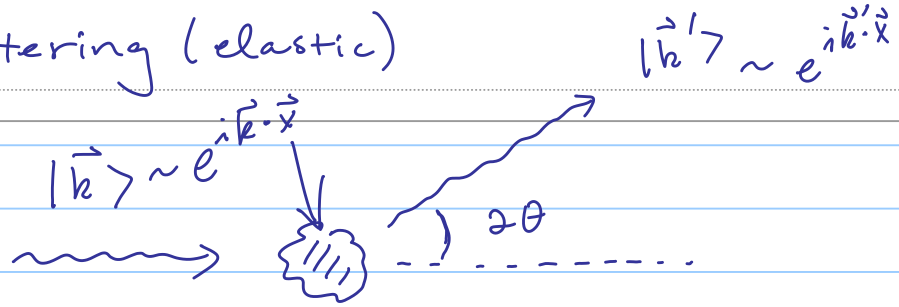
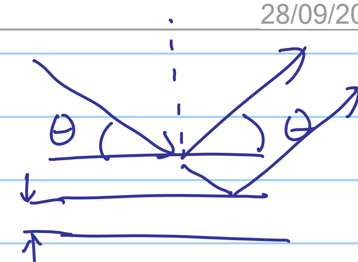
Scattering (elastic)

Note Title 28/09/2009





$$n\lambda = 2d\sin\theta$$

Bragg's law

Born approximation;

The scattering process is perturbation due to the scattering potential $U(\vec{x})$

$\Rightarrow$ Transition rate is square of the matrix element

$$W_{k,k'} = |M_{\vec{k},\vec{k}'}|^2 = |\langle\vec{k}|U|\vec{k}'\rangle|^2$$

$$\hookrightarrow \int d^3\vec{x}\, e^{-i\vec{k}\cdot\vec{x}}\, U(\vec{x})\, e^{i\vec{k}'\cdot\vec{x}}$$

For condensed matter systems $\quad U(\vec{x}) = \sum_\alpha U_\alpha(\vec{x}-\vec{x}_\alpha)$

$\vec{x}_1 \quad \vec{x}_2 \quad \vec{x}_3 \quad \cdots$

$\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \cdots\cdots \Rightarrow \vec{R}_\alpha \equiv \vec{x}-\vec{x}_\alpha$

$\vec{R}_2$

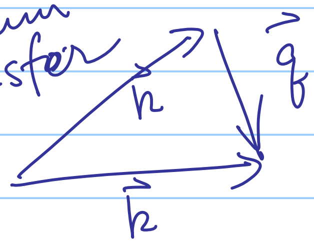
$$\langle\vec{k}|U|\vec{k}'\rangle = \sum_\alpha \int e^{-i\vec{k}\cdot\vec{x}}\, U_\alpha(\vec{x}-\vec{x}_\alpha)\, e^{i\vec{k}'\cdot\vec{x}}\, d^3\vec{x}$$

$$= \sum_\alpha \int e^{-i\vec{k}\cdot(\vec{R}_\alpha+\vec{x}_\alpha)}\, U_\alpha(\vec{R}_\alpha)\, e^{i\vec{k}'\cdot(\vec{R}_\alpha+\vec{x}_\alpha)}\, d^3\vec{R}_\alpha$$

$$\left(\vec{q} \equiv \vec{k}-\vec{k}'\right) \rightarrow \quad = \sum_\alpha \underbrace{\left(\int e^{-i\vec{q}\cdot\vec{R}_\alpha}\, U_\alpha(\vec{R}_\alpha)\, d^3\vec{R}_\alpha\right)}_{\text{F.T. of } U_\alpha(\vec{R}_\alpha)} e^{-i\vec{q}\cdot\vec{x}_\alpha}$$

momentum transfer

$\equiv U_\alpha(\vec{q})$: atomic form factor



$$\langle \vec{k} | U | \vec{k}' \rangle = \sum_{\alpha} U_\alpha(\vec{q}) \, e^{-i \vec{q} \cdot \vec{x}_\alpha}$$

$$|M_{kk'}|^2 = |\langle \vec{k} | U | \vec{k}' \rangle|^2 = \sum_{\alpha, \alpha'} U_\alpha(\vec{q}) \, U^*_{\alpha'}(\vec{q}) \, e^{-i \vec{q} \cdot (\vec{x}_\alpha - \vec{x}'_\alpha)}$$

$$\frac{d^2\sigma}{d\Omega} = \frac{2\pi}{\hbar} |M|^2 \propto |U_\alpha(\vec{q})|^2 \sum_{\alpha, \alpha'} e^{-i \vec{q} \cdot (\vec{x}_\alpha - \vec{x}'_\alpha)}$$

(U_α is identical for all atoms)

This is a single event $\Rightarrow$ need to average over ensembles (statistical mechanics sense)

$$\frac{d^2\sigma}{d\Omega} \propto \underbrace{|U(\vec{q})|^2}_{} \underbrace{\left\langle \sum_{\alpha \alpha'} e^{-i \vec{q} \cdot (\vec{x}_\alpha - \vec{x}'_\alpha)} \right\rangle}_{I(\vec{q}):\ \text{structure function.}}$$

$S(\vec{q}) \equiv \dfrac{I(\vec{q})}{N}$: structure factor

$S(\vec{q})$ does not depend on details of probe particles ($U(q)$ drops out)

We will see that this is an important quantity (F.T. of correlation function)

$$\frac{d^2\sigma}{d\Omega} \propto |U(\vec{q})|^2 \, S(\vec{q})$$

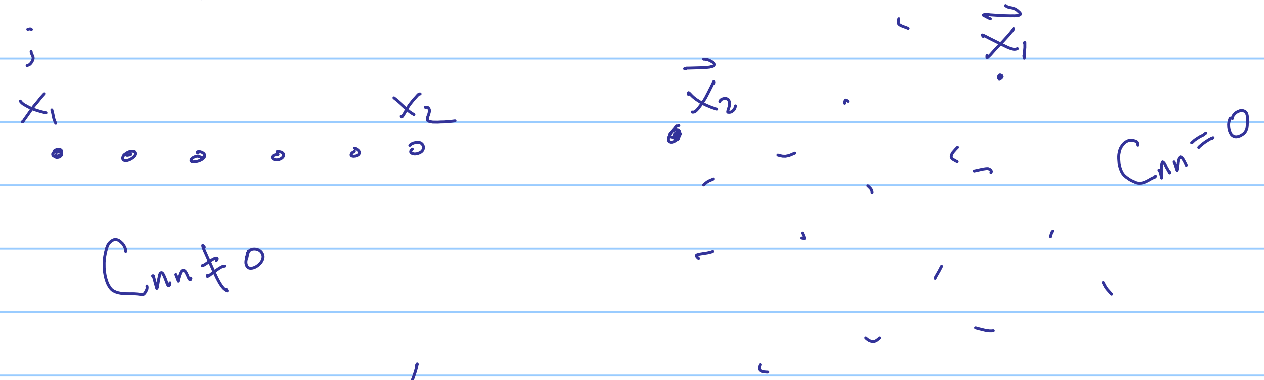
① number density operator $n(\vec{x}) = \sum_\alpha \delta(\vec{x} - \vec{x}_\alpha)$

$\langle n(\vec{x}) \rangle = \frac{N}{V}$ for isotropic homoge. fluid

↑ ensemble average.

② Correlation fn. (density)

$$C_{nn}(\vec{x}_1, \vec{x}_2) = \langle n(\vec{x}_1)\, n(\vec{x}_2) \rangle$$



$$C_{ss}(\vec{x}_1, \vec{x}_2) = \langle \vec{S}(\vec{x}_1) \cdot \vec{S}(\vec{x}_2) \rangle$$ (e.g. Spin-Spin correl. function)

$$C_{nn}(\vec{x}_1, \vec{x}_2) = \left\langle \sum_{\alpha, \alpha'} \delta(\vec{x}_1 - \vec{x}_\alpha)\, \delta(\vec{x}_2 - \vec{x}_{\alpha'}) \right\rangle$$

$$\boxed{\int e^{-i\vec{q}\cdot\vec{x}} \delta(\vec{x} - \vec{x}_\alpha)\, d\vec{x} = e^{-i\vec{q}\cdot\vec{x}_\alpha}}$$

$$I(\vec{q}) = \left\langle \sum_{\alpha, \alpha'} e^{-i(\vec{x}_\alpha - \vec{x}_{\alpha'})\cdot\vec{q}} \right\rangle$$

$$= \int d\vec{x}_1\, d\vec{x}_2 \left\langle \sum_{\alpha, \alpha'} \delta(\vec{x}_1 - \vec{x}_\alpha)\, \delta(\vec{x}_2 - \vec{x}_{\alpha'})\, e^{-i\vec{q}\cdot(\vec{x}_1 - \vec{x}_2)} \right\rangle$$

$$= \int d\vec{x}_1\, d\vec{x}_2\, \underbrace{e^{-i\vec{q}\cdot(\vec{x}_1 - \vec{x}_2)}} \underbrace{\langle n(\vec{x}_1)\, n(\vec{x}_2) \rangle}_{C_{nn}(\vec{x}_1, \vec{x}_2)} = \langle n(\vec{q})\, n(-\vec{q}) \rangle$$

C_{nn} is a fn of. $(\vec{x}_1 - \vec{x}_2)$ for iso. hom. fluid.

$\therefore$ $I(\vec{q})$ is F.T. of correlation fn.