor $S(\vec{q},\omega)$ depends only on the structure of the scatterer.

About the Dynamic Structure Factor

Let's consider the term inside $S(\vec{q},\omega)$, $\big\langle e^{-i\vec{q}\cdot\delta\vec{R}'} e^{i\vec{q}\cdot\delta\vec{R}(t)}\big\rangle$. For linear operators A and B, the relation

$$\big\langle e^A e^B\big\rangle = \exp\Big(\frac{1}{2}\big\langle A^2 + 2AB + B^2\big\rangle\Big) \tag{27}$$

holds (this is the Gaussian approximation), so

$$\Big\langle e^{-i\vec{q}\cdot\delta\vec{R}'} e^{i\vec{q}\cdot\delta\vec{R}(t)}\Big\rangle = \exp\Big\langle -\frac{1}{2}\Big[\vec{q}\cdot\delta\vec{R}'\Big]^2\Big\rangle \; \exp\Big\langle\Big[\vec{q}\cdot\delta\vec{R}'\Big]\Big[\vec{q}\cdot\delta\vec{R}(t)\Big]\Big\rangle \; \exp\Big\langle -\frac{1}{2}\Big[\vec{q}\cdot\delta\vec{R}(t)\Big]^2\Big\rangle \tag{28}$$

Since observable physical quantities depend only on relative coordinates and relative time,

$$\exp\Big\langle\Big[\vec{q}\cdot\delta\vec{R}'\Big]^2\Big\rangle \;=\; \exp\Big\langle\Big[\vec{q}\cdot\delta\vec{R}(t)\Big]^2\Big\rangle \;=\; 2W \;=\; \text{const.} \tag{29}$$

(This e^{-2W} is the Debye-Waller factor). Furthermore, by shifting the position coordinates, letting $\delta\vec{R}'\to\delta\vec{R}_0$, and rewriting $\delta\vec{R}\to\delta\vec{R}+\delta\vec{R}_0-\delta\vec{R}'$ as $\delta\tilde{\vec{R}}$,

$$\exp\Big\langle\Big[\vec{q}\cdot\delta\vec{R}'\Big]\Big[\vec{q}\cdot\delta\vec{R}(t)\Big]\Big\rangle = \exp\Big\langle\Big[\vec{q}\cdot\delta\vec{R}_0\Big]\Big[\vec{q}\cdot\delta\tilde{\vec{R}}(t)\Big]\Big\rangle \tag{30}$$

From these steps,

$$\begin{aligned} S(\vec{q},\omega) &= e^{-2W}\int\frac{dt}{2\pi}e^{i\omega t}\sum_{\tilde{\vec{R}}}e^{i\vec{q}\cdot\tilde{\vec{R}}}\exp\Big\langle\left[\vec{q}\cdot\delta\vec{R}_0\right]\left[\vec{q}\cdot\delta\tilde{\vec{R}}(t)\right]\Big\rangle \\ &= e^{-2W}\int\frac{dt}{2\pi}e^{i\omega t}\sum_{\vec{R}}e^{i\vec{q}\cdot\vec{R}}\exp\Big\langle\left[\vec{q}\cdot\delta\vec{R}_0\right]\left[\vec{q}\cdot\delta\vec{R}(t)\right]\Big\rangle \end{aligned} \tag{31}$$

(The transformation to the second line is just relabeling the summation variable from $\tilde{\vec{R}}$ to $\vec{R}$ for clarity.)

$$\exp\Big\langle\left[\vec{q}\cdot\delta\vec{R}_0\right]\left[\vec{q}\cdot\delta\vec{R}(t)\right]\Big\rangle = \sum_{m=0}^{\infty}\frac{1}{m!}\Big(\Big\langle\left[\vec{q}\cdot\delta\vec{R}_0\right]\left[\vec{q}\cdot\delta\vec{R}(t)\right]\Big\rangle\Big)^m \tag{32}$$

can be expanded. The m-th term here represents the contribution of m phonons; for example, $m=0$ is zero-phonon scattering (elastic scattering), and $m=1$ is called one-phonon scattering.