CROSS-SECTION / SCATTERING FUNCTION

$$\frac{d^2\sigma}{d\Omega\, dE} = C\,|F(\vec{\varkappa})|^2 \cdot S(\vec{\varkappa},\omega)$$

$\vec{k}_i - \vec{k}_f = \vec{\varkappa}$: MOMENTUM – } TRANSFER

$\hbar\omega$: ENERGY –

$F(\vec{\varkappa})$ FORM FACTOR OF "ELEMENTARY" SCATT. CENTER

$$C = \left(\frac{e^2}{mc^2}\right)^2 \left(\frac{k_f}{k_i}\right) (\vec{\varepsilon}_i \vec{\varepsilon}_f)^2$$ THOMSON - SCATT.

$$C = \frac{k_f}{k_i} \cdot \frac{\sigma_c}{4\pi}$$ COHERENT NEUTR./NUCL. SCATT.

$$C = \frac{k_f}{k_i} \left(\frac{e^2}{mc^2}\right)^2 \gamma^2$$ MAGN. NEUTR. SCATT.

"WEAKLY" INTERACTING PROBE — LINEAR RESPONSE

$$\boxed{S(\vec{\varkappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dt\, e^{-i\omega t} \underbrace{\sum_{i,j} \langle e^{-i\varkappa \vec{X}_i(0)}\, e^{i\vec{\varkappa}\vec{X}_j(t)} \rangle_T}_{Y(\vec{\varkappa},t)}}$$

INTERMEDIATE SCATT.-FCT.

$S(\vec{\varkappa},\omega)$: $\mathcal{F}_\tau^{-1}\{Y(\vec{\varkappa},\tau)\}$

$G(\vec{x},\tau)$: $\mathcal{F}_{\vec{\varkappa}}\{Y(\vec{\varkappa}\,\tau)\}$

$\exp(i[\vec{\varkappa}\vec{x} - \omega\tau])$

WRITE

$$S(\vec{\varkappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dt\, e^{-i\omega t} \langle \tilde{\rho}_{\vec{\varkappa}}(0)\, \tilde{\rho}^+_{\vec{\varkappa}}(\tau) \rangle_T$$

WITH $\tilde{\rho}_{-\vec{\varkappa}} = \tilde{\rho}^+_{\vec{\varkappa}}$

AND NON-COMMUT. $[\rho_{\vec{\varkappa}}(0)\, \rho^+_{\vec{\varkappa}}(\tau)] \neq 0$

DENSITY: $m(\vec{x})$ (NUCLEAR SCATTERING - DENSITY)

PAIR - CORRELATION

$$G(\vec{x}) = \int m(\vec{x}')\, m(\vec{x}'+\vec{x})\, d^3x'$$

$$m(\vec{x}) = \sum_j \delta(\vec{x} - \vec{X}_j)$$ FOR POINT SIZE SCATT. CENTERS (PSEUDO - POTENT)

$$G(\vec{x}) = \int d^3x' \sum_i \delta(\vec{x}' - \vec{X}_i) \sum_j \delta(\vec{x}' + \vec{x} - \vec{X}_j) = \sum_{i,j} \delta(\vec{x} - (\vec{X}_j - \vec{X}_i))$$

$$= N\delta(\vec{x}) + \underbrace{\sum_{i \neq j} \delta(\vec{x} - (\vec{X}_j - \vec{X}_i))}_{\text{PAIR - CORRELATION}}$$

$\vec{X}_i$: POSITION VECTORS (OPERATORS)

$\vec{X}_i(\tau)$ — DYNAMIC VARIABLES

$G(\vec{x}, \tau)$ "WHERE ARE THE ATOMS AND HOW DO THEY MOVE"

CORRELATION : $\vec{X}_i(0), \vec{X}_j(\tau)$ INVARIANCE τ - TRANSL. (STATIONARY SYSTEM)

i) CLASSICAL $[\vec{X}_i(0) \vec{X}_j(\tau)] = 0$

ii) Q.M. $[\vec{X}_i(0) \vec{X}_j(\tau)] \neq 0$

CONVOLUTION INTEGRAL NEEDS MORE CARE

DEFINITION δ - FCT.

HEISENBERG - REPRES.

$\boxed{\text{PROPERTIES OF } \tilde{\rho}_{\vec{x}}} \longrightarrow \partial_t \tilde{\rho}_{\vec{x}} = \frac{i}{\hbar} [\tilde{\rho}_{\vec{x}}, H]$

FROM DEFINITION

$\vec{X}$: HERMITIAN : $\tilde{\rho}_{-\vec{x}} = \tilde{\rho}^{+}_{\vec{x}}$

IT FOLLOWS :

i) $(\tilde{\rho}_{\vec{x}} \tilde{\rho}^{+}_{\vec{x}}(\tau))^* = \tilde{\rho}_{\vec{x}}(\tau) \tilde{\rho}^{+}_{\vec{x}}$

ii) $\tilde{\rho}_{\vec{x}}(-\tau) \tilde{\rho}^{+}_{x} = \tilde{\rho}_{x} \tilde{\rho}_{\vec{x}}^{+}(\tau)$ TIME TRANSL. (SAMPLE STATIONARY)

HENCE $\left.\begin{matrix} Re \\ Im \end{matrix}\right\} \langle \tilde{\rho}_{\vec{x}} \tilde{\rho}_{-\vec{x}}(\tau) \rangle_T \left\{\begin{matrix} \text{EVEN} \\ \text{ODD} \end{matrix}\right.$ IN TIME

AND

$$\int_{-\infty}^{+\infty} d\tau e^{-i\omega\tau} \langle \quad \rangle_T = S(\vec{x}, \omega) \in Re$$ (REAL) (ALWAYS)

BUT STILL : $\boxed{[\tilde{\rho}_{\vec{x}}(\tau) \tilde{\rho}^{+}] \neq 0}$ GENERALLY

HOWEVER, FOR $\langle \quad \rangle_T$ (AND ONLY FOR $\langle \quad \rangle_T$)

iii) $\langle \tilde{\rho}_{\vec{x}}(\tau) \tilde{\rho}^{+}_{\vec{x}} \rangle_T = \langle \tilde{\rho}^{+}_{\vec{x}} \tilde{\rho}_{\vec{x}}(\tau + i\hbar\beta) \rangle_T$
WITH $\beta = 1/kT$

$= \langle \tilde{\rho}^{+}_{x} \tilde{\rho}_{x}(\tau) \rangle_T$ FOR

i) $\hbar \longrightarrow 0$

ii) $kT \longrightarrow \infty$

Q.M. EFFECTS BURRIED

SPACE-TIME CORRELATION		MOMENTUM-ENERGY TRANSFER
$C(\vec{x},\tau)$		$S(\vec{\varkappa},\omega)$
$C_s(\vec{x},\tau)$		$S_i(\vec{\varkappa},\omega)$

$$\hbar\omega = \Delta E \sim \hbar / T$$

$$\hbar\vec{\varkappa} = \Delta\vec{p} \sim \hbar / Z$$

$\left.\begin{array}{ll} T & \text{LIFETIME} \\ Z & \text{SPATIAL EXTENS.} \end{array}\right\}$ OF FLUCTUATIONS

$\downarrow$

CRYSTAL STRUCTURE $\boxed{\text{PERSISTENT}}$ $\tau \longrightarrow \infty$

$C(\vec{x},\infty)$ AVERAGE POSITIONS OF SCATT. CENTERS	$\longleftrightarrow$	$S(\vec{\varkappa},0)$ COHERENT ELASTIC SCATTERING
$C_s(\vec{x},\infty)$?	$\longleftrightarrow$	$S_i(\vec{\varkappa};0)$ INCOHERENT ELASTIC SCATTERING

RIGID LATTICE (BRAVAIS)

$$\rho(\vec{x}) = \sum_{\ell} \delta(\vec{x} - \vec{\ell})$$

$$N \frac{\sigma_c}{4\pi} \delta(\hbar\omega) \int d^3x \, e^{i\vec{\varkappa}\vec{x}} C(\vec{x},\infty) = \frac{\sigma_c}{4\pi} \delta(\hbar\omega) \left| \int d^3x \, e^{i\vec{\varkappa}\vec{x}} \langle \rho(\vec{x}) \rangle \right|^2$$

$$\left.\frac{d\sigma}{d\Omega}\right|_{coh} = \frac{\sigma_c}{4\pi} \left| \sum_{\ell} e^{i\vec{\varkappa}\vec{\ell}} \right|^2 \sim \sum_{\tau} \delta(\vec{\varkappa} - \vec{\tau})$$

BRAGG-LINES

$$\left.\frac{d\sigma}{d\Omega}\right|_{inc} = \frac{\sigma_i}{4\pi} \sum_{j} \left| e^{i\vec{\varkappa}\vec{X}_j} \right|^2 = N \frac{\sigma_i}{4\pi}$$

ISOTROPE.

EINFACHES GITTER (OHNE BASIS)

$$\vec{x}_\ell = \ell_1 \vec{a}_1 + \ell_2 \vec{a}_2 + \ell_3 \vec{a}_3 \qquad \ell_i \in \mathbb{N}$$

$$\frac{2\pi}{\lambda} \vec{Q} = \vec{\varkappa}$$

SUMME ALLER STREUAMPLITUDEN:

$$\sum_{\ell_1 \ell_2 \ell_3} e^{i(\vec{\varkappa}\vec{x}_\ell)}$$

ℓ_1, ℓ_2, ℓ_3 ÜBER GANZEN KRISTALL

ALLE ELEMENTAR-AMPL. SIND GLEICH (HIER = 1 GESETZT)

INTENSITÄT: $\left| \sum_{\ell_1 \ell_2 \ell_3} e^{i(\vec{\varkappa}\vec{x}_\ell)} \right|^2$ KOHÄRENT !

$$\sum_{\ell_1 \ell_2 \ell_3}^{N_j - 1} e^{i(\vec{\varkappa}\vec{x}_\ell)} = \prod_{j=1}^{3} \left(\sum_{\ell_j}^{N_j-1} e^{i(\vec{\varkappa}\vec{a}_j)\ell_j} \right) \qquad (e^{a+b} = e^a \cdot e^b)$$

$\downarrow$

$\ell_j = 0, 1, 2, \ldots N_j - 1$

GEOM. FOLGE VON $q = e^{i(\vec{\varkappa}\vec{a}_j)}$

SUMME: $\frac{1 - q^{N_j}}{1 - q}$

$\downarrow$ ALSO

$$i \frac{e^{iN_j\left(\frac{\vec{\varkappa}\vec{a}_j}{2}\right)}}{e^{i\left(\frac{\vec{\varkappa}\vec{a}_j}{2}\right)}} \frac{\sin\left(N_j \frac{\vec{\varkappa}\vec{a}_j}{2}\right)}{\sin\left(\frac{\vec{\varkappa}\vec{a}_j}{2}\right)} \longleftarrow \frac{1 - e^{iN_j(\vec{\varkappa}\vec{a}_j)}}{1 - e^{i(\vec{\varkappa}\vec{a}_j)}}$$

$$e^{i\varphi} - e^{-i\varphi} = 2i \sin\varphi$$

$$\left| \quad \right|^2 = 1 \cdot \prod_{j=1}^{3} \frac{\sin^2\left(N_j \frac{\vec{\varkappa}\vec{a}_j}{2}\right)}{\sin^2\left(\frac{\vec{\varkappa}\vec{a}_j}{2}\right)}$$

MAXIMUM WENN ALLE NENNER VERSCHWINDEN ALSO

LAUE: $\boxed{(\vec{Q} \cdot \vec{a}_j) = \lambda m_j} \longleftarrow \frac{\vec{\varkappa}\vec{a}_j}{2} = \pi m_j$

ACHTUNG: $\left(\frac{\sin(Nx)}{\sin x}\right)^2$ FÜR $x = m\pi$ IST $\frac{0}{0}$

$$\left(\frac{\sin(Nx)}{\sin x}\right)^2_{x = m\pi} = N^2 \left(\frac{\cos Nx}{\cos x}\right)^2_{x = m\pi} = N^2$$

TYPISCH FÜR KOHERENTE STREUUNG !

NON-RIGID LATTICE

$$\boxed{\vec{X}_j(\tau) = \vec{l}_j + \vec{u}_j(\vec{l}_j, \tau)}$$

SOLID : $\langle \vec{u}_j(\vec{l}_j) \rangle_T = 0$

$$\rho(\vec{x}) = \sum_j \delta(\vec{x} - \vec{X}_j(\tau))$$

$$= \left(\frac{1}{2\pi}\right)^3 \int d^3\varkappa \sum_j e^{i\vec{\varkappa}(\vec{x} - \vec{l}_j)} \langle e^{-i\vec{\varkappa}\vec{u}_j(\vec{l}_j)} \rangle_T$$

$$\downarrow$$

$$e^{-\frac{1}{2}\langle (\vec{\varkappa}\vec{u}(\vec{l}))^2 \rangle_T}$$

BLOCH - RELATION

$$\langle e^{\hat{O}} \rangle_T = e^{\frac{1}{2}\langle \hat{O}^2 \rangle_T}$$

DEBYE - WALLER FACTOR :

$$\boxed{2W(\vec{\varkappa}) = \langle (\vec{\varkappa}\vec{u}(\vec{l}))^2 \rangle_T}$$

e.g. CUBIC LATTICE : $\langle (\vec{\varkappa}\vec{u}(\vec{l}))^2 \rangle = \frac{1}{6}\varkappa^2 \langle u^2 \rangle_T$

$$\langle \rho(\vec{x}) \rangle = \frac{3}{2\pi \langle u^2 \rangle} \sum_l \exp\left(\frac{|\vec{x} - \vec{l}|^2}{2\langle u^2 \rangle}\right)$$

GAUSSIAN DYNAMICAL FORM FACTOR

$$\left.\frac{d\sigma}{d\Omega}\right|_{coh} = \frac{N\sigma_c}{4\pi} \frac{(2\pi)^3}{v_0} \sum_{\tau} \delta(\vec{\varkappa} - \vec{\tau})\, e^{-2W(\vec{\varkappa})}$$

$$\left.\frac{d\sigma}{d\Omega}\right|_{inc} = \frac{N\sigma_i}{4\pi} e^{-2W(\vec{\varkappa})}$$

NOT ISOTROPIC

$$\updownarrow$$

$C_s(\vec{x}, \infty)$ CORREL. OF MOTIONAL RANGE

INELASTIC SCATTERING

CORREL. FCT :

$$\boxed{C(\vec{x},\tau) = C(\vec{x},\infty) + C'(\vec{x},\tau)}$$

PERSISTENT

$$\lim_{\tau\to\infty} C'(\vec{x},\tau) = 0$$

ELASTIC SCATT.

$$S(\vec{\varkappa},0)$$

$$C'(\vec{x},\tau) = \left(\frac{1}{2\pi}\right)^3 \sum_{ij} \int d^3\varkappa\, e^{-i\vec{\varkappa}\vec{x}}\, e^{-i\vec{\varkappa}(\vec{l}_i-\vec{l}_j)}\, e^{-2W(\vec{\varkappa})}$$

$$\cdot\left\{\exp\left[\langle \vec{\varkappa}\vec{u}(\vec{l}_i)\cdot\vec{\varkappa}\vec{u}(\vec{l}_j,\tau)\rangle_T\right] - 1\right\}$$

$C(\vec{x},\tau)$ $\qquad$ $C(\vec{x},\infty)$

UNDERSTANDING : !

$$\hat{A} = i\vec{\varkappa}\hat{\vec{u}}(\vec{l}_i) \qquad \vec{l}_i = l_1^{(i)}\vec{e}_1 + l_2^{(i)}\vec{e}_2 + l_3^{(i)}\vec{e}_3$$

$$\hat{B} = -i\vec{\varkappa}\hat{\vec{u}}(\vec{l}_j)$$

$$\langle e^{\hat{A}}\, e^{\hat{B}}\rangle_T = e^{\frac{1}{2}[\hat{A}\hat{B}]}\langle e^{\hat{A}+\hat{B}}\rangle_T$$

BLOCH RELATION

$$e^{\frac{1}{2}\langle(\hat{A}+B)^2\rangle_T}$$

$[\hat{A}\hat{B}]$ - C-NUMBER

$$A^2 + B^2 + AB + BA + AB - BA = \langle \underbrace{A^2 + B^2}_{\text{DEBYE-WALLER}} + \underbrace{2AB}_{\text{CORRELATION}} \rangle$$

LINEAR LATTICE DYNAMICS

EIGENMODE EXPANSION —— PHONONS

$$\vec{u}(\vec{l}_j, \tau) = \sum_{j,\vec{q}} \left(\frac{\hbar}{3NM\omega_j(\vec{q})}\right)^{1/2} \left[\vec{\alpha}^{(j)}(\vec{q})\, e^{i\vec{q}\vec{l}}\, \hat{a}_j(\vec{q},\tau) + \vec{\alpha}^{(j)*}(\vec{q})\, e^{-i\vec{q}\vec{l}}\, \hat{a}_j^+(\vec{q},\tau)\right]$$

HARMONIC REGIME :

$$\boxed{i\hbar\, \partial_t \hat{a}_j = [\hat{a}_j\, H] = \hbar\omega_j\, \hat{a}_j}$$

3N INDEPENDENT HARMONIC OSCILLATORS

$$\downarrow$$

DISPERSION RELATION $\omega_j(\vec{q})$

$$\hat{a}_j(\vec{q},t) = \hat{a}_j(\vec{q})\, e^{-i\omega_j(\vec{q})t}$$
$$\hat{a}_j^+(\vec{q},t) = \hat{a}_j^+(\vec{q})\, e^{i\omega_j(\vec{q})t}$$

$$[\hat{a}_i^+(\vec{q}), \hat{a}_j(\vec{q}')] = \delta_{ij}\, \delta_{\vec{q}\vec{q}'}$$

POPULATION

$$\langle \hat{a}_j^+(\vec{q})\, \hat{a}_{j'}(\vec{q}') \rangle_T = \delta_{jj'}\, \delta_{\vec{q}\vec{q}'}\, n_j(\vec{q})$$
$$\langle a_j(\vec{q})\, a_{j'}^+(\vec{q}') \rangle_T = \delta_{jj'}\, \delta_{\vec{q}\vec{q}'}\, (n_j(\vec{q}) + 1)$$

$$n_j(\vec{q}) = \left(e^{\beta\hbar\omega_j(\vec{q})} - 1\right)^{-1}$$

$$\boxed{2W(\vec{\kappa}) = \sum_{j\vec{q}} \frac{|\vec{\kappa}\cdot\vec{\alpha}^{(j)}(\vec{q})|^2}{\omega_j(\vec{q})} \left(2n_j(\vec{q}) + 1\right)}$$

ZERO POINT ENERGY

TRANSV.
LONGITUD. } MODES

OPTICAL — FOR LATTICE WITH BASIS

ACOUSTICAL

$$e^{\langle \hat{A}\hat{B} \rangle} = 1 + \langle \hat{A}\hat{B} \rangle + \frac{1}{2!}\langle \hat{A}\hat{B} \rangle^2 + \cdots\cdots$$

$$\left.\begin{array}{l} \hat{A} \sim \hat{u} \\ \hat{B} \sim \hat{u} \end{array}\right\} \text{CONTAINING } a, a^+$$

HENCE :

$\langle \hat{A}\hat{B} \rangle_T$ HAVE TERMS

$$\langle a^+ a \rangle_T \;\longrightarrow\; n \quad ; \quad \langle a a^+ \rangle_T \;\longrightarrow\; n+1$$

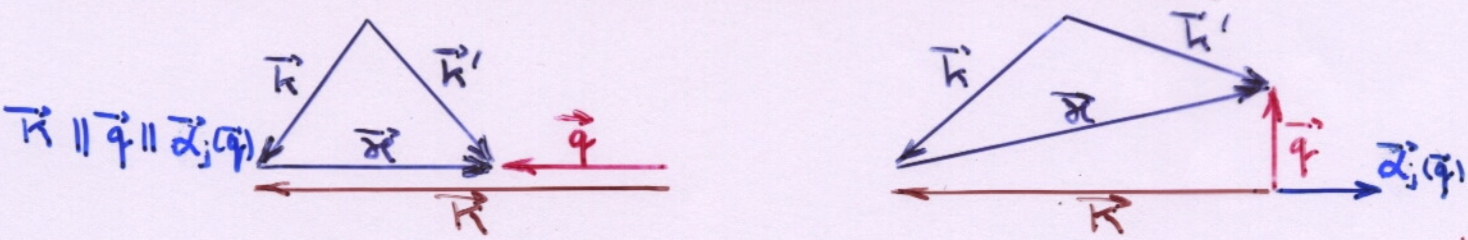
$S(\vec{\varkappa}, \omega)$ HAS TERMS PROPORT. TO :

i) $n_j(\vec{q})\,\delta(\omega + \omega_j(\vec{q}))\,\delta(\vec{\varkappa} + \vec{q} - \vec{K})$ ANTI-STOKES

ii) $(n_j(\vec{q}) + 1)\,\delta(\omega - \omega_j(\vec{q}))\,\delta(\vec{\varkappa} - \vec{q} - \vec{K})$ STOKES

ONE PHONON ANNIHILATION / CREATION

(HIGHER POWERS : MULTI-PHONON PROCESSES)



LONGIT. PHONON

TRANSV. PHONON

CONTROL BY PREFACTOR $\longrightarrow$ $\vec{\varkappa}\,\vec{\alpha}^{(j)}(\vec{q})$

"SELECTION RULE"

$\vec{K}$: RECIPR. LATTICE VECTOR (TRANSL. BY $\vec{K}$ – SAME OSCILL. DISPLACEMENT)

$$\boxed{E' = E \pm \hbar\omega_j(\vec{q}) \quad ; \quad \vec{k}' = \vec{k} \pm \vec{q} - \vec{K}}$$

PREFACTORES : $S(\vec{\varkappa}, \omega) \sim \frac{1}{\omega(\vec{q})}$

$\sim e^{-W(\vec{\varkappa})}$ T - DEPENDENT

CORRELATION FUNCTION

$$\boxed{C(\vec{x},\tau) = \frac{1}{N}\int d^3x' \, \langle \rho(\vec{x}',\tau)\, \rho(\vec{x}-\vec{x}',0) \rangle_T}$$

$$C(\vec{x},\tau) = \sum_{ij}\int d^3x' \langle \delta(\vec{x}'-\vec{X}_i(\tau))\, \delta(\vec{x}-\vec{x}'+\vec{X}_j(0)) \rangle_T$$

$$\rho(\vec{x},\tau) = \sum_j \delta(\vec{x}-\vec{X}_j(\tau))$$

$$C(\vec{x},\tau) = \left(\frac{1}{2\pi}\right)^3 \int d^3\varkappa \, e^{-i\vec{\varkappa}\vec{x}} \langle \qquad \rangle_T$$

$$\mathcal{F}_{\varkappa}$$

$$\boxed{\frac{1}{2\pi\hbar}\sum_{ij}\langle e^{i\vec{\varkappa}\vec{X}_i(\tau)}\, e^{-i\vec{\varkappa}\vec{X}_j(0)} \rangle_T}$$

INTERMEDIATE SCATT. FCT.

$$\mathcal{F}_{\tau}^{-1}$$

$$S(\omega,\vec{\varkappa}) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} d\tau \, e^{-i\omega\tau} \langle \qquad \rangle_T$$

$$\rho_{\varkappa}(\tau) = \sum_j e^{-i\vec{\varkappa}\vec{X}_j(\tau)}$$

$$\boxed{S(\omega,\vec{\varkappa}) = \frac{1}{2\pi\hbar}\frac{1}{N}\int_{-\infty}^{+\infty} d\tau \, e^{-i\omega\tau} \langle \rho_{\varkappa}(\tau)\, \rho_{\varkappa}^{+}(0) \rangle_T}$$

SCATTERING FUNCTION

(i,j) ,	$\omega = 0$	ABSOLUTE COHERENCE	ELASTIC
	$\omega \neq 0$	RELATIVE COHERENCE	INELASTIC
$(i=j)$,	$\left.\begin{matrix}\omega = 0 \\ \omega \neq 0\end{matrix}\right\}$	INCOHERENENT	$\left\{\begin{matrix}\text{ELASTIC} \\ \text{INELASTIC}\end{matrix}\right.$

$$\rho(\vec{x},\tau) = \sum_j \delta(\vec{x}-\vec{X}_j(\tau)) = \frac{1}{V}\sum_{\varkappa} \rho_{\varkappa} e^{i\vec{\varkappa}\vec{x}} \qquad \rho_{\varkappa}(\tau) = \sum_j e^{-i\vec{\varkappa}\vec{X}_j(\tau)}$$