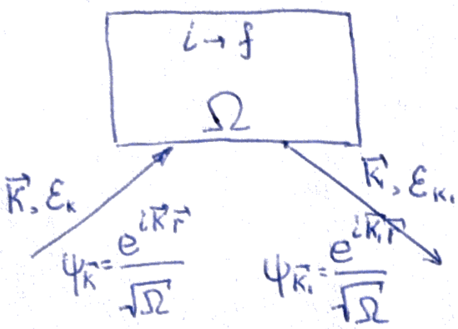
Neutron scattering on a crystal



Neutron scatters on a crystal with volume Ω.
The momentum of neutron changes: $\vec{K} \to \vec{K}_1$
The state of the crystal changes: $|i\rangle \to |f\rangle$

The probability (Fermi's golden rule):

$$W_{\substack{\vec{K}\to\vec{K}_1 \\ i\to f}} = \frac{2\pi}{\hbar} \left| M_{\substack{\vec{K}\to\vec{K}_1 \\ i\to f}} \right|^2 \cdot \delta(E_i + \varepsilon_K - E_f - \varepsilon_{K_1})$$

$$M_{\substack{\vec{K}\to\vec{K}_1 \\ i\to f}} = \langle f | \int_\Omega d\vec{r}\, \psi^*_{\vec{K}_1}(\vec{r}) \cdot U(\vec{r}) \psi_{\vec{K}}(\vec{r}) | i \rangle$$

$$U(\vec{r}) = \sum_n U_n(\vec{r} - \vec{R}_n) \leftarrow$$ interaction of neutrons with atoms in the crystal

$$\int_\Omega d\vec{r} \cdot \frac{e^{-i\vec{K}_1\vec{r}}}{\sqrt{\Omega}} \cdot \sum_n U_n(\vec{r} - \vec{R}_n) \cdot \frac{e^{i\vec{K}\vec{r}}}{\sqrt{\Omega}} = \sum_n \frac{1}{\Omega} \cdot \int_\Omega d\vec{r} \cdot U_n(\vec{r} - \vec{R}_n) e^{i(\vec{K} - \vec{K}_1)\vec{r}}$$

$\vec{r} - \vec{R}_n = \vec{r}'$

$\vec{K}_1 - \vec{K} = \vec{q}$ - change of neutron momentum

$\varepsilon_{K_1} - \varepsilon_K = \hbar\omega$ - change of neutron energy

$$= \sum_n \frac{1}{\Omega} \int_\Omega d\vec{r}' \cdot U_n(\vec{r}') e^{-i\vec{q}(\vec{r}' + \vec{R}_n)}$$

$$= \sum_n e^{-i\vec{q}\vec{R}_n} \cdot \underbrace{\frac{1}{\Omega} \int_\Omega d\vec{r}' \, U_n(\vec{r}') e^{-i\vec{q}\vec{r}'}}_{}$$

$U_n(\vec{q})$ - Fourier component of $U(\vec{r})$

N.B. For neutrons, $U_n(\vec{r}) \propto \delta(\vec{r})$,
so $U_n(\vec{q}) = \frac{1}{\Omega} \cdot \frac{2\pi\hbar^2}{m_n} \cdot b_n = const$
$\uparrow$ scattering length

Reminder:
$$\begin{cases} \varphi(\vec{r}) = \sum_{\vec{q}} \varphi(\vec{q}) e^{i\vec{q}\vec{r}} \\ \varphi(\vec{q}) = \frac{1}{\Omega} \int d\vec{r} \cdot \varphi(\vec{r}) e^{-i\vec{q}\vec{r}} \end{cases}$$

$$M_{\substack{\vec{K}\to\vec{K}_1 \\ i\to f}} = \langle f | \sum_n e^{-i\vec{q}\vec{R}_n} U_n(\vec{q}) | i \rangle = \sum_n U_n(\vec{q}) \cdot \langle f | e^{-i\vec{q}\vec{R}_n} | i \rangle$$

$$W_{\substack{\vec{k}\to\vec{k}_1 \\ i\to f}} = \frac{2\pi}{\hbar}\cdot \underbrace{\sum_n U_n(\vec{q})\langle f|e^{-i\vec{q}\vec{R}_n}|i\rangle}_{M} \cdot \underbrace{\sum_{n_1} U_{n_1}(-\vec{q})\langle i|e^{i\vec{q}\vec{R}_{n_1}}|f\rangle}_{M^*} \cdot \underbrace{\frac{1}{2\pi\hbar}\cdot\int_{-\infty}^{+\infty} dt\, e^{\frac{i}{\hbar}(E_i-E_f-\hbar\omega)t}}_{\delta(E_i-E_f+\underline{\varepsilon_k-\varepsilon_{k_1}})}$$

$$= \frac{1}{\hbar^2}\sum_{nn_1} U_n(\vec{q})U_{n_1}(-\vec{q})\cdot \int_{-\infty}^{+\infty} dt\cdot e^{-i\omega t}\cdot\langle i|e^{+i\vec{q}\vec{R}_{n_1}}|f\rangle\cdot e^{-\frac{i}{\hbar}E_f t}\cdot\langle f|e^{-i\vec{q}\vec{R}_n}|i\rangle\cdot e^{\frac{i}{\hbar}E_i t}$$

Reminder: $\hat{H}|f\rangle = E_f\cdot|f\rangle \Rightarrow \underbrace{\hat{H}\dots\hat{H}}_{n}|f\rangle = \hat{H}^n|f\rangle = (E_f)^n|f\rangle \Rightarrow e^{-\frac{i}{\hbar}\hat{H}t}|f\rangle = e^{-\frac{i}{\hbar}E_f t}|f\rangle$

$$= \frac{1}{\hbar^2}\cdot\sum_{nn_1} U_n(\vec{q})U_{n_1}(-\vec{q})\cdot\int_{-\infty}^{+\infty} dt\cdot e^{-i\omega t}\langle i|e^{i\vec{q}\vec{R}_n}e^{-\frac{i}{\hbar}\hat{H}t}|f\rangle\cdot\langle f|e^{-i\vec{q}\vec{R}_n}e^{\frac{i}{\hbar}\hat{H}t}|i\rangle$$

We don't know the initial state of the crystal, therefore we have to average over all possible initial states i.

$\varpi_i = \frac{1}{2}e^{-\frac{E_i}{kT}}$ ← probability of the crystal to be in the state "i"

We also have to average over all possible states f.

Due to the delta-function in Fermi's golden rule, we will authomatically take into account only such states "f" that satisfy the conservation of energy.

Thus $W_{\vec{k}\to\vec{k}_1} = \sum_i \varpi_i\cdot\sum_f W_{\substack{\vec{k}\to\vec{k}_1\\ i\to f}}$

$$W_{\vec{k}\to\vec{k}_1} = \frac{1}{\hbar^2}\sum_{nn_1} U_n(\vec{q})U_{n_1}(-\vec{q})\cdot\int_{-\infty}^{+\infty} dt\, e^{-i\omega t}\cdot\sum_i \varpi_i\cdot\sum_f\langle i|e^{i\vec{q}\vec{R}_n}e^{-\frac{i}{\hbar}\hat{H}t}|f\rangle\langle f|e^{-i\vec{q}\vec{R}_n}e^{\frac{i}{\hbar}\hat{H}t}|i\rangle$$

Reminder: $\sum_f \langle i|\hat{A}|f\rangle\langle f|\hat{B}|i\rangle = \langle i|\hat{A}\hat{B}|i\rangle$

$\hat{A}(t) = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}(0)e^{-\frac{i}{\hbar}\hat{H}t}$ - Heisenberg's representation of the operator $\hat{A}$

$$W_{\vec{k}\to\vec{k}_1} = \frac{1}{\hbar^2}\sum_{nn_1} U_n(\vec{q})U_{n_1}(-\vec{q})\cdot\int_{-\infty}^{+\infty} dt\cdot e^{-i\omega t}\cdot\underbrace{\sum_i \varpi_i\cdot\langle i|e^{i\vec{q}\hat{\vec{R}}_{n_1}(0)}e^{-i\vec{q}\hat{\vec{R}}_n(t)}|i\rangle}_{\langle\langle e^{i\vec{q}\hat{\vec{R}}_{n_1}(0)}e^{-i\vec{q}\hat{\vec{R}}_n(t)}\rangle\rangle}$$

double averaging: over state "i"
over all states

For a simple monoatomic crystal: $\hat{\vec{R}}_n = \vec{n} + \hat{\vec{u}}_n$, $\hat{\vec{u}}_n = \sum_{\xi} \hat{\vec{u}}_{n\xi}$, $u_{n\xi} \sim \frac{1}{\sqrt{N}}$ - small

$$\langle i| e^{i\vec{q}\hat{\vec{R}}_{n_1}(0)} e^{-i\vec{q}\hat{\vec{R}}_n(t)} |i\rangle = \langle i| e^{i\vec{q}\vec{n}_1} e^{i\vec{q}\hat{\vec{u}}_{n_1}(0)} e^{-i\vec{q}\vec{n}} e^{-i\vec{q}\hat{\vec{u}}_n(t)} |i\rangle$$

$$= e^{i\vec{q}(\vec{n}_1-\vec{n})} \cdot \langle i| e^{i\vec{q}\sum_{\xi_1}\hat{\vec{u}}_{n_1\xi_1}(0)} \cdot e^{-i\vec{q}\sum_{\xi}\hat{\vec{u}}_{n\xi}(t)} |i\rangle = e^{i\vec{q}(\vec{n}_1-\vec{n})} \langle i| \prod_{\xi_1} e^{i\vec{q}\hat{\vec{u}}_{n\xi_1}(0)} \cdot \prod_{\xi} e^{-i\vec{q}\hat{\vec{u}}_{n\xi}(t)} |i\rangle$$

$$= e^{i\vec{q}(\vec{n}_1-\vec{n})} \cdot \langle i| \prod_{\xi_1} \left(1 + i\vec{q}\hat{\vec{u}}_{n_1\xi_1}(0) - \frac{1}{2}\left(\vec{q}\hat{\vec{u}}_{n_1\xi_1}(0)\right)^2 + \ldots\right) \cdot \prod_{\xi} \left(1 - i\vec{q}\hat{\vec{u}}_{n\xi}(t) - \frac{1}{2}\left(\vec{q}\cdot\hat{\vec{u}}_{n\xi}(t)\right)^2 + \ldots\right) |i\rangle$$

$$\approx e^{i\vec{q}(\vec{n}_1-\vec{n})} \prod_{\xi_1}\prod_{\xi} \langle i| 1 + i\vec{q}\hat{\vec{u}}_{n_1\xi_1}(0) - i\vec{q}\hat{\vec{u}}_{n\xi}(t) - \frac{1}{2}\left(\vec{q}\hat{\vec{u}}_{n_1\xi_1}(0)\right)^2 - \frac{1}{2}\left(\vec{q}\hat{\vec{u}}_{n\xi}(t)\right)^2 + \vec{q}\hat{\vec{u}}_{n_1\xi_1}(0)\cdot\vec{q}\hat{\vec{u}}_{n\xi}(t) |i\rangle$$

$$\vec{q}\hat{\vec{u}}_{n\xi} = q^\alpha \hat{u}^\alpha_{n\xi}, \quad \langle i|\vec{q}\hat{\vec{u}}_{n\xi}|i\rangle = q^\alpha \cdot \underbrace{\langle i|\hat{u}^\alpha_{n\xi}|i\rangle}_{=0} = 0$$

Debye-Waller factor

$$(\vec{q}\hat{\vec{u}}_{n\xi})^2 = q^\alpha q^\beta \hat{u}^\alpha_{n\xi}\hat{u}^\beta_{n\xi}; \quad \langle i|(\vec{q}\hat{\vec{u}}_{n\xi})^2|i\rangle = q^\alpha q^\beta \underbrace{\langle i|\hat{u}^\alpha_{n\xi}\hat{u}^\beta_{n\xi}|i\rangle}_{} = \frac{1}{3}q^2\langle u^2_{n\xi}\rangle = Z_{n\xi}(q)$$

$$= \delta^{\alpha\beta}\langle i|\hat{u}^\alpha_{n\xi}\hat{u}^\beta_{n\xi}|i\rangle = \frac{1}{3}\delta^{\alpha\beta}\langle i|\hat{u}^2_{n\xi}|i\rangle = \frac{1}{3}\delta^{\alpha\beta}\cdot\langle u^2_{n\xi}\rangle$$

for cubic symmetry

$$\langle i|\vec{q}\hat{\vec{u}}_{n_1\xi_1}(0)\cdot\vec{q}\hat{\vec{u}}_{n\xi}(t)|i\rangle = D_{\substack{n_1 n\\ \xi_1 \xi}}(t) \text{ - correlator}$$

$$\approx e^{i\vec{q}(\vec{n}_1-\vec{n})} \prod_{\xi_1}\prod_{\xi} \left(1 - \frac{1}{2}Z_{n_1\xi_1}(\vec{q}) - \frac{1}{2}Z_{n\xi}(\vec{q}) + D_{\substack{n_1 n\\ \xi_1 \xi}}(t)\right)$$

$$\approx e^{i\vec{q}(\vec{n}_1-\vec{n})} \cdot \Big(1 - \underbrace{\frac{1}{2}\sum_{\xi_1} Z_{n_1\xi_1}(\vec{q})}_{Z_n(\vec{q}) = \frac{1}{3}q^2\langle u^2_n\rangle} - \underbrace{\frac{1}{2}\sum_{\xi} Z_{n\xi}(\vec{q})}_{Z_n(\vec{q})} + \underbrace{\sum_{\xi_1\xi} D_{\substack{n_1 n\\ \xi_1 \xi}}(t)}_{D_{n_1 n}(t)}\Big)$$

$$\approx e^{i\vec{q}(\vec{n}_1-\vec{n})}\, e^{-Z_n(\vec{q})}\, (1 + D_{n_1 n}(t))$$

The potential $U_n(\vec{r})$ (and the Fourier components $U_n(\vec{q})$) depends on the isotopes and direction of the nuclear spin. In a paramagnetic situation, we have to average over isotopes and spins

$$U_n(\vec{q}) = \underset{\substack{\uparrow \\ \text{average}}}{\overline{U}(\vec{q})} + \underset{\substack{\uparrow \\ \text{fluctuation}}}{\Delta U_n(\vec{q})} \qquad \left(\overline{\Delta U_n(\vec{q})} = 0 \right)$$

$$\overline{U_n(\vec{q})\, U_{n_1}(-\vec{q})} = \overline{[U(\vec{q}) + \Delta U_n(\vec{q})][U(-\vec{q}) + \Delta U_{n_1}(-\vec{q})]} = \underbrace{U(\vec{q})U(-\vec{q})}_{|U(\vec{q})|^2} + 0 + 0 + \underbrace{\overline{\Delta U_n(\vec{q})\,\Delta U_{n_1}(-\vec{q})}}_{\delta_{nn_1} \cdot \overline{|\Delta U_n(\vec{q})|^2}}$$

$$\overline{W_{\vec{k}\to\vec{k}_1}} = \frac{1}{\hbar^2} \sum_{n\,n_1} \left\{ |U(\vec{q})|^2 + \delta_{nn_1} \overline{|\Delta U_n(\vec{q})|^2} \right\} \int_{-\infty}^{+\infty} dt \cdot e^{-i\omega t} \cdot e^{i\vec{q}(\vec{n}_1-\vec{n})} e^{-2_n(\vec{q})} (1 + D_{n_1 n}(t))$$

$$= \frac{1}{\hbar^2} \sum_{n\,n_1} e^{i\vec{q}(\vec{n}_1-\vec{n})} \cdot e^{-2(\vec{q})} \cdot \Big\{ \underbrace{|U(\vec{q})|^2}_{\text{coherent}} + \underbrace{\delta_{nn_1} \overline{|\Delta U_n(\vec{q})|^2}}_{\text{incoherent}} \Big\} \cdot \Big\{ \underbrace{2\pi \cdot \delta(\omega)}_{\text{elastic}} + \underbrace{D_{n_1 n}(\omega)}_{\text{inelastic}} \Big\}$$

$$D_{n_1 n}(\omega)=\int_{-\infty}^{+\infty}dt\, e^{-i\omega t}\langle\langle \vec{q}\,\hat{\vec{u}}_{n_1}(0)\cdot\vec{q}\,\hat{\vec{u}}_n(t)\rangle\rangle = q^\alpha q^\beta\int_{-\infty}^{+\infty}dt\, e^{-i\omega t}\langle\langle \hat{u}^\alpha_{n_1}(0)\cdot\hat{u}^\beta_n(t)\rangle\rangle$$

Reminder: $$\hat{u}^\beta_n(t)=\sum_\xi\sqrt{\frac{\hbar}{2NM\omega_\xi}}\left(\ell^\beta_\xi e^{i\vec{f}\vec{n}}\underbrace{\hat{b}_\xi(t)}_{e^{\frac{i}{\hbar}\hat{H}t}\hat{b}_\xi e^{-\frac{i}{\hbar}\hat{H}t}}+\ell^{*\beta}_\xi e^{-i\vec{f}\vec{n}}\hat{b}^+_\xi(t)\right)$$

$$=q^\alpha q^\beta\sum_{\xi\xi_1}\frac{\hbar}{2NM\sqrt{\omega_\xi\omega_{\xi_1}}}\cdot\int_{-\infty}^{+\infty}dt\cdot e^{-i\omega t}\cdot\Big\{\ell^\alpha_{\xi_1}\ell^\beta_\xi e^{i\vec{f}_1\vec{n}_1}e^{i\vec{f}\vec{n}}\cdot\langle\langle\hat{b}_{\xi_1}(0)\,\hat{b}_\xi(t)\rangle\rangle$$

$$+\ell^\alpha_{\xi_1}\ell^{*\beta}_\xi e^{i\vec{f}_1\vec{n}_1}e^{-i\vec{f}\vec{n}}\cdot\langle\langle\hat{b}_{\xi_1}(0)\,\hat{b}^+_\xi(t)\rangle\rangle$$

$$+\ell^{*\alpha}_{\xi_1}\ell^\beta_\xi e^{-i\vec{f}_1\vec{n}_1}e^{i\vec{f}\vec{n}}\cdot\langle\langle\hat{b}^+_{\xi_1}(0)\,\hat{b}_\xi(t)\rangle\rangle$$

$$+\ell^{*\alpha}_{\xi_1}\ell^{*\beta}_\xi e^{-i\vec{f}_1\vec{n}_1}e^{i\vec{f}\vec{n}}\cdot\langle\langle\hat{b}^+_{\xi_1}(0)\,\hat{b}^+_\xi(t)\rangle\rangle\Big\}$$

It can be seen that $\langle i|\hat{b}_{\xi_1}(0)\,\hat{b}_\xi(t)|i\rangle=\langle i|\hat{b}^+_{\xi_1}(0)\,\hat{b}^+_\xi(t)|i\rangle=0$.

The mixed terms are non-zero only if $\xi=\xi_1$. Let us evaluate $\langle i|\hat{b}_\xi(0)\,\hat{b}^+_\xi(t)|i\rangle$

$$\langle i|\hat{b}_\xi e^{\frac{i}{\hbar}\hat{H}t}\hat{b}^+_\xi\underbrace{e^{-\frac{i}{\hbar}\hat{H}t}|i\rangle}_{e^{-\frac{i}{\hbar}E_it}|i\rangle}=e^{-\frac{i}{\hbar}E_it}\langle i|\hat{b}_\xi e^{\frac{i}{\hbar}\hat{H}t}\cdot\underbrace{\hat{b}^+_\xi|i\rangle}_{\sqrt{n_\xi+1}\cdot|\{i,n_\xi+1\}\rangle}=\sqrt{n_\xi+1}\,e^{-\frac{i}{\hbar}E_it}\langle i|\hat{b}_\xi\underbrace{e^{\frac{i}{\hbar}\hat{H}t}|\{i,n_\xi+1\}\rangle}_{e^{\frac{i}{\hbar}(E_i+\hbar\omega_\xi)t}|\{i,n_\xi+1\}\rangle}$$

$$=\sqrt{n_\xi+1}\,e^{-\frac{i}{\hbar}E_it}\cdot e^{\frac{i}{\hbar}(E_i+\hbar\omega_\xi)t}\cdot\langle i|\underbrace{\hat{b}_\xi|\{i,n_\xi+1\}\rangle}_{\sqrt{n_\xi+1}\cdot|i\rangle}=(n_\xi+1)\cdot e^{i\omega_\xi t}\cdot\underbrace{\langle i|i\rangle}_{1}$$

Averaging over all initial states gives: $\langle\langle\hat{b}_{\xi_1}(0)\,\hat{b}^+_\xi(t)\rangle\rangle=\delta_{\xi\xi_1}\cdot(\bar{n}_\xi+1)\,e^{i\omega_\xi t}$

Analogously, $\langle\langle\hat{b}^+_{\xi_1}(0)\,\hat{b}_\xi(t)\rangle\rangle=\delta_{\xi\xi_1}\cdot\bar{n}_\xi\cdot e^{-i\omega_\xi t}$.

$$D_{n_1n}(\omega)=q^\alpha q^\beta\cdot\sum_\xi\frac{\hbar}{2NM\omega_\xi}\Big\{\ell^\alpha_\xi\ell^{*\beta}_\xi e^{i\vec{f}(\vec{n}_1-\vec{n})}(\bar{n}_\xi+1)\cdot\underbrace{\int_{-\infty}^{+\infty}dt\,e^{-i\omega t}e^{i\omega_\xi t}}_{2\pi\delta(\omega-\omega_\xi)}+\ell^{*\alpha}_\xi\ell^\beta_\xi e^{-i\vec{f}(\vec{n}_1-\vec{n})}\cdot\bar{n}_\xi\cdot\underbrace{\int_{-\infty}^{+\infty}dt\,e^{-i\omega t}e^{-i\omega_\xi t}}_{2\pi\delta(\omega+\omega_\xi)}\Big\}$$

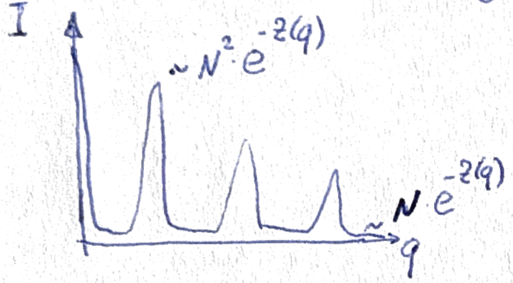
$$=\sum_\xi\frac{2\pi\hbar}{2NM\omega_\xi}|\vec{q}\,\vec{\ell}_\xi|^2\cdot\Big\{\underbrace{e^{i\vec{f}(\vec{n}_1-\vec{n})}(\bar{n}_\xi+1)\cdot\delta(\omega-\omega_\xi)}_{\text{creation of a phonon}}+\underbrace{e^{-i\vec{f}(\vec{n}_1-\vec{n})}\cdot\bar{n}_\xi\cdot\delta(\omega+\omega_\xi)}_{\text{annihilation of a phonon}}\Big\}$$

$$W_{el}^{coh}(\vec q,\omega) = \frac{1}{\hbar^2}\underbrace{\sum_n\sum_{n_1} e^{i\vec q(\vec n_1-\vec n)}}_{N^2\cdot\delta_{\vec q,\vec G}} \cdot e^{-2(\vec q)}\cdot|U(\vec q)|^2\cdot 2\pi\delta(\omega) = \frac{2\pi}{\hbar^2}\delta(\omega)\cdot|N\cdot U(\vec q)|^2\cdot e^{-2(\vec q)}\cdot\delta_{\vec q,\vec G}$$

coherent elastic scattering gives sharp Bragg peaks at $\vec q=\vec G$.

$$W_{el}^{inc}(\vec q,\omega)=\frac{1}{\hbar^2}\sum_n\underbrace{\sum_{n_1} e^{i\vec q(\vec n_1-\vec n)}\cdot\delta_{nn_1}}_{1}\cdot e^{-2(\vec q)}\overline{|\Delta U_n(\vec q)|^2}\cdot 2\pi\delta(\omega) = \frac{2\pi}{\hbar^2}\delta(\omega)\cdot\sum_n\overline{|\Delta U_n(\vec q)|^2}\cdot e^{-2(\vec q)}$$

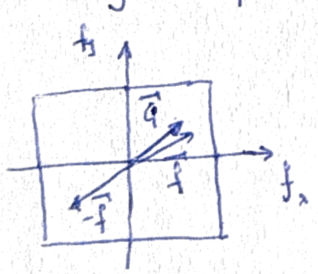
incoherent elastic scattering gives a background between the Bragg peaks



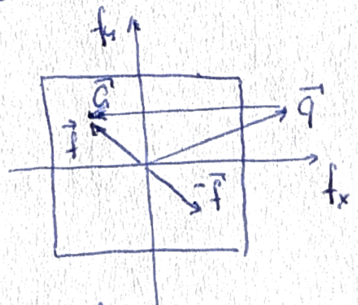
$$W_{inel}^{coh}(\vec q,\omega)=\frac{1}{\hbar^2}e^{-2(\vec q)}|U(\vec q)|^2\cdot\sum_s\frac{2\pi\hbar}{2MN\omega_s}|\vec q\vec l_s|^2\cdot\Big\{\overbrace{\sum_{nn_1}e^{i(\vec f+\vec q)(\vec n_1-\vec n)}}^{N^2\cdot\delta_{\vec f+\vec q,\vec G}=N^2\cdot\delta_{\vec f,\vec G-\vec q}}(\bar n_s+1)\,\delta(\omega-\omega_s)+$$

$$+\underbrace{\sum_{nn_1}e^{-i(\vec f-\vec q)(\vec n_1-\vec n)}}_{N^2\cdot\delta_{\vec f-\vec q,\vec G}=N^2\cdot\delta_{\vec f,\vec G+\vec q}}\cdot\bar n_s\cdot\delta(\omega+\omega_s)\Big\}$$

Regardless of the momentum transfer $\vec q$ of a neutron, the phonon with a quasi-momentum $\vec f\in 1^{st}$ Brillouin zone would be created (annihilated), such that $\vec f=\vec G\pm\vec q$ lies in the 1^{st} Brillouin zone.



normal-process



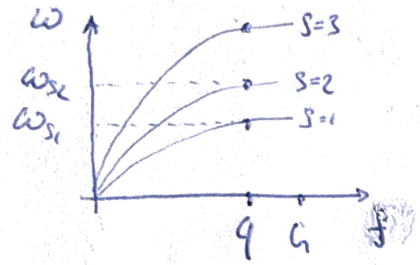
umklapp-process

For simplicity, let us assume a normal process ($\vec{G}=0$)

$$W^{coh}_{inel} = \frac{2\pi}{\hbar}|N U(\vec q)|^2 \cdot e^{-2(\vec q)} \cdot \sum_s \frac{|\vec q\cdot \vec\ell_s(\vec q)|^2}{2NM\omega_s(\vec q)} \cdot \Big\{\underbrace{(\bar n(\omega_s(\vec q))+1)\cdot\delta(\omega-\omega_s)}_{\text{creation of a phonon}} + \underbrace{\bar n(\omega_s(\vec q))\cdot \delta(\omega+\omega_s(\vec q))}_{\text{absorption of phonon.}}\Big\}$$

At a fixed $\vec q$, the scattering will occur only at phonon frequencies.

Thus, one can experimentally measure phonon dispersion



$$W^{inc.}_{inel.}(\vec q,\omega) = \frac{1}{\hbar^2}\underbrace{\sum_{nn_1} e^{i\vec q(\vec r_1-\vec r)}\cdot\delta_{nn_1}}_{\sum_n} e^{-2(\vec q)}\cdot\overline{|\Delta U_n(\vec q)|^2}\cdot\underbrace{D_{nn_1}(\omega)}_{D_{nn}(\omega)}$$

$$D_{nn}(\omega) = \sum_s \frac{2\pi\hbar}{2NM\omega_s}|\vec q\,\vec\ell_s|^2\cdot\{(\bar n_s+1)\cdot\delta(\omega-\omega_s)+\bar n_s\cdot\delta(\omega+\omega_s)\}$$

$$= q^\alpha q^\beta\cdot\underbrace{\sum_s \frac{2\pi\hbar}{2NM\omega_s}\cdot\ell_s^\alpha\,\ell_s^{*\beta}\,\{(\bar n_s+1)\,\delta(\omega-\omega_s)+\bar n_s\,\delta(\omega+\omega_s)\}}_{T^{\alpha\beta}}$$

$T^{\alpha\beta}$ - in a cubic crystal, $T^{\alpha\beta} = T\cdot\delta^{\alpha\beta}$

$$T^{\alpha\alpha} = T\cdot\underbrace{\delta^{\alpha\alpha}}_{3} = 3T \Rightarrow T = \frac{1}{3}T^{\alpha\alpha}$$

$$T^{\alpha\alpha} = \sum_s \frac{2\pi\hbar}{2NM\omega_s}\cdot\underbrace{\ell_s^\alpha\,\ell_s^{*\alpha}}_{|\vec\ell_s|^2=1 \text{ (for a monoatomic crystal)}}\cdot\{\ldots\}$$

$$D_{nn}(\omega) = \underbrace{q^\alpha q^\beta\cdot\delta^{\alpha\beta}}_{q^2}\cdot\frac{1}{3}\sum_s\frac{2\pi\hbar}{2NM\omega_s}\cdot\{(\bar n_s+1)\cdot\delta(\omega-\omega_s)+\bar n_s\cdot\delta(\omega+\omega_s)\}$$

$$= q^2\cdot\frac{2\pi\hbar}{2M}\cdot\int_0^{\omega_{max}} d\omega_1\cdot\underbrace{\frac{1}{3N}\cdot\sum_s\delta(\omega_s-\omega_1)}_{g(\omega_1)\text{ - density of phonon states}}\left\{\frac{\overline{n(\omega_1)}+1}{\omega_1}\delta(\omega-\omega_1)+\frac{\overline{n(\omega_1)}}{\omega_1}\cdot\delta(\omega+\omega_1)\right\}$$

$$= q^2\cdot\frac{\pi\hbar}{M}\cdot\int_0^{\omega_{max}} d\omega_1\cdot g(\omega_1)\left\{\frac{\overline{n(\omega_1)}+1}{\omega_1}\delta(\omega-\omega_1)+\frac{\overline{n(\omega_1)}}{\omega_1}\delta(\omega+\omega_1)\right\}$$

$$D_{nn}(\omega) = q^2 \frac{\pi\hbar}{M} \cdot \left\{ g(\omega) \cdot \frac{\overline{n(\omega)}+1}{\omega} + \underbrace{g(-\omega)}_{g(-\omega)=g(\omega)} \cdot \frac{\overline{n(-\omega)}}{-\omega} \right\}$$

$$\frac{\overline{n(-\omega)}}{-\omega} = -\frac{1}{\omega} \cdot \frac{1}{e^{-\frac{\hbar\omega}{kT}} - 1} = \frac{1}{\omega} \cdot \frac{e^{\frac{\hbar\omega}{kT}}}{e^{\frac{\hbar\omega}{kT}} - 1} = \frac{\overline{n(\omega)}+1}{\omega}$$

$$\overline{n(\omega)}+1 = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1} + 1 = \frac{e^{\frac{\hbar\omega}{kT}}}{e^{\frac{\hbar\omega}{kT}} - 1}$$

$$D_{nn}(\omega) = q^2 \cdot \frac{2\pi\hbar}{M} \cdot g(\omega) \cdot \frac{\overline{n(\omega)}+1}{\omega}$$

$$W^{inc.}_{inel.}(\vec{q},\omega) = \frac{2\pi q^2}{\hbar \cdot M} \cdot \sum_n \overline{|b U_n(\vec{q})|^2} \cdot e^{-2(\vec{q})} \cdot \frac{\overline{n(\omega)}+1}{\omega} \cdot g(\omega) \propto g(\omega).$$

Incoherent inelastic scattering allows one to experimentally measure the density of phonon states $g(\omega)$.