1) **Dynamic Scattering function $S(Q, \omega)$**

Physical property: the probability for scattering a neutron with a given momentum and energy transfer.

The dynamic structure is exactly what is probed in **coherent inelastic** neutron scattering.

The differential cross section is :

$$\frac{d^2\sigma}{d\Omega d\omega} = a^2 \left(\frac{E_f}{E_i}\right)^{\frac{1}{2}} S(Q,\omega)$$

Compare to S(Q) in SANS, independent of ω in **elastic scattering**:

$$S(\vec{Q}) = \frac{1}{N}\left\langle \left| \int dr \cdot e^{-i\vec{Q}\cdot\vec{r}} n_{unc}(\vec{r}) \right|^2 \right\rangle$$

Where n is nuclear density. (no energy transfer in elastic scattering thus independent of omega), to see how to get S(Q)

At a nucleus located at $\vec{R}_i$ the incident wave is $e^{i\vec{k}_0 . \vec{R}_i}$

so the scattered wave is $\psi_{scat} = \sum e^{i\vec{k}_0 . \vec{R}_i} \left[\frac{-b_i}{|\vec{r} - \vec{R}_i|} e^{i\vec{k}' . (\vec{r} - \vec{R}_i)} \right]$

$$\therefore \frac{d\sigma}{d\Omega} = \frac{vdS|\psi_{scat}|^2}{vd\Omega} = \frac{dS}{d\Omega}\left| b_i e^{i\vec{k}'.\vec{r}} \sum \frac{1}{|\vec{r} - \vec{R}_i|} e^{i(\vec{k}_0 - \vec{k}').\vec{R}_i} \right|^2$$

If we measure far enough away so that $r >> R_i$ we can use $d\Omega = dS/r^2$ to get

$$\frac{d\sigma}{d\Omega} = \sum_{i,j} b_i b_j e^{i(\vec{k}_0 - \vec{k}').(\vec{R}_i - \vec{R}_j)} = \sum_{i,j} b_i b_j e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)}$$

where the wavevector transfer Q is defined by $\vec{Q} = \vec{k}' - \vec{k}_0$

$\frac{d\sigma}{d\Omega} = \langle b \rangle^2 N.S(\vec{Q})$ for an assembly of similar atoms where $S(\vec{Q}) = \frac{1}{N}\left\langle \sum_{i,j} e^{-i\vec{Q}.(\vec{R}_i - \vec{R}_j)} \right\rangle_{\text{ensemble}}$

Now $\sum_i e^{-i\vec{Q}.\vec{R}_i} = \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \sum_i \delta(\vec{r} - \vec{R}_i) = \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \rho_N(\vec{r})$ where ρ_N is the nuclear number density

so $$S(\vec{Q}) = \frac{1}{N}\left\langle \left| \int d\vec{r}.e^{-i\vec{Q}.\vec{r}} \rho_N(\vec{r}) \right|^2 \right\rangle$$

or $S(\vec{Q}) = \frac{1}{N}\int d\vec{r}' \int d\vec{r}.e^{-i\vec{Q}.(\vec{r} - \vec{r}')} \langle \rho_N(\vec{r})\rho_N(\vec{r}')\rangle = \frac{1}{N}\int d\vec{R} \int d\vec{r} e^{-i\vec{Q}.\vec{R}} \langle \rho_N(\vec{r})\rho_N(\vec{r} - \vec{R})\rangle$

ie $$S(\vec{Q}) = 1 + \int d\vec{R}.g(\vec{R}).e^{-i\vec{Q}.\vec{R}}$$

where $g(\vec{R}) = \sum_{i \neq 0} \langle \delta(\vec{R} - \vec{R}_i + \vec{R}_0) \rangle$ is a function of $\vec{R}$ only.

g(R) is known as the **static pair correlation function**. It gives the probability that there is an atom, i, at distance R from the origin of a coordinate system at time t, given that there is also a (different) atom at the origin of the coordinate system

2) **Intermediate scattering function $I(Q, t)$ (What we measure in NSE)**

Usage: From a quantum mechanic model view, when the neutron beam went through the coil, neutron wave function is split by magnetic fields, these two wave arrive at the sample with a time different t, and if the molecules move in the sample between the arrival of the first and the second wave packet then the coherence is lost, and I(Q, t) is used to reflect this lost in coherence

$$I(Q,t) = \frac{1}{N}\langle \rho_{\bar{k}}(t)\rho_{-\bar{k}}(0)\rangle$$

3) **Van hove function G(r,t)**

Physical property (in different situation):

- **Inelastic coherent scattering:** probability of finding a particle at position r at time t when there is a particle at r=0 and t=0 (time-dependent pair correlation function), in this situation, intensity of scattering is proportional to the spatial and time Fourier transform of G.
- **Inelastic incoherent scattering:** the probability of finding a particle at position r at time t when the same particle was at r=0 at t=0. (self-correlation function),), in this situation, intensity of scattering is proportional to the spatial and time Fourier transform of G.
- **elastic coherent scattering:** the probability of finding a particle at position r if there is simultaneously a particle at r=0 (pair correlation function), in this situation, intensity of scattering is proportional to the spatial Fourier transform of G.

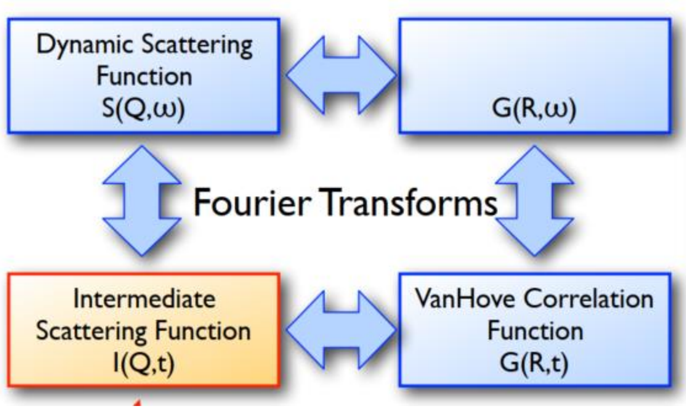
The van Hove function for a spatially uniform system containing N point particles is defined as:

$$G(\vec{r},t) = \left\langle \frac{1}{N}\int \sum_{i=1}^{N}\sum_{j=1}^{N}\delta[\vec{r}\,' + \vec{r} - \vec{r}_j(t)]\delta[\vec{r}\,' - \vec{r}_i(0)]d\vec{r}\,' \right\rangle$$

Or can be rewritten as:

$$G(\vec{r},t) = \left\langle \frac{1}{N}\int \rho(\vec{r}\,' + \vec{r},t)\rho(\vec{r}\,',0)d\vec{r}\,' \right\rangle$$

4) **relationship between S and I,G**



$$P_x(Q,t) = \langle \cos\varphi \rangle = \frac{\int S(Q,\omega)\cos(\omega t)\,d\omega}{\int S(Q,\omega)\,d\omega} = \frac{\mathrm{Re}al(I(Q,t))}{I(Q,0)}$$

$$I(Q,t) = F[S(Q,\omega)]$$

$$I(Q,t) = \int G(\vec{r},t)\exp(-i\vec{k}\cdot\vec{r})\,d\vec{r} \quad (spatial\ Fourier\ transform)$$