Scattering and correlation function. General treatment

let N scatters at $\vec{r}_j$ interact with incoming particles so that the interaction potential is:

$$H_I(\vec{x}) = \sum_{j=1}^{N} V(\vec{r}_j - \vec{x}) = \int d^d y \, n(\vec{y}) \, V(\vec{x} - \vec{y})$$

with a density $$n(\vec{y},t) = \sum_{j=1}^{N} \delta(\vec{y} - \vec{r}_j(\vec{t}))$$

The scattering cross section $\frac{d^2\sigma}{d\Omega \, d\epsilon_f}$ per unit solid angle and per unit energy

is given, to first order in H, by Fermi's golden rule:

$$\frac{d^2\sigma(i\to f)}{d^2\Omega \, d\epsilon_f} = \frac{1}{V} \frac{k_f}{k_i} \left(\frac{m}{2\pi\hbar^2}\right)^2 \left| \langle k_f \, f | H_I | i \, \vec{k}_i \rangle \right|^2 \cdot \delta(\hbar\omega - E_f - E_i)$$

volume

($d^2\Omega$) is the solid angle in $\vec{k}$ space.

$d\vec{k}_f = d\Omega \, k_f^2 \, dk_f$ for the emerging particles.

where k_i and k_f are the incident and outgoing wavevector of the beam, and we consider the inelastic case in which $\hbar\omega = \epsilon_f - \epsilon_i$ is the energy imparted on the system by the scattering

ϵ_i, ϵ_f energies of the ~~se~~ incoming particle.

$E_i ; E_f$ initial and final energies of the system of particles that undergoes the scattering:

$$\epsilon_i + E_i = \epsilon_f + E_f$$

The $|i\rangle$ and $|f\rangle$ refer to the initial and final state of the system of particles described by n. So:

$$\langle k_f \cdot f | = \langle k_f | \otimes \langle f |$$

and we will take $|k_i\rangle$ and $|k_f\rangle$ as plane waves.

The matrix element:

$$\langle k_f f | H_I | i k_i \rangle = \langle k_f f | \sum_{j=1}^{N} \int \frac{d^3 q}{(2\pi)^3} V(q) e^{iq(\vec{r}_j - \vec{x})} | i k_i \rangle$$

$$= \int \frac{d^3 q}{(2\pi)^3} V(q) \underbrace{\langle k_f | e^{-iqx} | k_i \rangle}_{\text{this refers to the scattering particles}} \underbrace{\langle f | \sum_{j=1}^{N} e^{iqr_j} | i \rangle}_{\text{this refers to the state } \Omega \text{ the scatterers}}$$

• The matrix element for the incoming and outgoing particle states is easy:

$$\langle k_f | e^{-iqx} | k_i \rangle = \int d^3x' \, \langle k_f | e^{-iqx} | x' \rangle \langle x' | k_i \rangle =$$

$$= \int d^3x' \, \underbrace{\langle k_f | e^{-iqx'} x' \rangle}_{e^{-iqx'} \langle k_f | x' \rangle} \langle x' | k_i \rangle$$

If we assume plane waves, the position representation wavefunction of a plane wave of wavevector k_i is:

$$\langle x' | k_i \rangle = e^{ik_i x'}$$

$$\Rightarrow \langle k_f | e^{-iqx} | k_i \rangle =$$

$$= \int d^3x' \, e^{-iqx'} e^{ik_f x'} e^{ik_i x'} = (2\pi)^3 \delta(k_i - k_f - q)$$

Really, conservation of momentum in the collision.

We define: $\hbar k = \hbar k_i - \hbar k_f$ so that:

$$\langle k_f f | H_I | i k_i \rangle = \int \frac{d^3 q}{\cancel{(2\pi)^3}} V(q) \cancel{(2\pi)^3} \delta(k - q) \langle f | \sum_{j=1}^{N} e^{iqr_j} | i \rangle$$

$$= V(k) \langle f | \sum_{j=1}^{N} e^{ikr_j} | i \rangle$$

which is entirely dependent on the structure of the scattering medium

We next conduct a thermal average $p_i = \frac{e^{-\beta E_i}}{Z}$

so that we properly

calculate the total scattering probability averaged over all possible initial states

of the medium:

$$\frac{d^2\sigma}{d\Omega\, d\epsilon_f} = \frac{1}{V}\frac{k_f}{k_i}\left(\frac{m}{2\pi\hbar^2}\right)^2 |V(k)|^2 \sum_{if} p_i \left| \langle f | \sum_{j=1}^{N} e^{ikr_j} | i \rangle \right|^2 \delta(\hbar\omega - E_f + E_i)$$

We now define:

$$\bar{S}_T(\vec{k},\omega) = \frac{2\pi\hbar}{V} \sum_{if} \delta(\hbar\omega - E_f + E_i)\, p_i \left| \langle f | \sum_{j=1}^{N} e^{ikr_j} | i \rangle \right|^2$$

so that the scattering cross section is:

$$\frac{d^2\sigma}{d\Omega\, d\epsilon_f} = \frac{1}{2\pi\hbar}\frac{k_f}{k_i}\left(\frac{m}{2\pi\hbar^2}\right)^2 |V(k)|^2\, \bar{S}_T(\vec{k},\omega)$$

of course this is a function of the scattering wavevector $\vec{k}$, and of the frequency ω — inelastic scattering $\omega \neq 0$.

We now focus on the quantity $\bar{S}_T(\vec{k},\omega)$ which is independent of the incident beam, and depends only on the scattering medium.

Write $2\pi\hbar\, \delta(\hbar\omega - E_f - E_i) = \int_{-\infty}^{\infty} dt\, e^{i(\omega - (E_f - E_i)/\hbar)t}$

$$\bar{S}_T(\vec{k},\omega) = \frac{1}{V}\sum_{if}\int_{-\infty}^{\infty} dt\, e^{i(\omega-(E_f-E_i)/\hbar)t} \langle i | \sum_{k=1} e^{-ikr_j} | f \rangle \langle f | \sum e^{ikr_j} | i \rangle$$

We now use: $H|i\rangle = E_i |i\rangle$

so that $e^{-i(E_f - E_i)t/\hbar} \langle i | \sum e^{-ikr_j} | f \rangle =$

$$= \langle i | \sum e^{-i(E_f - E_i)t/\hbar} e^{-ikr_j} | f \rangle =$$

$$= \langle i | e^{iE_i t/\hbar} \sum e^{-ikr_j} e^{-iE_f t/\hbar} | f \rangle =$$

~~But one has $r_j(t) = e$~~

using $H|i\rangle = E_i|i\rangle$

$$= \langle i | e^{iHt/\hbar} \left(\sum e^{-ikr_j} \right) e^{-iHt/\hbar} | f \rangle$$

and now one can define the time dependent operator $\vec{r}_j(t) = e^{iHt/\hbar} r_j e^{-iHt/\hbar}$

Therefore: $\bar{S}_T(\vec{k}, \omega) = \frac{1}{V} \int_{-\infty}^{\infty} dt\, e^{i\omega t} \sum_{i,f} p_i \langle f | \sum_\ell e^{ikr_\ell} | i \rangle \cdot$

$$\cdot \langle i | \sum_j e^{-ikr_j(t)} | f \rangle$$

In order to make contact with more standard treatments, one introduces the density: $n(x,t) = \sum_{j=1}^{N} \delta(x - r_j(t))$

so that its Fourier transform:

$$n_k(t) = \frac{1}{\sqrt{V}} \int d^3x\, e^{-ikx} n(x,t) = \frac{1}{\sqrt{V}} \sum_{j=1}^{N} e^{-ikr_j(t)}$$

$$\Rightarrow \bar{S}_T(\vec{k}, \omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} \sum_{i,f} p_i \langle f | n_{-k}(0) | i \rangle \langle i | n_k(t) | f \rangle$$

$\sum_f |f\rangle\langle f| = 1$

$$= \int_{-\infty}^{\infty} dt\, e^{-i\omega t} \underbrace{\sum_i p_i \langle i | n_k(t) n_{-k}(0) | i \rangle}_{\text{the thermal average - after the trace -}}$$

$$\Rightarrow \boxed{\bar{S}_T(\vec{k}, \omega) = \int_{-\infty}^{\infty} dt\, e^{-i\omega t} \langle n_k(t) n_{-k}(0) \rangle}$$

$\bar{S}_T$ is the (ω, k) Fourier transform of the density-density correlation function.