Dynamic Structure Factor [nln89]

Inelastic scattering of particles (electrons, neutrons, photons,...) involves momentum transfer, $\hbar\mathbf{q} = \hbar\mathbf{k}_\mathrm{f} - \hbar\mathbf{k}_\mathrm{i}$, and energy transfer, $\hbar\omega = E_\mathrm{f} - E_\mathrm{i}$, between scattered particles and collective excitations in the system.

Scattering cross section is proportional to dynamic structure factor:

$$\frac{d^2\sigma}{d\omega d\Omega} \propto S_{AA}(\mathbf{q},\omega).$$

Target system: $\mathcal{H}_0|\lambda\rangle = E_\lambda|\lambda\rangle$.

Interaction with scattering radiation: $A(\mathbf{q},t) = \int d^3r\, e^{-\imath\mathbf{k}_\mathrm{i}\cdot\mathbf{r}} V(\mathbf{r},t) e^{\imath\mathbf{k}_\mathrm{f}\cdot\mathbf{r}}$.

Scattering events produce transitions $|\lambda\rangle \to |\lambda'\rangle$ in target system.

Transition rates: $T(\mathbf{q},\omega) = |\langle\lambda|A(\mathbf{q})|\lambda'\rangle|^2 \delta(\hbar\omega - E_{\lambda'} + E_\lambda)\delta_{\mathbf{q}-\mathbf{k}_{\lambda'}+\mathbf{k}_\lambda+\mathbf{Q}}$.

Dynamic structure factor: $S_{AA}(\mathbf{q},\omega) = \dfrac{2\pi}{Z}\displaystyle\sum_{\lambda,\lambda'} e^{-\beta E_\lambda} T(\mathbf{q},\omega)$.

Electron scattering (Coulomb interaction with target charge density):

$$V(\mathbf{r},t) = \frac{e\rho(\mathbf{R},t)}{|\mathbf{r}-\mathbf{R}|} \quad \Rightarrow \; S_{\rho\rho}(\mathbf{q},\omega) = \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t} \langle \rho(\mathbf{q},t)\rho(-\mathbf{q},0)\rangle.$$

Nuclear neutron scattering (contact interaction with target particle density):

$$V(\mathbf{r},t) = a\delta(\mathbf{r}-\mathbf{R})n(\mathbf{R},t) \quad \Rightarrow \; S_{nn}(\mathbf{q},\omega) = \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t} \langle n(\mathbf{q},t)n(-\mathbf{q},0)\rangle.$$

Magnetic neutron scattering (interaction with target magnetisation):

$$V(\mathbf{r},t) = S_\mu(\mathbf{r}) V_{\mu\nu}(\mathbf{r}-\mathbf{R}) M_\nu(\mathbf{R},t)$$

$$\Rightarrow \; S_{\mu\nu}(\mathbf{q},\omega) = \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t} \langle M_\mu(\mathbf{q},t) M_\nu(-\mathbf{q},0)\rangle.$$

Light scattering (interaction with inhomogeneities in dielectric function):

$$\epsilon(\mathbf{r},t) \quad \Rightarrow \; S_{\epsilon\epsilon}(\mathbf{q},\omega) = \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t} \langle \epsilon(\mathbf{q},t)\epsilon(-\mathbf{q},0)\rangle.$$