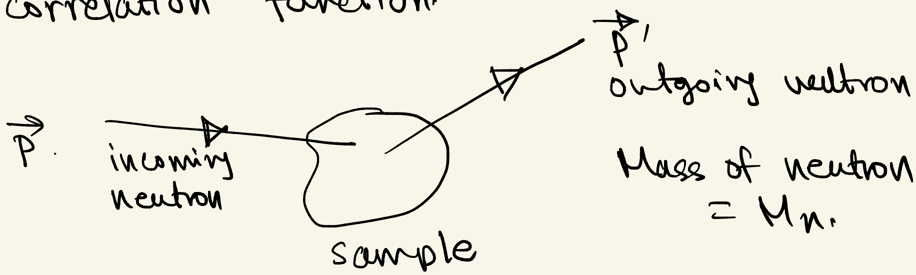
Neutron Scattering and Structure Factor

Here we will relate the scattering cross-section in neutron scattering to unequal time density-density correlation function.



Mass of neutron $= M_n$.

By energy-momentum conservation, $\vec{p}\,' - \vec{p}$ momentum and $\frac{p^2}{2M_n} - \frac{p'^2}{2M_n}$ energy is dumped into the sample.

We assume that initially the system is an eigenstate $|E_i\rangle$ and afterwards in eigenstate $|E_f\rangle$. Energy conservation $\Rightarrow E_f - E_i = \frac{p^2}{2M_n} - \frac{p'^2}{2M_n}$

$\equiv \omega$.

The scattering rate is given by,

$$\Gamma_{\vec{p}\vec{p}'} = \Big(\sum_{i,f} e^{-\beta E_i} \, \Gamma_{if} \Big) \Big/ \sum_i e^{-\beta E_i}$$

where $\Gamma_{if} = 2\pi\, \delta(E_f - E_i - \omega)\, |\langle \varphi_f | H_{int} | \varphi_i \rangle|^2$

where H_{int} is the interaction Hamiltonian between the neutron and the sample and $|\varphi_i\rangle$, $|\varphi_f\rangle$ are the initial and final states of the total system (= neutron + sample).

We assume that the total Hamiltonian is

$$H = H_s + \sum_p \frac{p^2}{2M_n} a_n^\dagger(p) a_n(p) + \overbrace{\sum_r a_n^\dagger(r) a_n(r)\, b^\dagger(r) b(r)}^{H_{int}}$$

$$\sum_r a_n^\dagger(r) a_n(r)\, b^\dagger(r) b(r) = \sum_r \rho_n(r) \rho_s(r)$$

where $a_n^\dagger$ is the creation operator for neutron and $b^\dagger(r)$ is that for sample's constituents (could be bosons or fermions). H_s is sample Hamiltonian (e.g. Bose-Hubbard Hamiltonian).

By assumption,

$$|\varphi_i\rangle = |E_i\rangle\, |p\rangle_n$$
$$|\varphi_f\rangle = |E_f\rangle\, |p'\rangle_n$$

$\Rightarrow \Gamma_{if}$

$$= 2\pi\, \delta(E_f - E_i - \omega) \left| \sum_r \langle E_f | \rho_s(r) | E_i \rangle \langle p' | \rho_n(r) | p \rangle \right|^2$$

Now $\quad \langle p' | \rho_n(r) | p \rangle = e^{i(p-p')\cdot r}$

further, $\sum_r \rho_s(r)\, e^{i(p-p')\cdot r} = \rho_s(-q)$

where $q = p' - p$.

$$\Rightarrow \Gamma_{if} = 2\pi\, \delta(E_f - E_i - \omega) \; |\langle E_f | \rho_s(-q) | E_i \rangle|^2$$

$$\Rightarrow \Gamma = \sum_f \Gamma_{if}\, e^{-\beta E_i} / Z \qquad \left(Z = \sum_i e^{-\beta E_i} \right)$$

$$= \sum_f \frac{e^{-\beta E_i} |\langle E_i | \rho_s(q) | E_f \rangle|^2 \int e^{it(E_f - E_i - \omega)} dt}{Z}$$

$$= \Big[\sum_{fi} e^{-\beta E_i} \langle E_i | \rho_s(q) | E_f \rangle \langle E_f | \rho_s(-q) | E_i \rangle \int dt\, e^{it(E_f - E_i)}\, e^{-i\omega t} \Big] / Z$$

Now recall $\quad O(t) = e^{iHt}\, O\, e^{-iHt}$

$$\Rightarrow \quad \langle E_f | \rho_s(-q) | E_i \rangle e^{it(E_f - E_i)}$$
$$= \langle E_f | \rho_s(-q, t) | E_i \rangle$$

$\Rightarrow \Gamma$

$$= \sum_i e^{-\beta E_i} \frac{\int \langle E_i | \rho_s(q,0)\, \rho_s(-q,t) | E_i \rangle \, dt\, e^{-i\omega t}}{Z}$$

$$= \int \langle\langle \rho_s(q)\, \rho_s(-q,t) \rangle\rangle\, e^{-i\omega t}\, dt$$

$$\stackrel{\text{def}}{=} S(q,\omega)$$

where $\langle\langle \quad \rangle\rangle$ denotes thermal averaging

Therefore, the neutron's scattering rate is proportional to dynamical density-density correlation fn ("Structure factor").

The static structure factor is just the equal-time correlation fn $\langle\langle \rho_s(q)\, \rho_s(-q) \rangle\rangle$

$$= \int S(q,\omega)\, d\omega$$

$S(q,\omega)$ may be interpreted as the spectral density of excitations that are generated when the system is perturbed by density operator.

Let's consider the following quantity, called 'oscillator strength', $f(\vec{q})$

$= \int \omega S(\omega, \vec{q})\, d\omega$. This is heuristically the average energy of excitations generated due to density perturbation.

One can show that $f(\vec{p}) = \dfrac{p^2}{2M}$ where M is the mass of the sample constituents. See Girvin-Yang for the derivation.

Let's define $\Delta(q) = \dfrac{f(\vec{q})}{S(\vec{q})} = \dfrac{q^2}{2M\, S(\vec{q})}$

which heuristically is the average energy of excitations. To make this a bit more precise, let's consider 'single mode approximation'.

Single Mode Approximation:

Recall our discussion of Goldstone thm, where we constructed a low energy eigenstate of the form:

$$|\vec{k}\rangle = \int d^d x \; e^{-i\vec{k}\cdot\vec{x}} \; J_0(\vec{x}) \, |g.s.\rangle$$

where $J_0(x)$ is the density of the conserved quantity Q i.e. $Q = \int_x J_0(x)$.

If the conserved quantity is $\int_r \rho(r)$ where $\rho(r)$ is local density, then the states of the above form are said to be obtained via 'Single mode approximation'.

$$\text{i.e.} \quad |\vec{k}\rangle = \rho_k \, |g.s.\rangle.$$

If this state is the only one that contributes to the dynamical structure factor, then

$$S(\vec{q}, \omega) = S(\vec{q})\ \delta(\omega - E(\vec{q}))$$

where $E(\vec{q})$ is the energy of the excitation thus generated.

[Recall $S(\vec{q}, \omega)$ at $T = 0$ is

$$= \sum_f |\langle E_0 | \rho_q | E_f \rangle|^2 \ \delta(\omega - (E_f - E_0))$$

and here we are assuming that only one term in this sum, namely that corresponding to $E_f = E(\vec{q})$ contributes]

$$\Rightarrow \int S(\vec{q}, \omega)\, d\omega = S(\vec{q})$$

and $\int \omega\, S(\vec{q}, \omega)\, d\omega = E(\vec{q}) \cdot S(\vec{q})$

Using $\int \omega\, S(\bar{q}, \omega)\, d\omega = \dfrac{q^2}{2M}$

$$\Rightarrow \boxed{E(\vec{q}) = \frac{q^2}{2M\, S(\vec{q})}}$$

See Expt. papers on Canvas that use this