A quantum approach to scattering

- Scattering cross sections
- Two-photon processes: 2nd .vs. charge
- X-ray scattering, elastic and inelastic
- Static and dynamic scattering functions
- Phonon scattering - theory
- Phonon scattering - experiments

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Scattering cross sections

Elastic scattering cross-section

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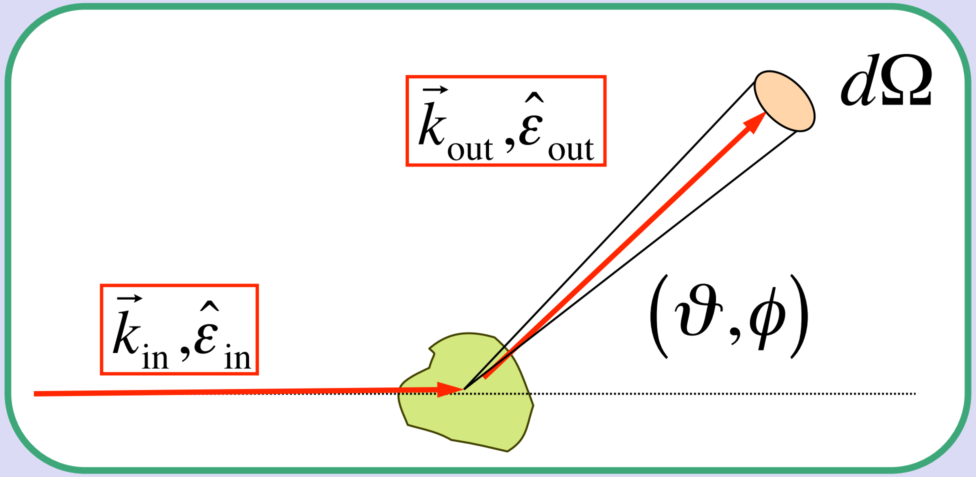

Static scattering function

Structural sample properties

Differential scattering cross-section

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_0 S(\vec{K})$$

Intrinsic cross-section

Probe - sample coupling

?

- X-rays
- electrons
- neutrons

Inelastic scattering cross-section

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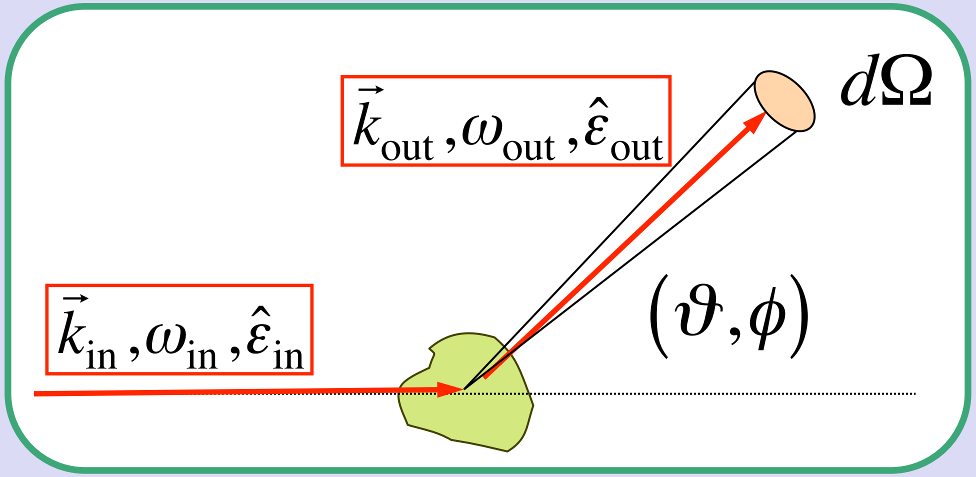

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \left(\frac{d\sigma}{d\Omega}\right)_0 S(\vec{K}, \omega)$$

Double differential scattering cross-section

Dynamic scattering function

Dynamical sample properties

Intrinsic cross-section

Probe - sample coupling

Intrinsic cross-sections for scattering by atoms

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X-rays
(neglecting polarisation factor)

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = r_e^2 \left|f_0\left(\vec{K},Z\right)\right|^2 = \left|f_X\left(\vec{K},Z\right)\right|^2$$

Radiation–matter interaction

$$f_0\left(\vec{K}\right) = \int \rho_e(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV$$

Electrons

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = \left|f_{\mathrm{el}}\left(\vec{K},Z\right)\right|^2$$

Potential scattering
Born approx.

$$f_{\mathrm{el}}\left(\vec{K}\right) \approx \int \Phi(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}\, dV$$

Thermal neutrons

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = |b|^2$$

Fermi pseudo-potential

$$V(\vec{r}) \;\propto\; b\,\delta(\vec{r})$$

Formal scattering theory

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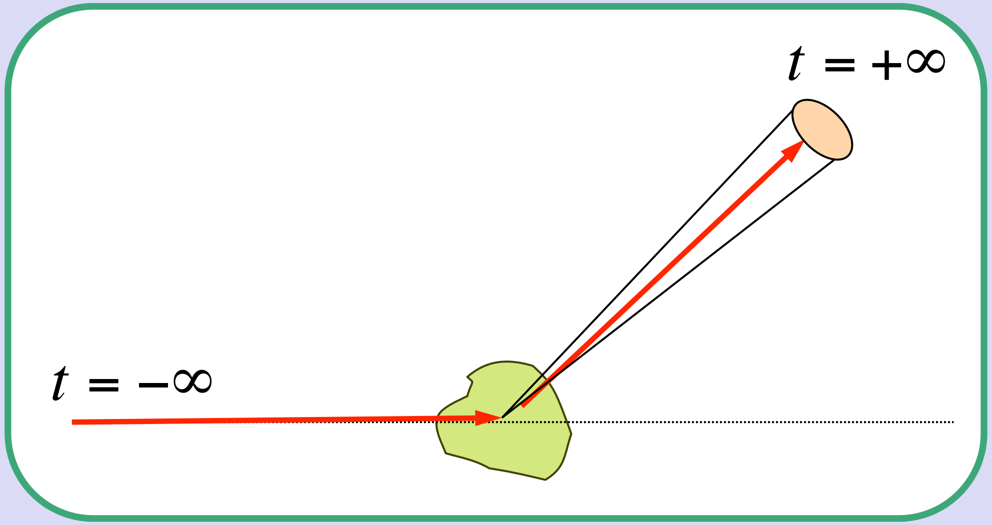

Adiabatic switching of the interaction

Scattering amplitude and S matrix

$$\langle \Phi_f | \mathcal{S} | \Phi_i \rangle = \langle \Phi_f | \tilde{U}(-\infty, +\infty) | \Phi_i \rangle$$

a) $|\Phi_f\rangle$ and $|\Phi_i\rangle$ are the final and initials states of the entire system (probe+ sample)
b) $\tilde{U}$ is the evolution operator from $-\infty$ to $+\infty$ in the interaction picture

Two-photon processes - scattering

Time-dependent perturbation theory

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Transition amplitudes

$$c_{fi} = \left\langle \Phi_f \middle| U\left(t_f, t_i\right) \middle| \Phi_i \right\rangle = c_{fi}^{(1)} + c_{fi}^{(2)} + \ldots.$$

Approximations:

Zero-order

$$\tilde{c}_{fi}^{(0)} = \delta_{fi}$$

First-order

$$\tilde{c}_{fi}^{(1)} = \frac{1}{i\hbar} \int_{t_i}^{t_f} d\tau \; e^{iE_f \tau/\hbar} \, \langle \Phi_f | \, H_{\rm int} \, | \Phi_i \rangle \; e^{-iE_i \tau/\hbar}$$

Second-order

$$\tilde{c}_{fi}^{(2)} = \left(\frac{1}{i\hbar}\right)^2 \int_{t_1}^{t_f} d\tau_2 \int_{t_i}^{t_1} d\tau_1$$
$$\sum_{\Phi_1} e^{iE_f \tau_2/\hbar} \, \langle \Phi_f | \, H_{\rm int} \, | \Phi_1 \rangle \, e^{-iE_1(\tau_2 - \tau_1)/\hbar} \, \langle \Phi_1 | \, H_{\rm int} \, | \Phi_i \rangle \, e^{-iE_i \tau_1/\hbar}$$

....

n interaction factors
n+1 free evolution factors

Interaction Hamiltonian

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Non-relativistic Hamiltonian

$$H_{\text{tot}} = H_{\text{at}} + H_{\text{rad}} + H_{\text{int}}$$

$$H_{\text{at}} = \sum_j \frac{P_j^2}{2m} + V(\vec{r}_1 \ldots \vec{r}_N)$$

$$H_{\text{rad}} = \sum_{\vec{k}s} \hbar\omega_{\vec{k}s} \left[a^\dagger a + \frac{1}{2} \right] .$$

1st order (interaction)

$$H_{\text{int},1} = \frac{e}{m} \sum_j \vec{P}_j \cdot \vec{A}(\vec{r}_j)$$

2nd order (interaction)

$$H_{\text{int},2} = \frac{e^2}{2m} \sum_j |\vec{A}(\vec{r}_j)|^2$$

Photon scattering

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Photon scattering = two-photon processes ➔ 2nd order processes .vs. e

charge

1st-order approximation

2nd-order interaction

$$c_{fi}^{(1)} = -2\pi i \langle \Phi_f | H_{I,2} | \Phi_i \rangle$$

$$H_{I,2} = \frac{e^2}{2m} \sum_j \left| \vec{A}(\vec{r}_j) \right|^2$$

Type γ

2nd-order approximation

1st-order interaction

$$c_{fi}^{(2)} = -2\pi i \sum_\ell \lim_{\eta \to 0} \frac{\langle \Phi_f | H_{I,1} | \ell \rangle \langle \ell | H_{I,1} | \Phi_i \rangle}{E_f - E_\ell + i\eta}$$

$$H_{I,1} = \frac{e}{m} \sum_j \vec{P}_j \cdot \vec{A}(\vec{r}_j)$$

Type α, β

$$\vec{A}(\vec{r}) = \sum_{\vec{k}s} \sqrt{\frac{\hbar}{2\varepsilon_0 V \omega_{\vec{k}s}}} \left[a_{\vec{k}s} e^{i\vec{k}\cdot\vec{r}} + a_{\vec{k}s}^{+} e^{-i\vec{k}\cdot\vec{r}} \right] \varepsilon_{\vec{k}s}$$

Scattering type α

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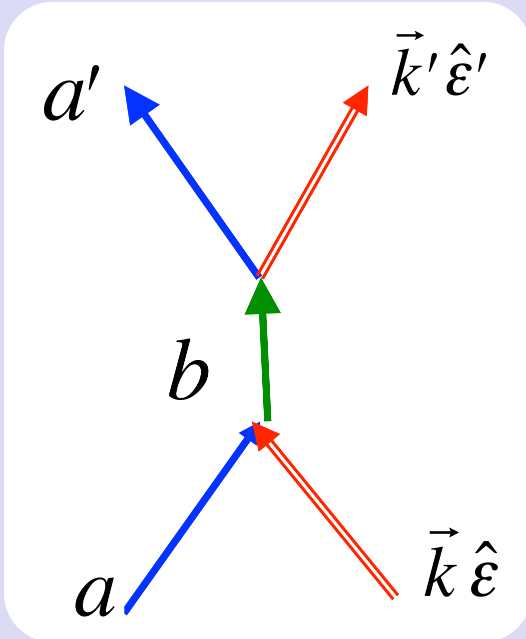
1st-order interaction
2nd-order approximation

$$|\Phi_f\rangle = |a';\vec{k}'\hat{\varepsilon}'\rangle$$



$$|\Phi_i\rangle = |a;\vec{k}\hat{\varepsilon}\rangle$$

Energy

$$E_i = E_f = E_a + \hbar\omega = E_{a'} + \hbar\omega'$$

Transition amplitude

$$c_{fi}^{(2)} = -2\pi i \sum_b \lim_{\eta \to 0} \frac{\langle a';\vec{k}'\hat{\varepsilon}'|H_{I,1}|b;0\rangle\langle b;0|H_{I,1}|a;\vec{k}\hat{\varepsilon}\rangle}{E_a + \hbar\omega - E_b + i\eta}$$

$\underbrace{E_a + \hbar\omega}$: $E_i = E_f$

E_b: Intermediate-state energy

Scattering type α – elastic

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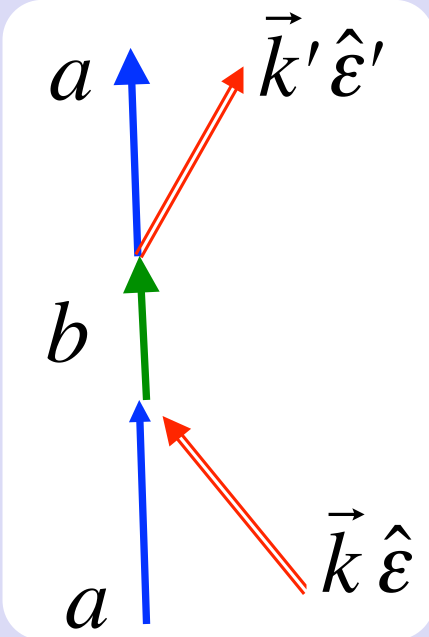
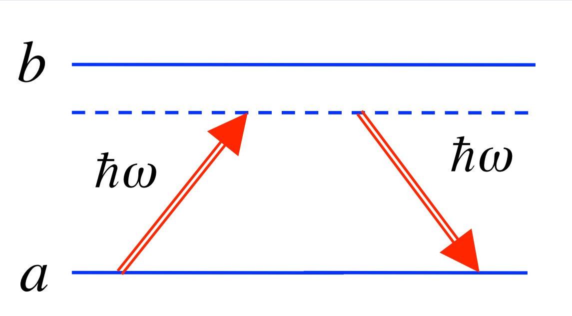
1st-order interaction
2nd-order approximation

$\hbar\omega << E_{ion}$



Elastic scattering: $\hbar\omega = \hbar\omega'; \quad a' = a$

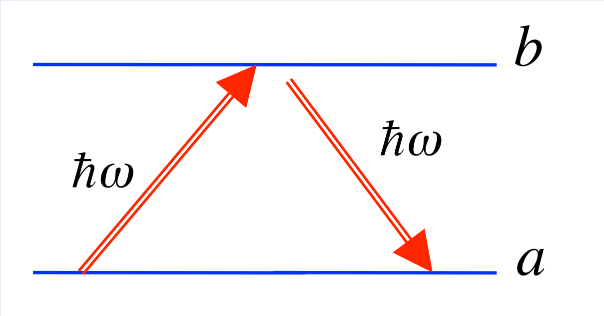
$$c_{fi}^{(2)} = -2\pi i \sum_b \lim_{\eta\to 0} \frac{\langle a;\vec{k}'\hat{\varepsilon}'|H_{I,1}|b;0\rangle\langle b;0|H_{I,1}|a;\vec{k}\hat{\varepsilon}\rangle}{E_a + \hbar\omega - E_b + i\eta}$$



non-resonant

$\hbar\omega < |E_b - E_a|$

Rayleigh



resonant

$\hbar\omega = |E_b - E_a|$

Scattering type α - inelastic

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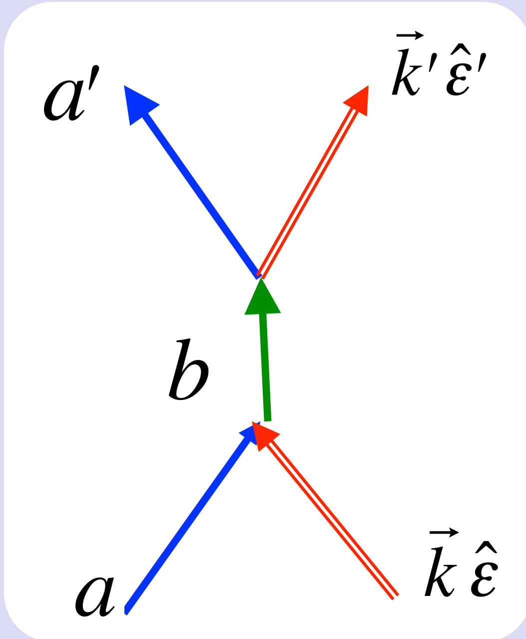
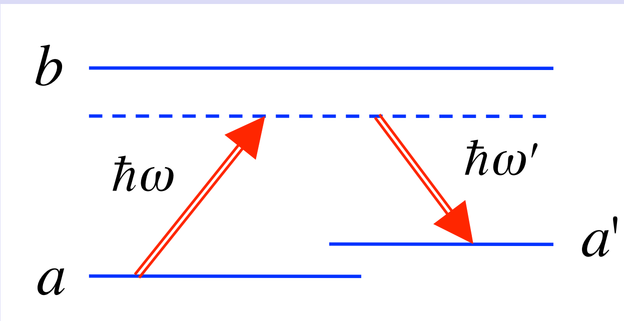
1st-order interaction
2nd-order approximation

$$\hbar\omega << E_{ion}$$

Inelastic scattering: $\hbar\omega \neq \hbar\omega'; \quad a' \neq a$

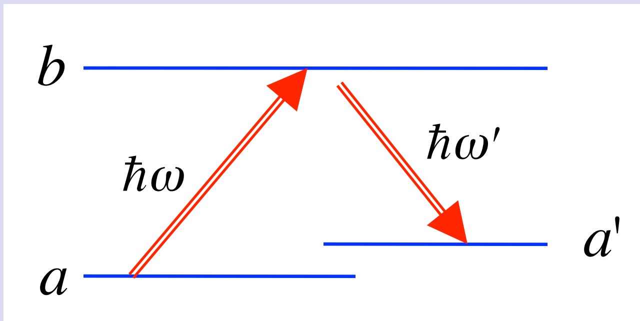
$$c_{fi}^{(2)} = -2\pi i \sum_b \lim_{\eta\to 0} \frac{\langle a';\vec{k}'\hat{\varepsilon}'|H_{I,1}|b;0\rangle\langle b;0|H_{I,1}|a;\vec{k}\hat{\varepsilon}\rangle}{E_a + \hbar\omega - E_b + i\eta}$$





non-resonant

Raman



resonant

Scattering type β

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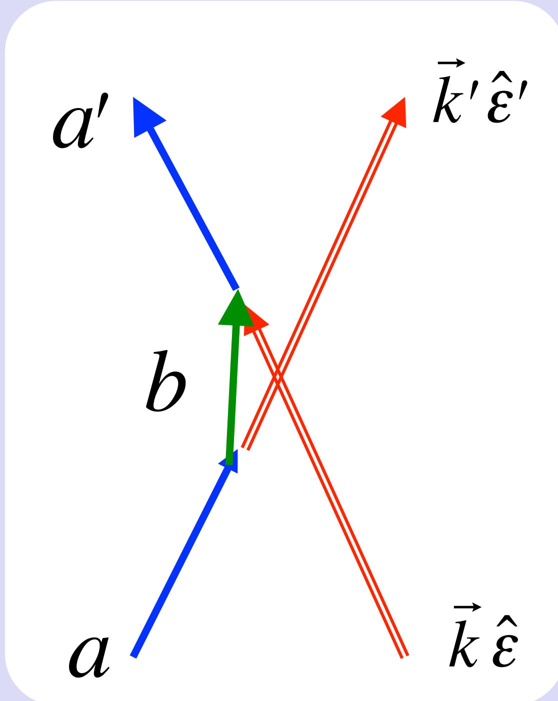
1st-order interaction
2nd-order approximation

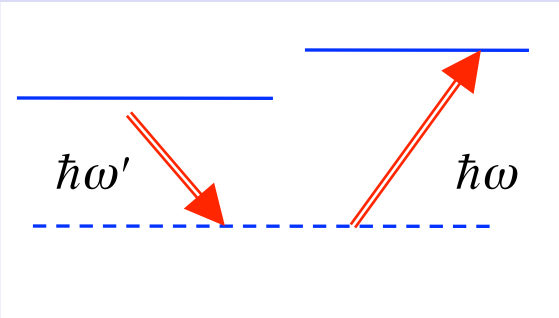
$$|\Phi_f\rangle = |a';\vec{k}'\hat{\varepsilon}'\rangle$$



$$|\Phi_i\rangle = |a;\vec{k}\hat{\varepsilon}\rangle$$

Energy

$$E_i = E_f = E_a + \hbar\omega = E_{a'} + \hbar\omega'$$



Transition amplitude

$$c_{fi}^{(2)} = -2\pi i \sum_b \lim_{\eta\to 0} \frac{\langle a';\vec{k}'\hat{\varepsilon}'|H_{I,1}|b;\vec{k}\hat{\varepsilon},\vec{k}'\hat{\varepsilon}'\rangle\langle b;\vec{k}\hat{\varepsilon},\vec{k}'\hat{\varepsilon}'|H_{I,1}|a;\vec{k}\hat{\varepsilon}\rangle}{E_a - \hbar\omega' - E_b + i\eta}$$

Scattering type γ

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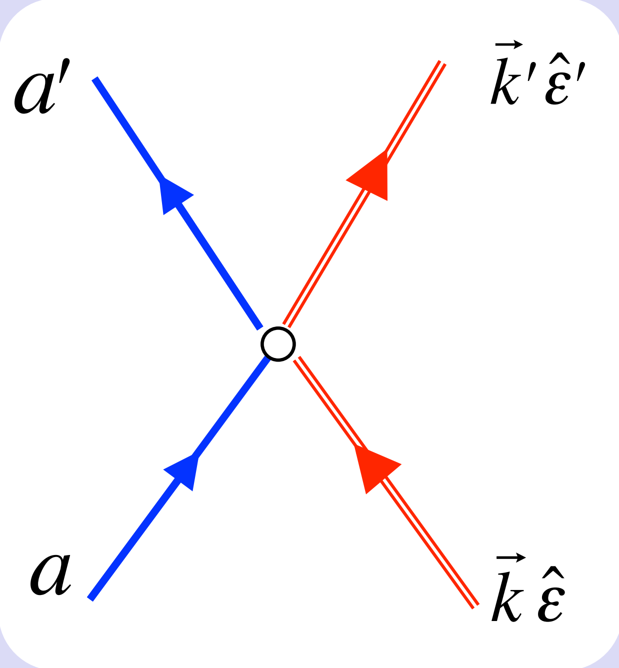
2nd-order interaction
1st-order approximation

$$\left|\Phi_f\right\rangle = \left|a';\vec{k}'\hat{\varepsilon}'\right\rangle$$



$$\left|\Phi_i\right\rangle = \left|a;\vec{k}\hat{\varepsilon}\right\rangle$$

Energy

$$E_i = E_f = E_a + \hbar\omega = E_{a'} + \hbar\omega'$$

Transition amplitude

$$c_{fi}^{(1)} = -2\pi i\left\langle a';\vec{k}'\hat{\varepsilon}'\middle|H_{I,2}\middle|a;\vec{k}\hat{\varepsilon}\right\rangle$$

Scattering type γ - elastic

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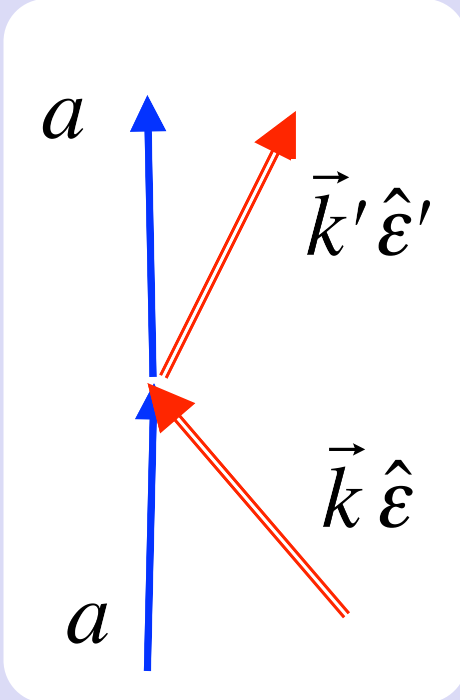
2nd-order interaction

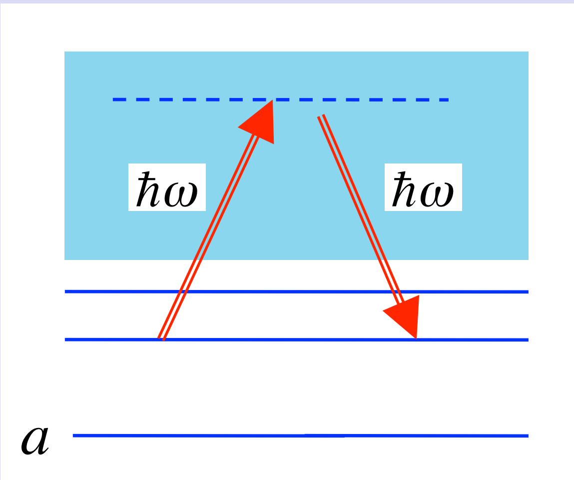
1st-order approximation

Transition amplitude

$$c_{fi}^{(1)} = -2\pi i \left\langle a; \vec{k}'\hat{\varepsilon}' \middle| H_{I,2} \middle| a; \vec{k}\hat{\varepsilon} \right\rangle$$

Elastic scattering: $\hbar\omega = \hbar\omega'; \quad a' = a$





Thomson

$$\hbar\omega >> E_{ion}$$

Scattering type γ - inelastic

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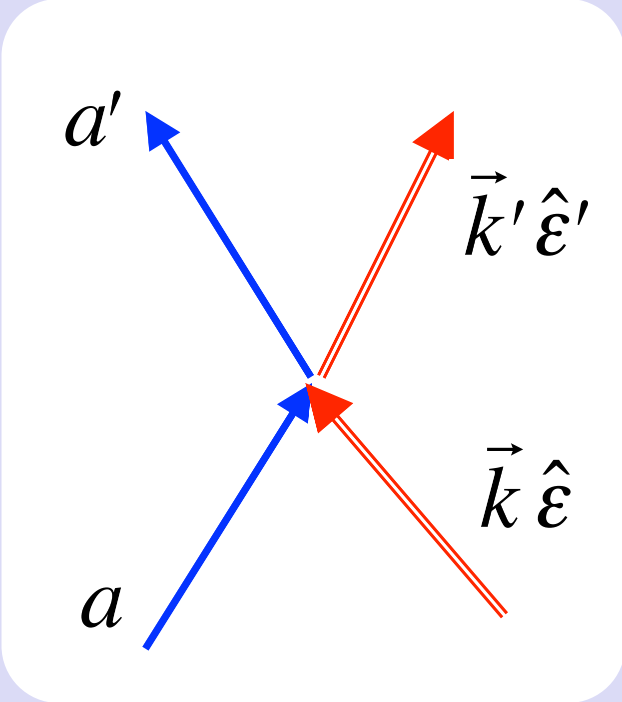
2nd-order interaction

1st-order approximation

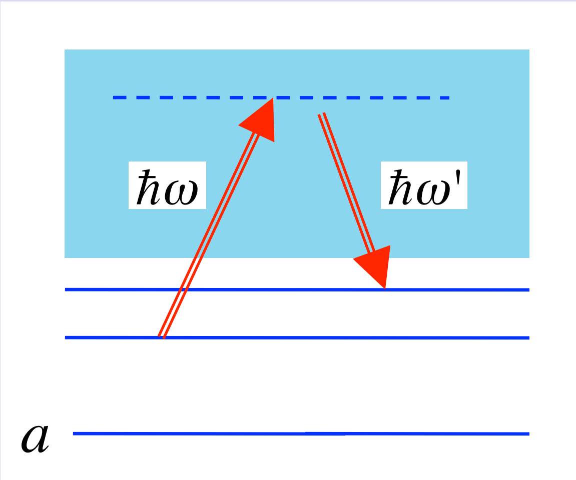


Transition amplitude

$$c_{fi}^{(1)} = -2\pi i \left\langle a';\vec{k}'\hat{\varepsilon}' \middle| H_{I,2} \middle| a;\vec{k}\hat{\varepsilon} \right\rangle$$

Inelastic scattering:

$$\hbar\omega \neq \hbar\omega'; \quad a' \neq a$$



Compton

$$\hbar\omega >> E_{ion}$$

X-ray scattering

X-ray scattering

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$$c_{fi}^{(1)} + c_{fi}^{(2)} = -2\pi i \langle a';\vec{k}'\hat{\varepsilon}' | H_{I,2} | a;\vec{k}\hat{\varepsilon}\rangle$$

γ

$$H_{I,2} = \frac{e^2}{2m}\sum_j \left|\vec{A}(\vec{r}_j)\right|^2$$

$\hbar\omega >> E_{ion}$

$$-2\pi i \sum_b \lim_{\eta\to 0} \frac{\langle a';\vec{k}'\hat{\varepsilon}' | H_{I,1} | b;0\rangle\langle b;0 | H_{I,1} | a;\vec{k}\hat{\varepsilon}\rangle}{E_a + \hbar\omega - E_b + i\Gamma/2}$$

$$-2\pi i \sum_b \lim_{\eta\to 0} \frac{\langle a';\vec{k}'\hat{\varepsilon}' | H_{I,1} | b;\vec{k}\hat{\varepsilon},\vec{k}'\hat{\varepsilon}'\rangle\langle b;\vec{k}\hat{\varepsilon},\vec{k}'\hat{\varepsilon}' | H_{I,1} | a;\vec{k}\hat{\varepsilon}\rangle}{E_a - \hbar\omega' - E_b + i\Gamma/2}$$

α,β

$$H_{I,1} = \frac{e}{m}\sum_j \vec{P}_j \cdot \vec{A}(\vec{r}_j)$$

$\hbar\omega << E_{ion}$

Vector potential

$$\vec{A}(\vec{r}) = \sum_{\vec{k}s} \sqrt{\frac{\hbar}{2\varepsilon_0 V \omega_{\vec{k}s}}} \left[a_{\vec{k}s}\, e^{i\vec{k}\cdot\vec{r}} + a_{\vec{k}s}^{+} e^{-i\vec{k}\cdot\vec{r}}\right]\hat{\varepsilon}_{\vec{k}s}$$

Many photons

$$\vec{A}(\vec{r}) = \sqrt{\frac{\hbar}{2\varepsilon_0 V}} \left[\frac{\hat{\varepsilon}\, a_{\vec{k}s}\, e^{i\vec{k}\cdot\vec{r}} + \hat{\varepsilon}\, a_{\vec{k}s}^{+} e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{\omega}} + \frac{\hat{\varepsilon}'\, a_{\vec{k}'s'}\, e^{i\vec{k}'\cdot\vec{r}} + \hat{\varepsilon}'\, a_{\vec{k}'s'}^{+} e^{-i\vec{k}'\cdot\vec{r}}}{\sqrt{\omega'}}\right]$$

Two photons

X-ray scattering: γ

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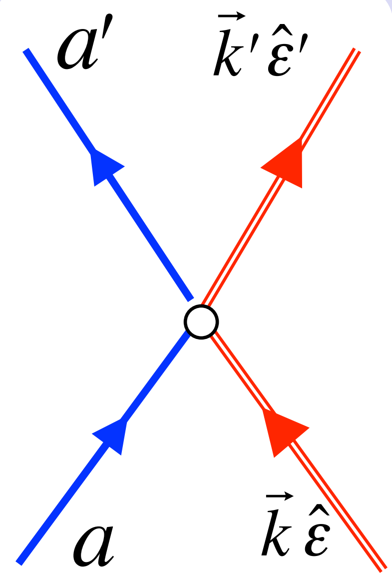
$$H_{\mathrm{I},2} = \frac{e^2}{2m}\sum_j \left|\vec{A}(\vec{r}_j)\right|^2$$

$$= \frac{e^2}{2m}\,\frac{\hbar}{2\varepsilon_0 V}\,\frac{1}{\sqrt{\omega\,\omega'}}(\hat{\varepsilon}\cdot\hat{\varepsilon}')\sum_j\left[a_{\vec{k}s}\,e^{i\vec{k}\cdot\vec{r}_j}\,a^{+}_{\vec{k}'s'}\,e^{-i\vec{k}'\cdot\vec{r}_j} + a^{+}_{\vec{k}'s'}\,e^{i\vec{k}\cdot\vec{r}_j}\,a_{\vec{k}s}\,e^{-i\vec{k}'\cdot\vec{r}_j}\right]$$



1 photon created + 1 photon deleted

transition amplitude

$$c^{(1)}_{\mathrm{fi}} \approx \left\langle a';\vec{k}'\hat{\varepsilon}'\right|H_{\mathrm{I},2}\left|a;\vec{k}\hat{\varepsilon}\right\rangle = \frac{e^2}{2m}\,\frac{\hbar}{\varepsilon_0 V}\,\frac{1}{\sqrt{\omega\omega'}}(\varepsilon\cdot\varepsilon')\left\langle a'\right|\sum_j e^{i\vec{K}\cdot\vec{r}_j}\left|a\right\rangle$$

$$e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_j} = e^{i\vec{K}\cdot\vec{r}_j}$$

X-ray scattering: γ

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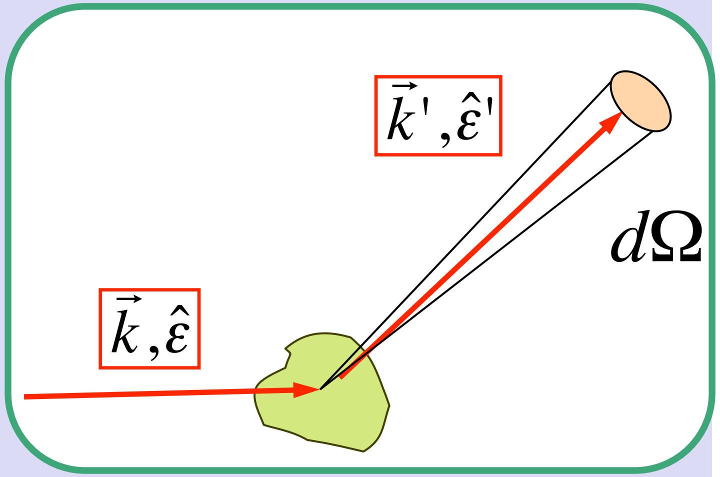
Transition probability per unit time

$$w_{\mathrm{fi}}^{(1)} = \frac{2\pi}{\hbar} \left| \left\langle a';\vec{k}'\hat{\varepsilon}' \right| H_{\mathrm{I},2} \left| a;\vec{k}\hat{\varepsilon} \right\rangle \right|^2 g\left(E_f\right)$$

Golden rule



Number of available final states

$$dN = \frac{V}{8\pi^3} k'^2\, dk'\, \Delta\Omega = g\left(E_f\right) dE_f$$

Density of final states

$$g\left(E_f\right) = \frac{V}{8\pi^3} \frac{\omega'^2}{\hbar c^3} \Delta\Omega$$

$$w_{\mathrm{fi}}^{(1)} = \frac{c}{V} \left(\frac{e^2}{4\pi\varepsilon_0 c^2 m} \right)^2 \frac{\omega'}{\omega} \left(\hat{\varepsilon}\cdot\hat{\varepsilon}'\right)^2 \left| \left\langle a' \right| \sum_j e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_j} \left| a \right\rangle \right|^2 \Delta\Omega$$

X-ray elastic scattering γ

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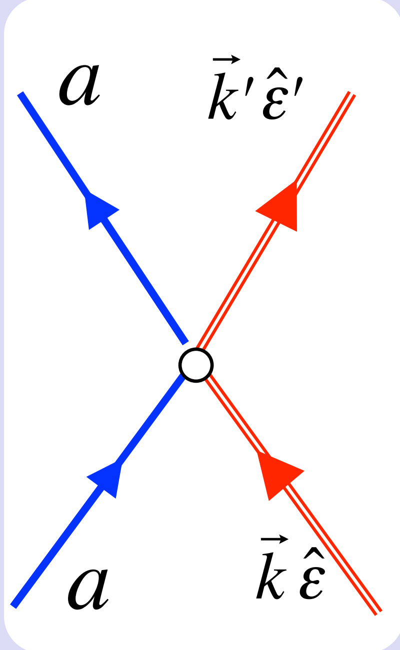
Transition probability per unit time

$$w_{\rm fi}^{(1)} = \frac{c}{V}\left(\frac{e^2}{4\pi\varepsilon_0 c^2 m}\right)^2 \frac{\omega'}{\omega}(\hat{\varepsilon}\cdot\hat{\varepsilon}')^2 \left|\langle a'|\sum_j e^{i\vec{K}\cdot\vec{r}_j}|a\rangle\right|^2 \Delta\Omega$$



elastic scattering

$a' = a, \quad \omega' = \omega$

$$\langle a|\sum_j e^{i\vec{K}\cdot\vec{r}_j}|a\rangle = \int |\psi|^2 e^{i\vec{K}\cdot\vec{r}}\, dV = f_0(\vec{K})$$

$$w_{\rm fi}^{(1)} = \frac{c}{V}\left(\frac{e^2}{4\pi\varepsilon_0 c^2 m}\right)^2 (\hat{\varepsilon}\cdot\hat{\varepsilon}')^2 \left|f_0(\vec{K},Z)\right|^2 \Delta\Omega$$

$$\left(\frac{d\sigma}{d\Omega}\right)_0 = \frac{w_{\rm fi}^{(1)}}{\Phi_{in}}\frac{1}{\Delta\Omega} = r_e^2 (\hat{\varepsilon}\cdot\hat{\varepsilon}')^2 \left|f_0(\vec{K},Z)\right|^2$$

= classical result

X-ray elastic scattering

α

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$$c_{fi}^{(2)} = -2\pi i \sum_b \lim_{\eta\to 0} \frac{\langle a;\vec{k}'\hat{\varepsilon}' | H_{I,1} | b;0\rangle\langle b;0 | H_{I,1} | a;\vec{k}\hat{\varepsilon}\rangle}{E_a + \hbar\omega - E_b + i\Gamma/2}$$

$$H_{I,1} = \frac{e}{m}\sum_j \vec{P}_j \cdot \vec{A}(\vec{r}_j)$$

$$c_{fi}^{(2)} \approx c_{fi}^{(1)} \left(\frac{E_{\text{ion}}}{\hbar\omega}\right)^2$$

Resonant scattering

Scattering functions

Static and dynamic scattering functions γ

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$$E_{A,out} + \hbar\omega_{out} = E_{A,in} + \hbar\omega_{in}$$

A = material system

Inelastic scattering

$$\frac{d^2\sigma}{d\Omega\, d\omega_{out}} = r_0^2 \left(\hat{\varepsilon}_{out} \cdot \hat{\varepsilon}_{in}\right)^2 \frac{\omega_{out}}{\omega_{in}} \left| \left\langle A_{out} \left| \sum_j e^{-i\vec{K}\cdot\vec{r}_j} \right| A_{in} \right\rangle \right|^2$$

$S(\vec{K},\omega)$ Dynamic scattering function

Elastic scattering

$$\frac{d\sigma}{d\Omega} = r_0^2 \left(\hat{\varepsilon}_{out} \cdot \hat{\varepsilon}_{in}\right)^2 \left| \left\langle A \left| \sum_j e^{-i\vec{K}\cdot\vec{r}_j} \right| A \right\rangle \right|^2$$

$\omega_{out} = \omega_{in}$

$A_{out} = A_{in} = A$

$S(\vec{K})$ Static scattering function

Static scattering function

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$$S(\vec{K}) = \left| \langle A | \sum_j e^{-i\vec{K}\cdot\vec{r}_j} | A \rangle \right|^2 = \left| \sum_j \langle j | e^{-i\vec{K}\cdot\vec{r}_j} | j \rangle \right|^2$$

$$= \left| \sum_j \int \left| \psi_j(\vec{r}) \right|^2 e^{-i\vec{K}\cdot\vec{r}_j} \, d\vec{r}_j \right|^2$$

$$= \left| \int \sum_j \rho_j(\vec{r}) \, e^{-i\vec{K}\cdot\vec{r}_j} \, d\vec{r}_j \right|^2$$

$$= \left| \int \rho(\vec{r}) \, e^{-i\vec{K}\cdot\vec{r}} \, d\vec{r} \right|^2$$

j: electrons (X scatt.); nuclei (n scattering)

→ Fourier transform of number density

The inversion problem

$$S(\vec{K}) \rightarrow \rho(\vec{r})$$

- Finite K range
- Finite K resolution
- Phase problem

Equal-time correlation function

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$$S(\vec{K}) = \left| \int \rho(\vec{r})\, e^{i\vec{K}\cdot\vec{r}} d\vec{r} \right|^2 = \int \rho(\vec{r}_1)\, e^{i\vec{K}\cdot\vec{r}_1} d\vec{r}_1 \;\times\; \int \rho(\vec{r}_2)\, e^{-i\vec{K}\cdot\vec{r}_2} d\vec{r}_2$$

$$= \int d\vec{r}_2 \int d\vec{r}_1\, \rho(\vec{r}_1)\, \rho(\vec{r}_2)\, e^{i\vec{K}\cdot(\vec{r}_1 - \vec{r}_2)}$$

$$= \int d\vec{R} \int d\vec{r}_1\, \rho(\vec{r}_1)\, \rho(\vec{r}_1 + \vec{R})\, e^{i\vec{K}\cdot\vec{R}}$$

$$\vec{R} = \vec{r}_2 - \vec{r}_1$$

$$S(\vec{K}) = \int G(\vec{R})\, e^{i\vec{K}\cdot\vec{R}} d\vec{R}$$

$$G(\vec{R}) = \int d\vec{r}_1\, \rho(\vec{r}_1)\, \rho(\vec{r}_1 + \vec{R})$$

Density-density autocorrelation function
or
Equal-time correlation function

Probability density that given a particle @ $\vec{r}_1$
another particle is @ $\vec{r}_1 + \vec{R}$

S(K) for a monatomic crystal

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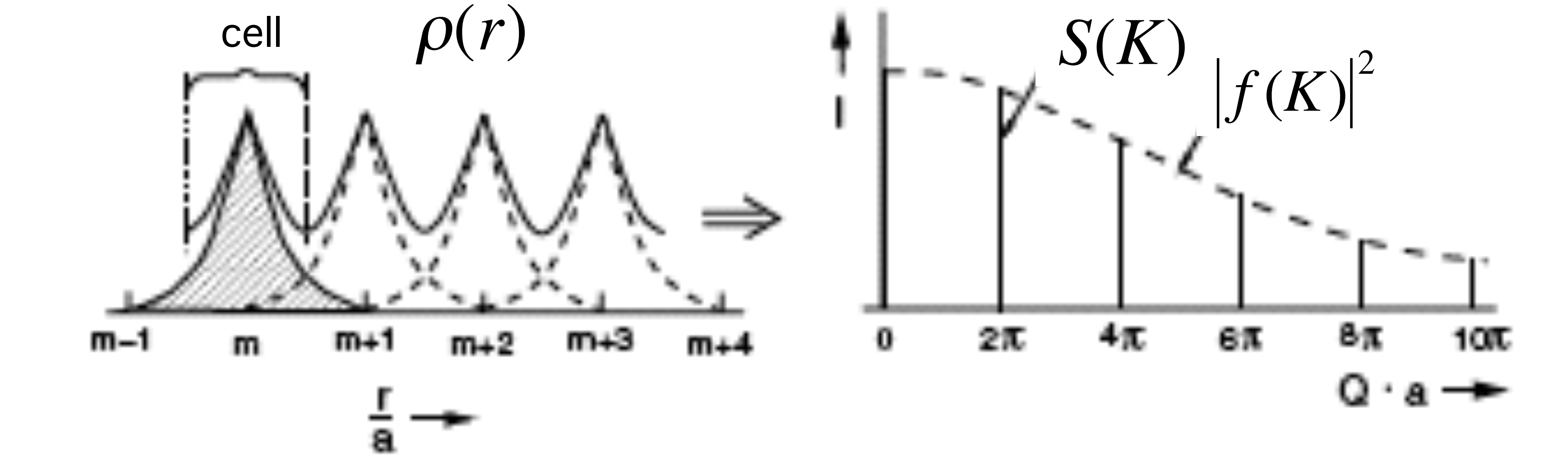
Real space

Reciprocal space



$$S(\vec{K}) = \left|A_{eu}(\vec{K})\right|^2 = \left|f(\vec{K})\right|^2 \sum_{mn} e^{i\vec{K}\cdot\vec{R}_{mn}}$$

m,n = atom indices

atomic scattering factor

S(K) for a two-atomic crystal

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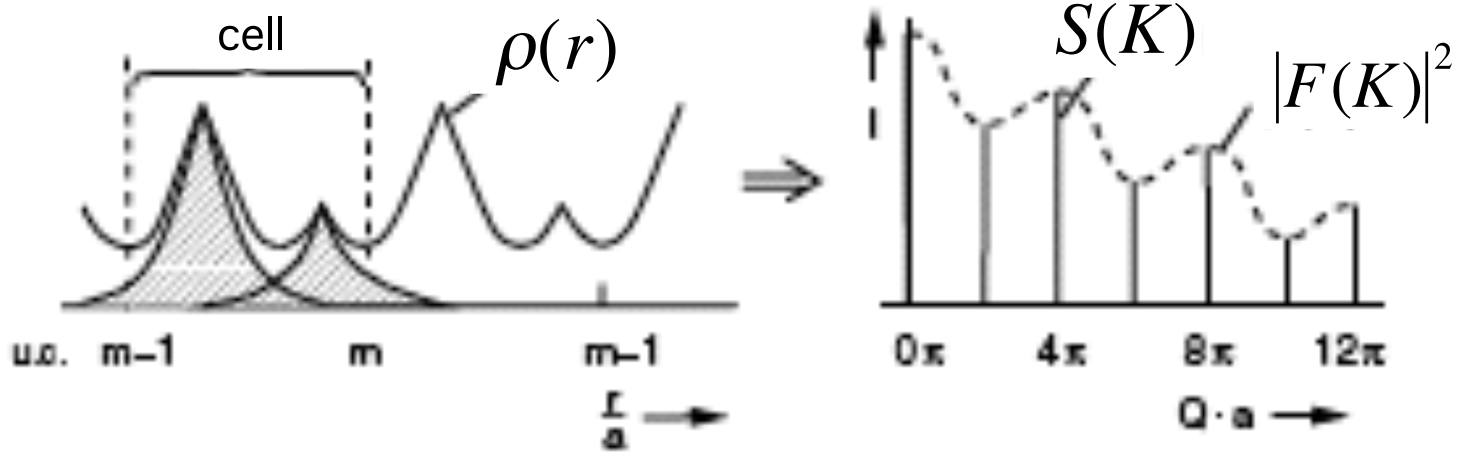
Real space

Reciprocal space



$$S(\vec{K}) = \left|A_{eu}(\vec{K})\right|^2 = \left|F(\vec{K})\right|^2 \sum_{mn} e^{i\vec{K}\cdot\vec{R}_{mn}}$$

structure factor

m,n = cell indices

S(K) for a monatomic liquid

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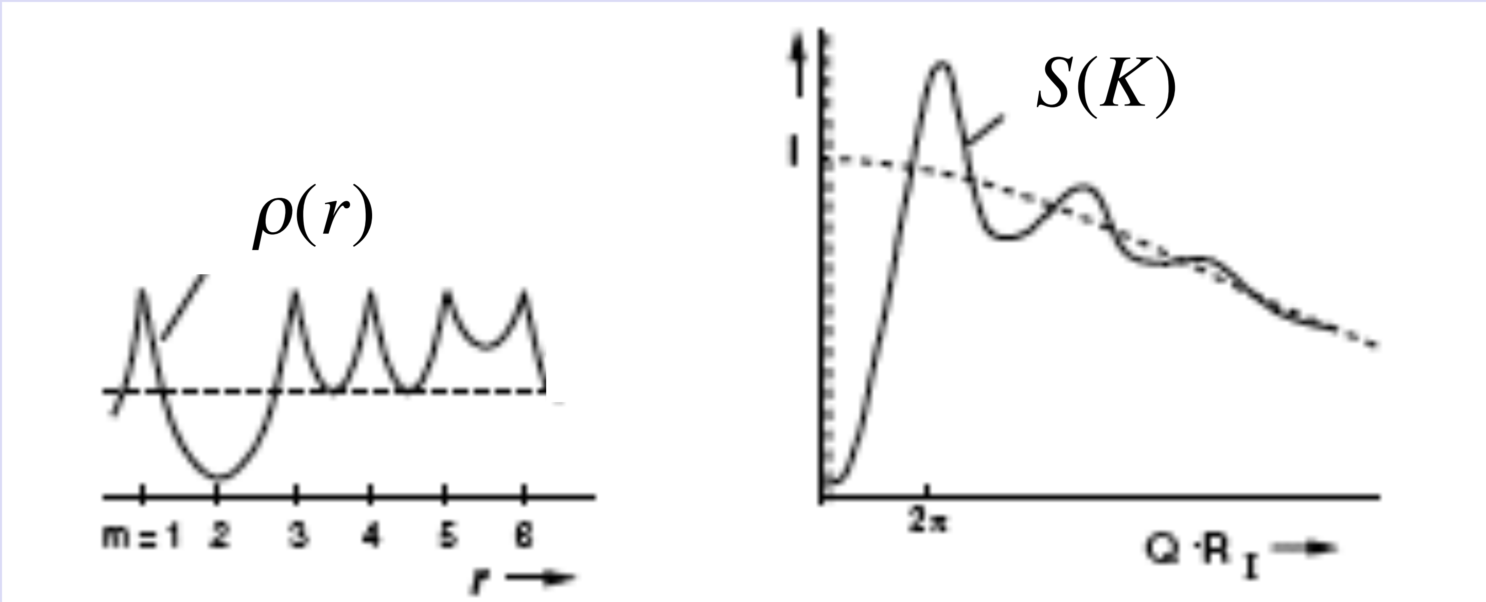
Real space

Reciprocal space



$$S(K) = \sum_{m,n} f_m f_n \left\langle e^{i\vec{K}\cdot\vec{R}_{mn}} \right\rangle = \sum_{m,n} f_m f_n \frac{\sin(KR_{mn})}{KR_{mn}}$$

Dynamic scattering function

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Inelastic scattering (non-resonant)

$$\frac{d^2\sigma}{d\Omega\, d\omega_{\text{out}}} = r_0^2 \left(\hat{\varepsilon}_{\text{out}} \cdot \hat{\varepsilon}_{\text{in}}\right)^2 \frac{\omega_{\text{out}}}{\omega_{\text{in}}} \underbrace{\left| \left\langle A_{\text{out}} \right| \sum_j e^{-i\vec{K}\cdot\vec{r}_j} \left| A_{\text{in}} \right\rangle \right|^2}_{S(\vec{K},\omega)}$$

$$E_{\text{A,out}} + \hbar\omega_{\text{out}} = E_{\text{A,in}} + \hbar\omega_{\text{in}}$$

$$\omega = \omega_{\text{out}} - \omega_{\text{in}}$$

System excitations

- Single particle
- Collective

Characteristic length

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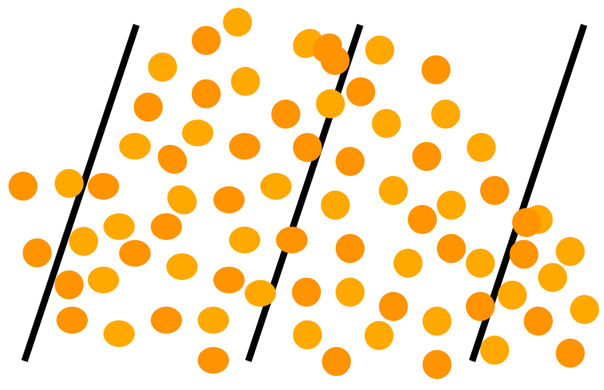
ξ = characteristic length describing the spatial inhomogeneity (e.g. the inter-particle distance)

$K\xi \leq 1$

$\frac{1}{K} \geq \xi$

Interference
Probe of collective behaviour

- phonons
- plasmons
- magnons

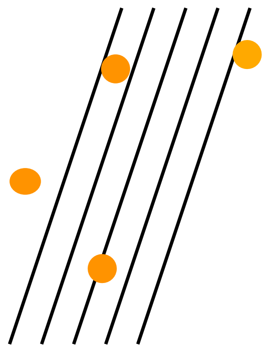


$K\xi >> 1$

$\frac{1}{K} << \xi$

Independent contribution of particles
Probe of single-particle properties

- Compton scattering $\hbar\omega >> E_b$
- inner-shell excitations $\hbar\omega \approx E_b$



Compton scattering from moving electrons

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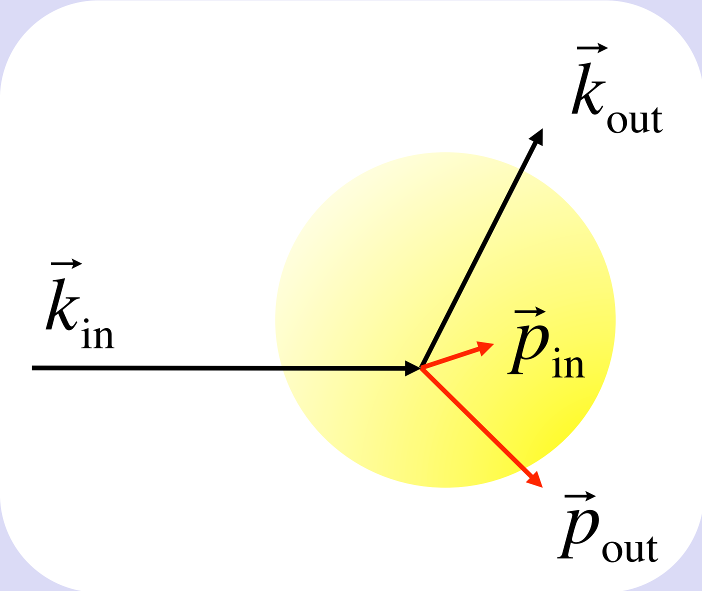

$$\hbar\omega_{in} + \frac{p_{in}^2}{2m} = \hbar\omega_{out} + \frac{p_{out}^2}{2m}$$

energy conservation

$$\hbar\vec{k}_{in} + \vec{p}_{in} = \hbar\vec{k}_{out} + \vec{p}_{out}$$

momentum conservation

Scattering vector

$$\vec{K} = \vec{k}_{in} - \vec{k}_{out}$$

$$\hbar\omega = \hbar\omega_{in} - \hbar\omega_{out} = \frac{(\hbar K)^2}{2m} - \frac{\hbar}{m}\vec{p}_{in}\cdot\vec{K}$$

Exchanged energy
=lost by field
=gained by electron

Atomic electron
momentum

One-dim. projection
of the momentum density

Compton scattering function

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$$S(\vec{K},\omega) = \left| \langle A_{out} | \sum_j e^{-i\vec{K}\cdot\vec{r}_j} | A_{in} \rangle \right|^2$$

Energy conservation

$$\delta\left(\hbar\omega - \frac{(\hbar K)^2}{2m} + \frac{\hbar}{m}\vec{p}_{in}\cdot\vec{K}\right)$$

One electron

$$S(\vec{K},\omega) = \frac{1}{V}\left|\int d^3\vec{r}\, \varphi_{out}(\vec{r})\, e^{-i\vec{K}\cdot\vec{r}}\, \varphi_{in}(\vec{r})\right|^2$$

$$= \frac{1}{V}\left|\int d^3\vec{r}\, e^{i\vec{p}_{out}\cdot\vec{r}/\hbar}\, e^{-i\vec{K}\cdot\vec{r}}\, \varphi_{in}(\vec{r})\right|^2$$

$$= \frac{1}{V}\left|\int d^3\vec{r}\, e^{i\vec{p}_{in}\cdot\vec{r}/\hbar}\, \varphi_{in}(\vec{r})\right|^2$$

$$\varphi_{out}(\vec{r}) = e^{i\vec{p}_{out}\cdot\vec{r}/\hbar}$$

outgoing plane wave

$$\vec{p}_{out} = \vec{p}_{in} + \hbar\vec{K}$$

(for a fixed K)

FT of the ground-state wavefunction
➔ momentum-space wave-function

$$\chi(\vec{p}_{in})$$

Compton profile

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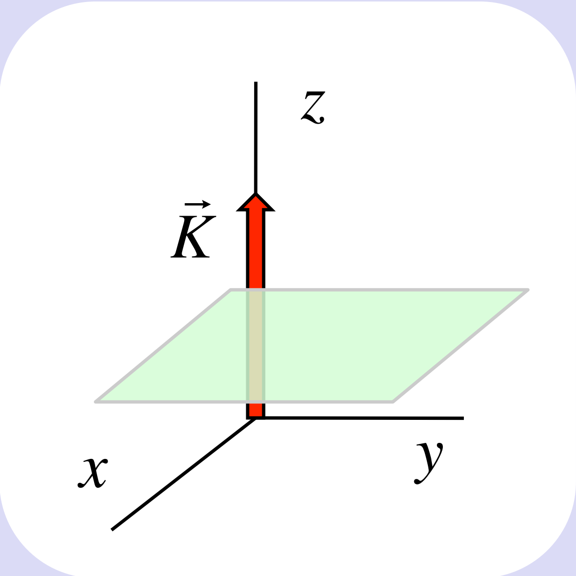
$$\rho(\vec{p}_{\rm in}) = \sum_j \left|\chi_j(\vec{p}_{\rm in})\right|^2$$

One atom

$$S(\vec{K},\omega) = \int d^3\vec{p}_{in}\, \rho(\vec{p}_{in})\, \delta\left(\hbar\omega - \frac{(\hbar K)^2}{2m} + \frac{\hbar}{m}\vec{p}_{in}\cdot\vec{K}\right)$$

distribution of electron momenta

Energy conservation (link between K and p_{in})



Compton profile

$$J(p_z) = \int dx\, dy\ \ \rho(\vec{p}_{in})$$

$$S(\vec{K},\omega)$$

Cross section

$$\frac{d^2\sigma}{d\Omega\, d\omega} = r_0^2 \left(\hat{\varepsilon}_{\rm out}\cdot\hat{\varepsilon}_{\rm in}\right)^2 \frac{\omega_{\rm out}}{\omega_{\rm in}} \frac{m}{|\vec{K}|} J(p_z)$$

Compton cross section and Compton profile

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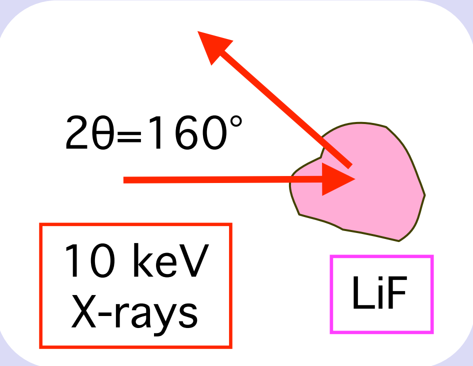
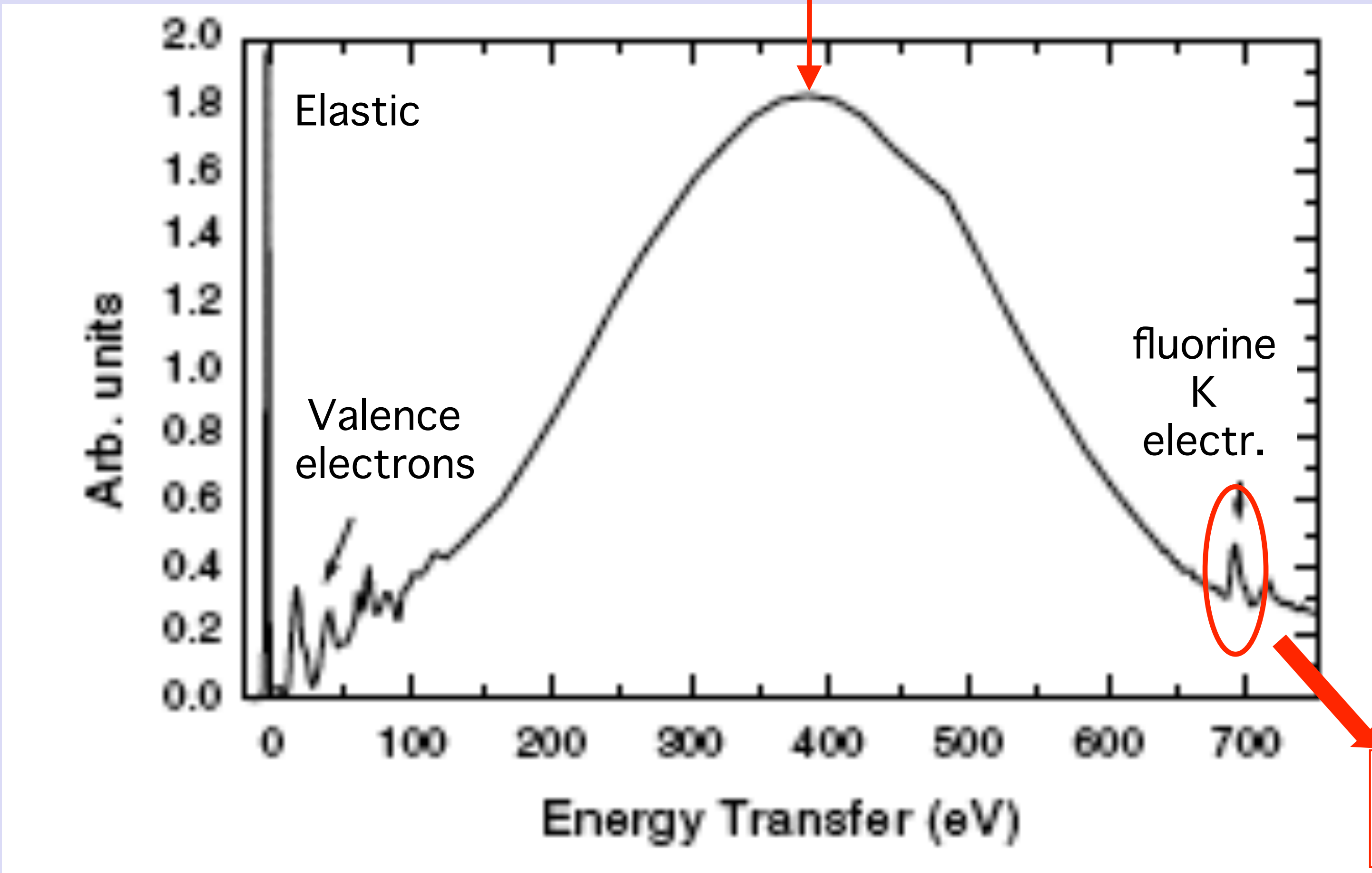


$$K \approx 10\ \text{Å}^{-1}$$

Rest electrons

$$\Delta E \approx \hbar\omega_0 \frac{\Delta\lambda}{\lambda_0} = 380\,\text{eV}$$



next
slide

X-ray Raman scattering

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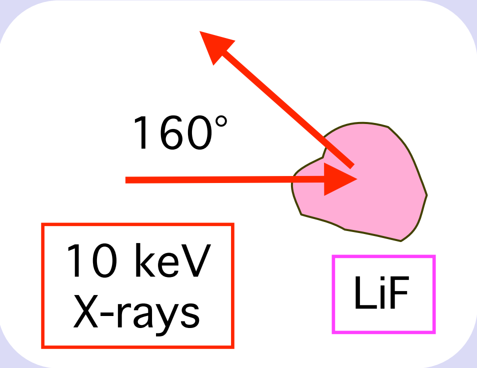
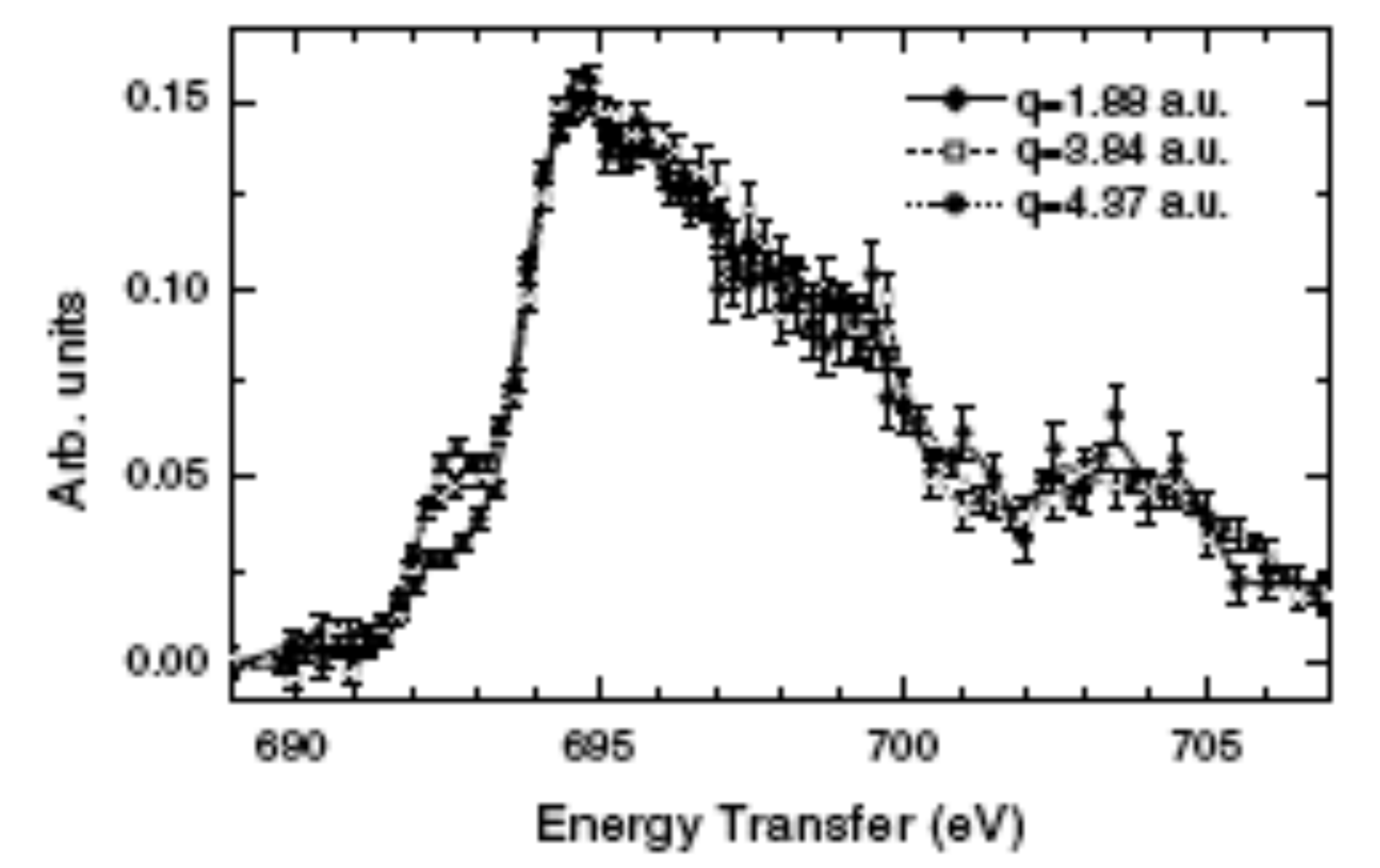


K edge of fluorine



Non-resonant X-ray Raman scattering

Excitations in condensed matter

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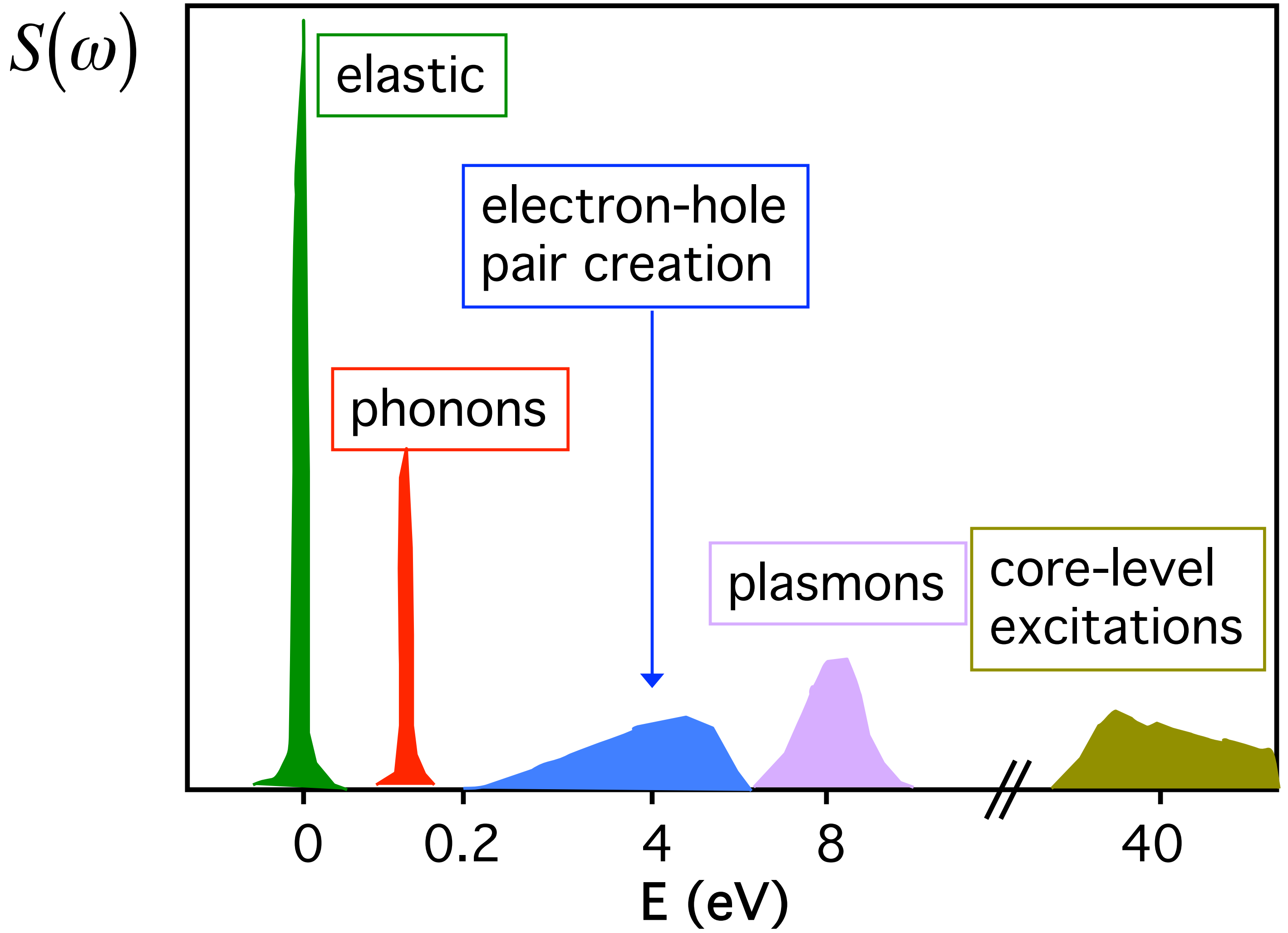

Energy transfer $\hbar\omega = \hbar\omega_{in} - \hbar\omega_{out}$

Space-time correlation function

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$$S(\vec{K},\omega) = \int G\left(\vec{R},t\right) e^{i\left(\vec{K}\cdot\vec{R}-\omega t\right)} d\vec{R}\, dt$$

Space-time correlation function

$$G(\vec{R},t) = \int d\vec{r}_1\; \rho\left(\vec{r}_1,0\right)\, \rho\left(\vec{r}_1 + \vec{R},t\right)$$

Probability density that: given a particle @ $\vec{r}_1\ ,t = 0$
another particle is @ $\vec{r}_1 + \vec{R}\ ,t$

Effects of atomic vibrations on diffraction patterns

Average over instantaneous displacements

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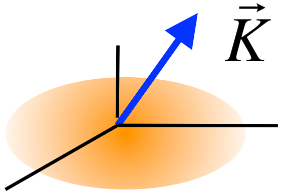
$$I_{\mathrm{e.u.}}\left(\vec{K}\right) = \left|f\left(\vec{K}\right)\right|^2 \sum_{mn} e^{i\vec{K}\cdot(\vec{r}_m - \vec{r}_n)} \left\langle e^{i\vec{K}\cdot(\vec{u}_m - \vec{u}_n)} \right\rangle$$

Gaussian distrib.

$$\left\langle e^{ix} \right\rangle = e^{-\frac{1}{2}\left\langle x^2 \right\rangle}$$

$$e^{-\frac{1}{2}\left\langle\left(\vec{K}\cdot\vec{u}_m\right)^2\right\rangle} \; e^{-\frac{1}{2}\left\langle\left(\vec{K}\cdot\vec{u}_n\right)^2\right\rangle} \; e^{\left\langle\left(\vec{K}\cdot\vec{u}_m\right)\left(\vec{K}\cdot\vec{u}_n\right)\right\rangle}$$

$$e^{-\frac{1}{2}\left\langle\left(\vec{K}\cdot\vec{u}_m\right)^2\right\rangle} \; e^{-\frac{1}{2}\left\langle\left(\vec{K}\cdot\vec{u}_n\right)^2\right\rangle} \left\{1 + \left[e^{\left\langle\left(\vec{K}\cdot\vec{u}_m\right)\left(\vec{K}\cdot\vec{u}_n\right)\right\rangle} - 1\right]\right\}$$



ellipsoid of atomic vibrations

Debye-Waller factor (monatomic crystals)

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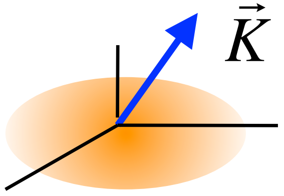


ellipsoid of atomic vibrations

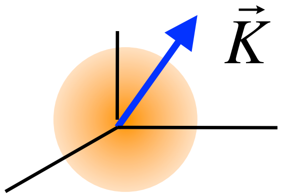
$$\left\langle \left(\vec{K}\cdot\vec{u}_m\right)^2 \right\rangle$$

Increases with
- increasing K
- increasing temperature

$$e^{-\frac{1}{2}\left\langle \left(\vec{K}\cdot\vec{u}_m\right)^2 \right\rangle}$$

Decreases with
- increasing K
- increasing temperature

Isotropic vibrations ➔ Debye-Waller factor



$$e^{-\frac{1}{2}\left\langle \left(\vec{K}\cdot\vec{u}_m\right)^2 \right\rangle} = e^{-W(T,K)}$$

Two equal atoms

$$e^{-\frac{1}{2}\left\langle \left(\vec{K}\cdot\vec{u}_m\right)^2 \right\rangle} \; e^{-\frac{1}{2}\left\langle \left(\vec{K}\cdot\vec{u}_n\right)^2 \right\rangle} = e^{-2W(T,K)}$$

Partition of total scattering intensity

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$$I_{\text{e.u.}}(\vec{K}) = \left|f(\vec{K})\right|^2 e^{-2W(K,T)} \sum_{mn} e^{i\vec{K}\cdot(\vec{r}_m-\vec{r}_n)}$$

$$+\left|f(\vec{K})\right|^2 e^{-2W(K,T)} \sum_{mn} e^{i\vec{K}\cdot(\vec{r}_m-\vec{r}_n)} \left[e^{\langle(\vec{K}\cdot\vec{u}_m)(\vec{K}\cdot\vec{u}_n)\rangle} - 1 \right]$$

Laue scattering

Diffuse scattering

$$e^{\langle[\vec{K}\cdot\vec{u}_m(0)][\vec{K}\cdot\vec{u}_n(t)]\rangle} = 1 + \left\langle \left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right] \right\rangle + \ldots.$$

$$I_{\text{e.u.}}(\vec{K}) = \left|f(\vec{K})\right|^2 e^{-2W(K,T)} \sum_{mn} e^{i\vec{K}\cdot(\vec{r}_m-\vec{r}_n)}$$

$$+\left|f(\vec{K})\right|^2 e^{-2W(K,T)} \sum_{mn} e^{i\vec{K}\cdot(\vec{r}_m-\vec{r}_n)} \left[\left\langle \left(\vec{K}\cdot\vec{u}_m\right)\left(\vec{K}\cdot\vec{u}_n\right) \right\rangle + \ldots.. \right]$$

Laue scattering

Diffuse scattering

Laue scattering

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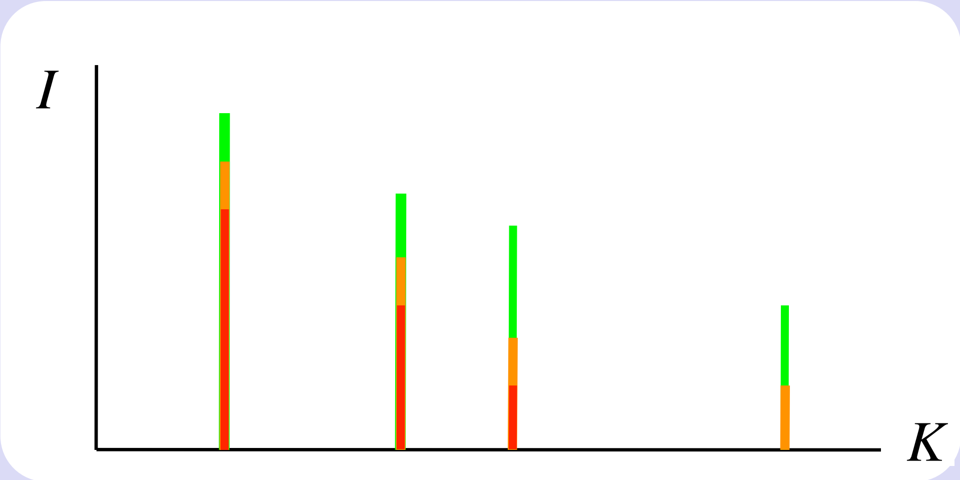
$$I_{\text{e.u.}}\left(\vec{K}\right) = \left|f\left(\vec{K}\right)\right|^2 e^{-2W(K,T)} \sum_{mn} e^{i\vec{K}\cdot(\vec{r}_m - \vec{r}_n)}$$

Debye_Waller factor

Reduction of Laue intensities

Decreases with
- increasing K
- increasing temperature



Energy lost for elastic scattering goes into diffuse scattering

Diffuse scattering

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X-rays exchange energy with crystal normal modes

1-phonon processes

2 or more phonons

$$\left|f\left(\vec{K}\right)\right|^2 e^{-2W\left(\vec{K}\right)} \sum_{mn} e^{i\vec{K}\cdot\left(\vec{r}_m-\vec{r}_n\right)}\left[\left\langle\left(\vec{K}\cdot\vec{u}_m\right)\left(\vec{K}\cdot\vec{u}_n\right)\right\rangle + \ldots..\right]$$

correlation significant
only for neighbouring atoms

sum limited to
neighbouring atoms

significant intensity for $\vec{K} \neq \vec{G}$

Scattering by crystal phonons

Dynamical scattering function (a)

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- Monatomic crystal
- Adiabatic approximation > Scattering from atoms

$$S(\vec{K},\omega) = \int G\left(\vec{R},t\right) e^{i\left(\vec{K}\cdot\vec{R}-\omega t\right)} d\vec{R}\, dt$$

$$G(\vec{R},t) = \int d\vec{r}_1\ \rho(\vec{r}_1,0)\ \rho\left(\vec{r}_1+\vec{R},t\right)$$

$$G\left(\vec{R},t\right) = \sum_{m,n} \int d\vec{r}\,'\ \delta\left[\vec{r}\,'-\vec{r}_m(0)\right]\ \delta\left[\vec{r}\,'+\vec{R}-\vec{r}_n(t)\right]$$

$$S\left(\vec{K},\omega\right) = \left|f\left(\vec{K}\right)\right|^2 \sum_{m,n} \int dt \left\langle e^{i\vec{K}\cdot\vec{r}_m(0)} e^{-i\vec{K}\cdot\vec{r}_n(t)} \right\rangle e^{-i\omega t}$$

$$\vec{r}(t) = \vec{r}^{\,0} + \vec{u}(t)$$

Dynamical scattering function for a crystal

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$$S(\vec{K},\omega) = \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot[\vec{r}_m^{\,0}-\vec{r}_n^{\,0}]} \int dt \left\langle e^{i\vec{K}\cdot[\vec{u}_m(0)-\vec{u}_n(t)]} \right\rangle e^{-i\omega t}$$

Gaussian distrib.

$$\left\langle e^{ix} \right\rangle = e^{-\frac{1}{2}\langle x^2 \rangle}$$

$$e^{-\frac{1}{2}\left\langle [\vec{K}\cdot\vec{u}_m(0)]^2 \right\rangle} \; e^{-\frac{1}{2}\left\langle [\vec{K}\cdot\vec{u}_n(t)]^2 \right\rangle} \; e^{\left\langle [\vec{K}\cdot\vec{u}_m(0)][\vec{K}\cdot\vec{u}_n(t)] \right\rangle}$$

Self-correlations

Pair-correlation

$$S(\vec{K},\omega) = \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle [\vec{K}\cdot\vec{u}]^2 \right\rangle} \int e^{\left\langle [\vec{K}\cdot\vec{u}_m(0)][\vec{K}\cdot\vec{u}_n(t)] \right\rangle} e^{-i\omega t} dt$$

Debye-Waller factor

$$e^{-\frac{1}{2}\left\langle (\vec{K}\cdot\vec{u}_m)^2 \right\rangle} \; e^{-\frac{1}{2}\left\langle (\vec{K}\cdot\vec{u}_n)^2 \right\rangle} = e^{-2W(T,K)}$$

Scattering function for a crystal (c)

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$$S(\vec{K},\omega) = \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int e^{\left\langle\left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right]\right\rangle} e^{-i\omega t} dt$$

$$e^{\left\langle\left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right]\right\rangle} = 1 + \left\langle\left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right]\right\rangle + \ldots.$$

$$S(\vec{K},\omega) = \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int 1\, e^{-i\omega t} dt$$

Elastic

$$+ \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int \left\{\left\langle\left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right]\right\rangle + \ldots\right\} e^{-i\omega t} dt$$

Inelastic

1st order

Elastic scattering

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$$S^{(0)}\left(\vec{K},\omega\right) = \left|f\left(\vec{K}\right)\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int e^{-i\omega t} dt$$

$$= \left|f\left(\vec{K}\right)\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \delta(\omega)$$

$$\omega = \omega_{\text{out}} - \omega_{\text{in}} = 0$$

$$S^{(0)}(\vec{K},\omega) = S(\vec{K})$$

Inelastic scattering – 1st order (a)

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$$S(\vec{K},\omega) = \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int 1\, e^{-i\omega t} dt$$

$$+ \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int \left\{\left\langle\left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right]\right\rangle\right\} e^{-i\omega t} dt + \ldots.$$

$$S^{(1)}(\vec{K},\omega) = \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int \left\langle\left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right]\right\rangle e^{-i\omega t} dt$$

$$\left\langle\left[\vec{K}\cdot\vec{u}_m(0)\right]\left[\vec{K}\cdot\vec{u}_n(t)\right]\right\rangle = \sum_{\alpha,\beta} K_\alpha K_\beta \left\langle u_{m\alpha}(0)\, u_{n\beta}(t)\right\rangle$$

α,β
cartesian coordinates

Atomic displacements and normal modes

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Atomic displacements

Mode eigenvectors

$$u_{m\alpha}(t) = \frac{1}{\sqrt{NM}} \sum_{\vec{q}s} \left[e_{m\alpha,\vec{q}s}\, e^{i\vec{q}\cdot R_m} Q_{\vec{q}s}(t) \right]$$

Normal coordinates

$$Q_{\vec{q}s}(t) = \sqrt{\frac{\hbar}{2\omega_{\vec{q}s}}} \left[a_{\vec{q}s} e^{-i\omega_{\vec{q}s} t} + a^{+}_{\vec{q}s} e^{i\omega_{\vec{q}s} t} \right]$$

$$u_{m\alpha}(t) = \sqrt{\frac{\hbar}{2NM}} \sum_{\vec{q}s} \frac{e_{m\alpha,\vec{q}s}}{\sqrt{\omega_{\vec{q}s}}} e^{i\vec{q}\cdot R_m} \left[a_{\vec{q}s} e^{-i\omega_{\vec{q}s} t} + a^{+}_{\vec{q}s} e^{i\omega_{\vec{q}s} t} \right]$$

Sum over normal modes

Annihilation and creation operators

Correlation term

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$$u_{m\alpha}(t) = \sqrt{\frac{\hbar}{2NM}} \sum_{\vec{q}s} \frac{e_{m\alpha,\vec{q}s}}{\sqrt{\omega_{\vec{q}s}}} e^{i\vec{q}\cdot R_m} \left[a_{\vec{q}s} e^{-i\omega_{\vec{q}s} t} + a^{+}_{\vec{q}s} e^{i\omega_{\vec{q}s} t} \right]$$

$$\left\langle u_{m\alpha}(0)\, u_{n\beta}(t) \right\rangle = \frac{\hbar}{2NM} \sum_{\vec{q}s} \left(\frac{1}{\omega_{\vec{q}s}} \right) e_{\alpha,\vec{q}s} e_{\beta,\vec{q}s}$$

$$\times \left[\left\langle n_{\vec{q}s} \right\rangle e^{-i\omega_{\vec{q}s} t} e^{i\vec{q}\cdot\vec{R}_{mn}} + \left\langle n_{\vec{q}s} + 1 \right\rangle e^{i\omega_{\vec{q}s} t} e^{-i\vec{q}\cdot\vec{R}_{mn}} \right]$$

One-phonon scattering

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$$S^{(1)}(\vec{K},\omega) = \left|f(\vec{K})\right|^2 \sum_{m,n} e^{i\vec{K}\cdot\vec{R}_{mn}} e^{-\left\langle\left[\vec{K}\cdot\vec{u}(t)\right]^2\right\rangle} \int \sum_{\alpha,\beta} K_\alpha K_\beta \left\langle u_{m\alpha}(0)\, u_{n\beta}(t)\right\rangle e^{-i\omega t}\, dt$$

$$\left\langle u_{m\alpha}(0)\, u_{n\beta}(t)\right\rangle = \sum_{\vec{q}s} \left(\frac{\hbar}{2NM\omega_{\vec{q}s}}\right) w_{\alpha,\vec{q}s} w_{\beta,\vec{q}s} \times \left[\left\langle n_{\vec{q}s}\right\rangle e^{-i\omega_{\vec{q}s}t} e^{i\vec{q}\cdot\vec{R}_{mn}} + \left\langle n_{\vec{q}s}+1\right\rangle e^{i\omega_{\vec{q}s}t} e^{-i\vec{q}\cdot\vec{R}_{mn}}\right]$$

energy gain
phonon annih.

energy loss
phonon creation

$S^{(1)}(\vec{K},\omega) \neq 0$ for

$$\omega = \omega_{\vec{q}s}$$

$$\vec{K} = \vec{G} \pm \vec{q}$$

Phonon scattering - experiments

Real and reciprocal space

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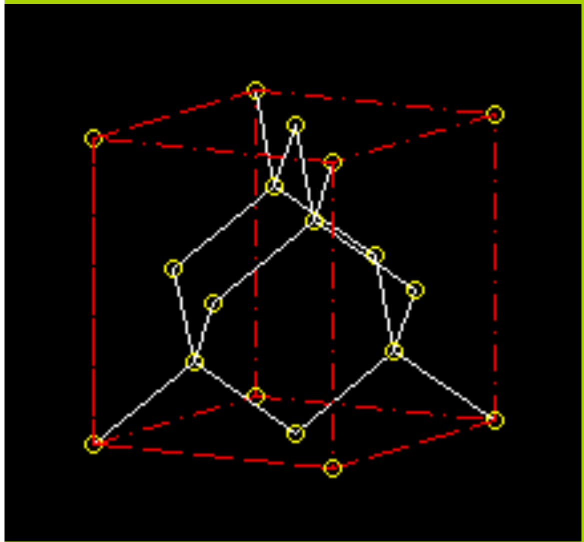
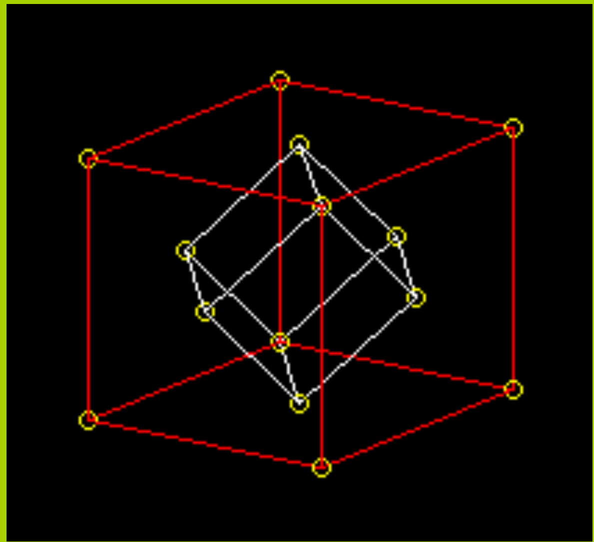


Diamond conventional unit cell (8 atoms/cell)

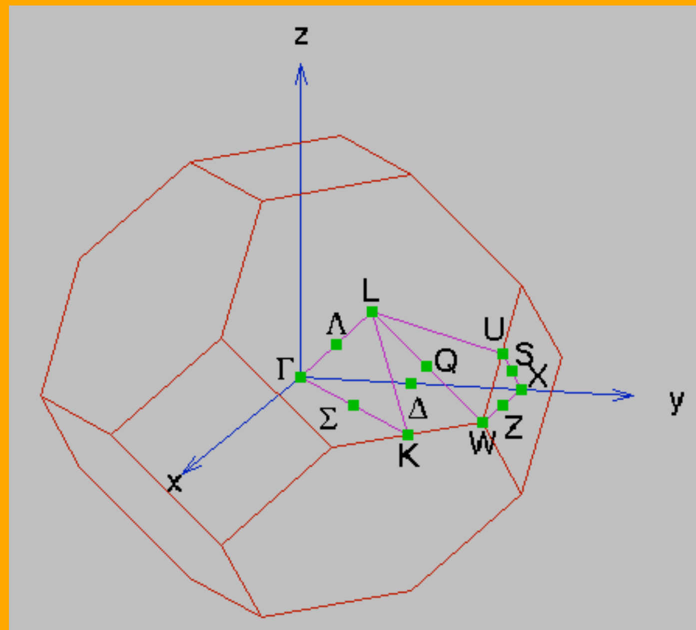


Primitive unit cell fcc + 2 atoms/cell

Real space

Reciprocal space

1st Brillouin zone



- Reciprocal space vectors $\vec{G}$
- Phonon wave-vectors $\vec{q}$

Phonon dispersion curves (Ge)

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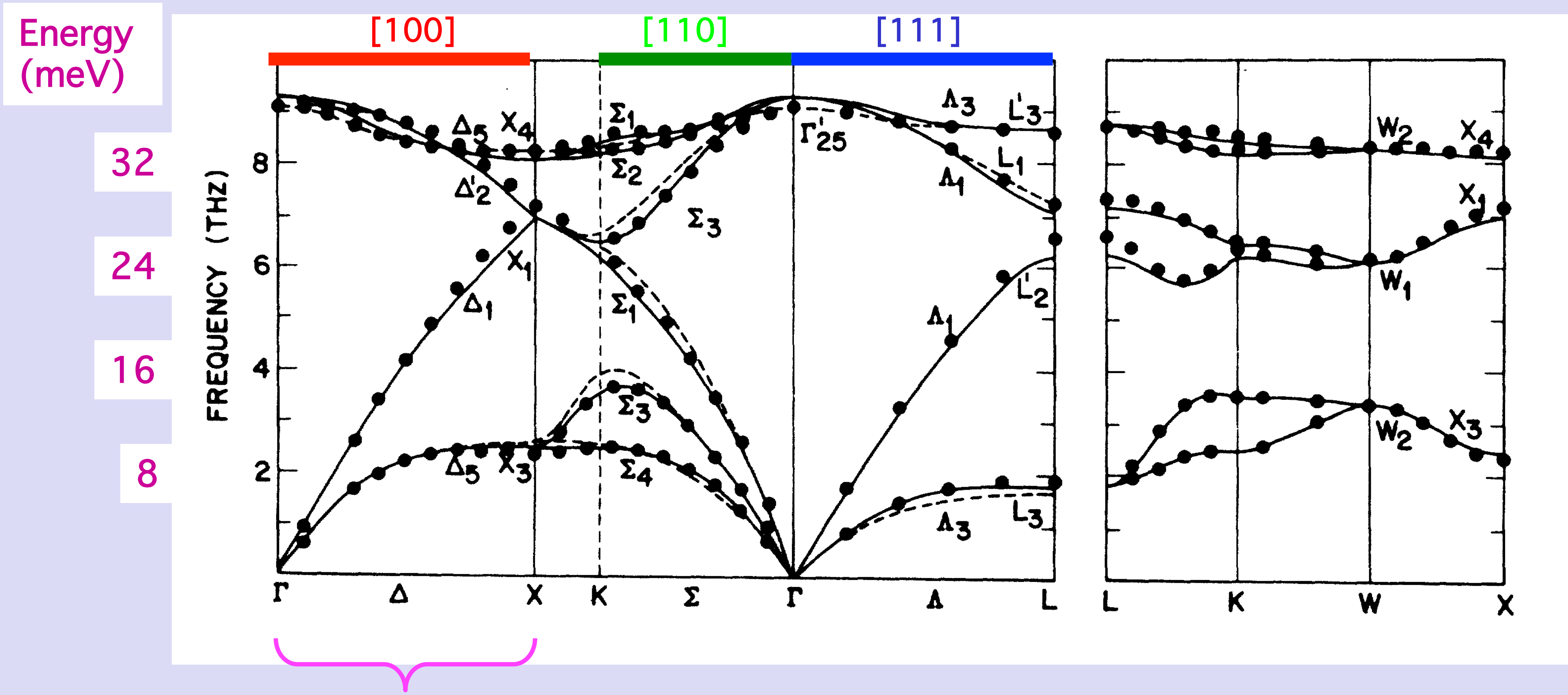

$$0 < q \le \frac{\pi}{a}$$

$$\omega = \omega_{\vec{q}\lambda}$$

$$\vec{K} = \vec{G} \pm \vec{q}$$

Neutrons and X-rays

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$$E_{\text{tot}}^2 = (pc)^2 + \left(m_0 c^2\right)^2$$

Photons

$$m = 0$$

$$E = pc$$

$$\hbar\omega = \hbar k\, c$$

$$k[\text{Å}^{-1}] = \frac{E[\text{keV}]}{1.97}$$

$$E = 12.4 \text{ keV}$$

$$E = \hbar\omega$$

$$\vec{p} = \hbar\vec{k}$$

$$\lambda = 1\text{Å}$$

Thermal neutrons

$$m_0 c^2 >> E_k$$

$$E_k = \frac{p^2}{2m}$$

$$\hbar\omega = \frac{(\hbar k)^2}{2m}$$

$$k[\text{Å}^{-1}] = \left[\frac{E[\text{meV}]}{2.07}\right]^{1/2}$$

$$E = 81.7 \text{ meV}$$

Phonon probes: X .vs. n

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$$\lambda = 1\,\mathring{A}$$

Thermal neutrons

$$E = 81.7\ \text{meV}$$

Natural probe for phonons

Limitations

- Large samples required
- Weak signal from some isotopes (like H)
- Limited velocity .vs. phase velocity of phonons

Photons

$$E = 12.4\ \text{keV}$$

Complementary probe

$$\frac{\Delta E}{E} \approx 10^{-8} \div 10^{-7}$$

⇒ Technical problems

Inelastic X-ray scattering

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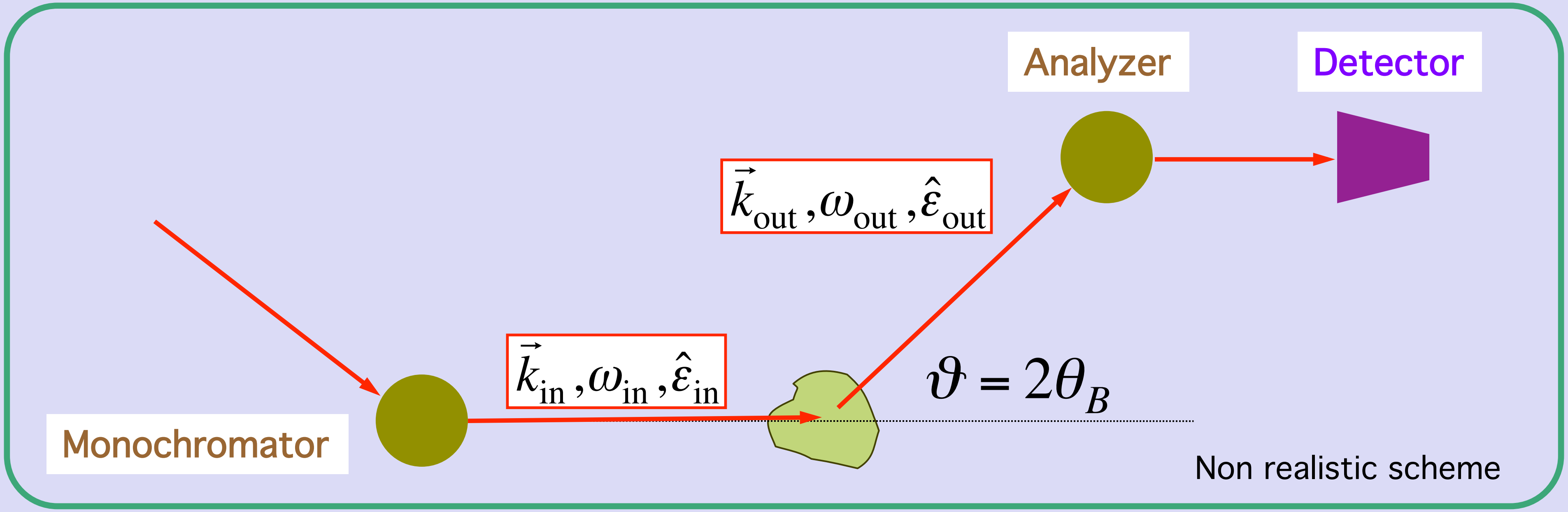
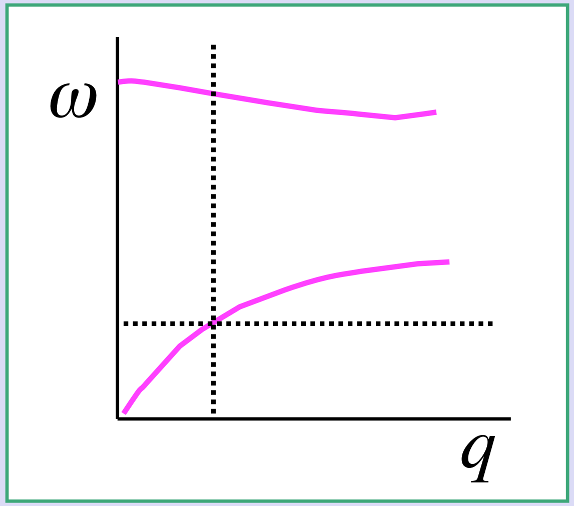


$$\omega << \omega_{in} \quad \Rightarrow \quad k_{out} \approx k_{in} \quad \Rightarrow \quad K = 2k_{in} \sin\theta_B$$

- Scattering angle ⇒ momentum transfer
- Analyzer ⇒ energy transfer

$$\vec{K} = \vec{G} \pm \vec{q}$$

$$\omega = \omega_{\vec{q}\lambda}$$



Energy resolution

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$$\frac{\Delta E}{E} = \frac{\omega}{\omega_{\text{in}}} \approx 10^{-8} \div 10^{-7}$$

Perfect unstrained crystal

Crystal contribution
(Darwin width)

$$\frac{\Delta E}{E} \propto \frac{r_e \lambda^2}{\sin^2 \theta_B}$$

Monochromator
&
analyzer

$$\theta_B = \vartheta / 2$$

Geometry contribution
(beam divergence)

$$\frac{\Delta E}{E} \propto \cot\theta_B \, \Delta\theta_B$$

High-order reflections

Minimum for

$$\theta_B = 90^\circ \rightarrow \vartheta = 180^\circ$$

Back-scattering geometry

Back-scattering geometry

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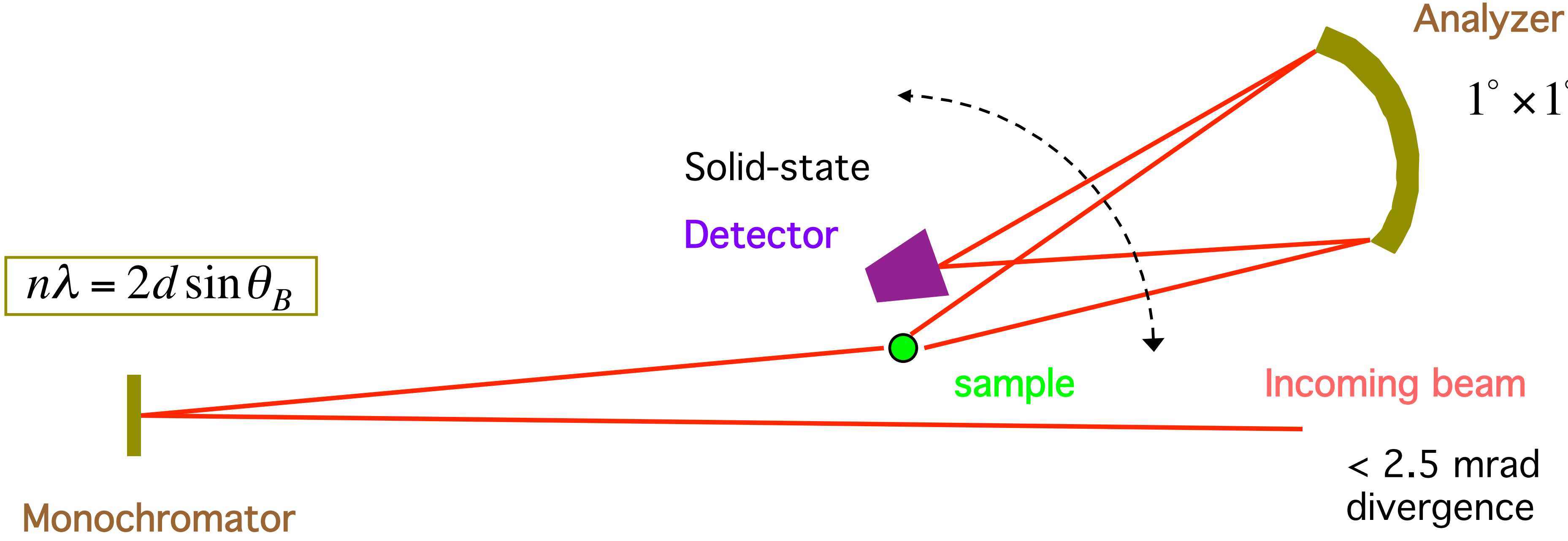
ESRF - Grenoble

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

Array of spherically bent crystals

ω_{out} fixed



< 2.5 mrad divergence

ω_{in} varied by thermally varying d (1 K $\Rightarrow$ 51 meV)

$$\Delta E = \hbar\omega \approx 1\ \text{meV}$$

In-line monochromator

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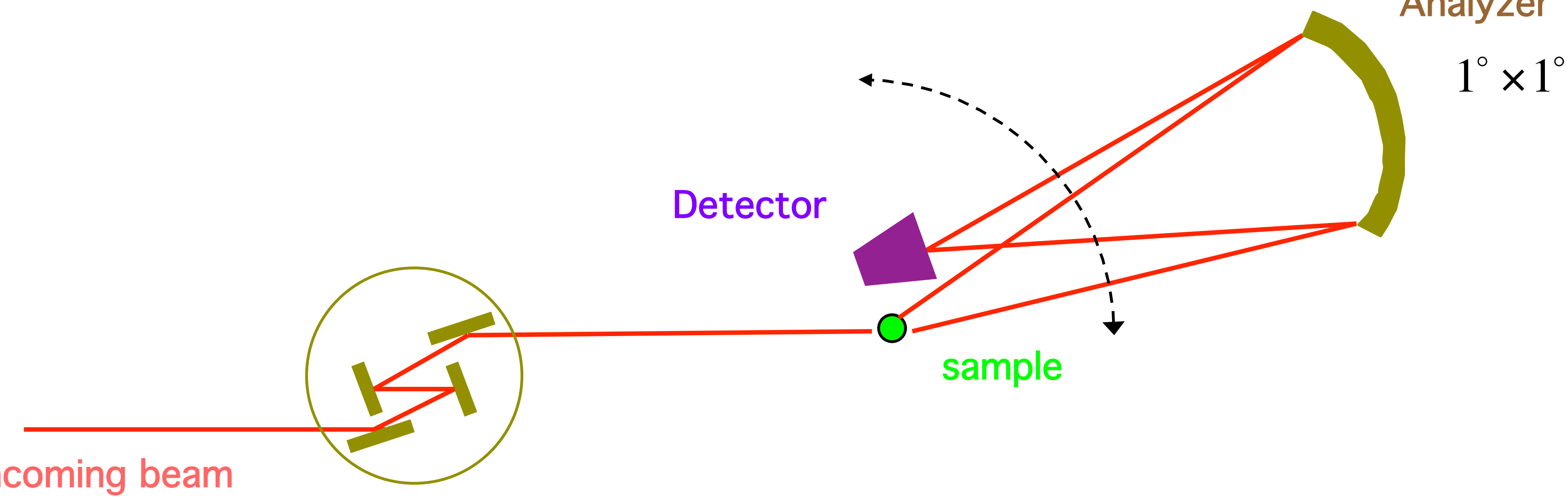
Array of spherically bent crystals ω_{out} fixed



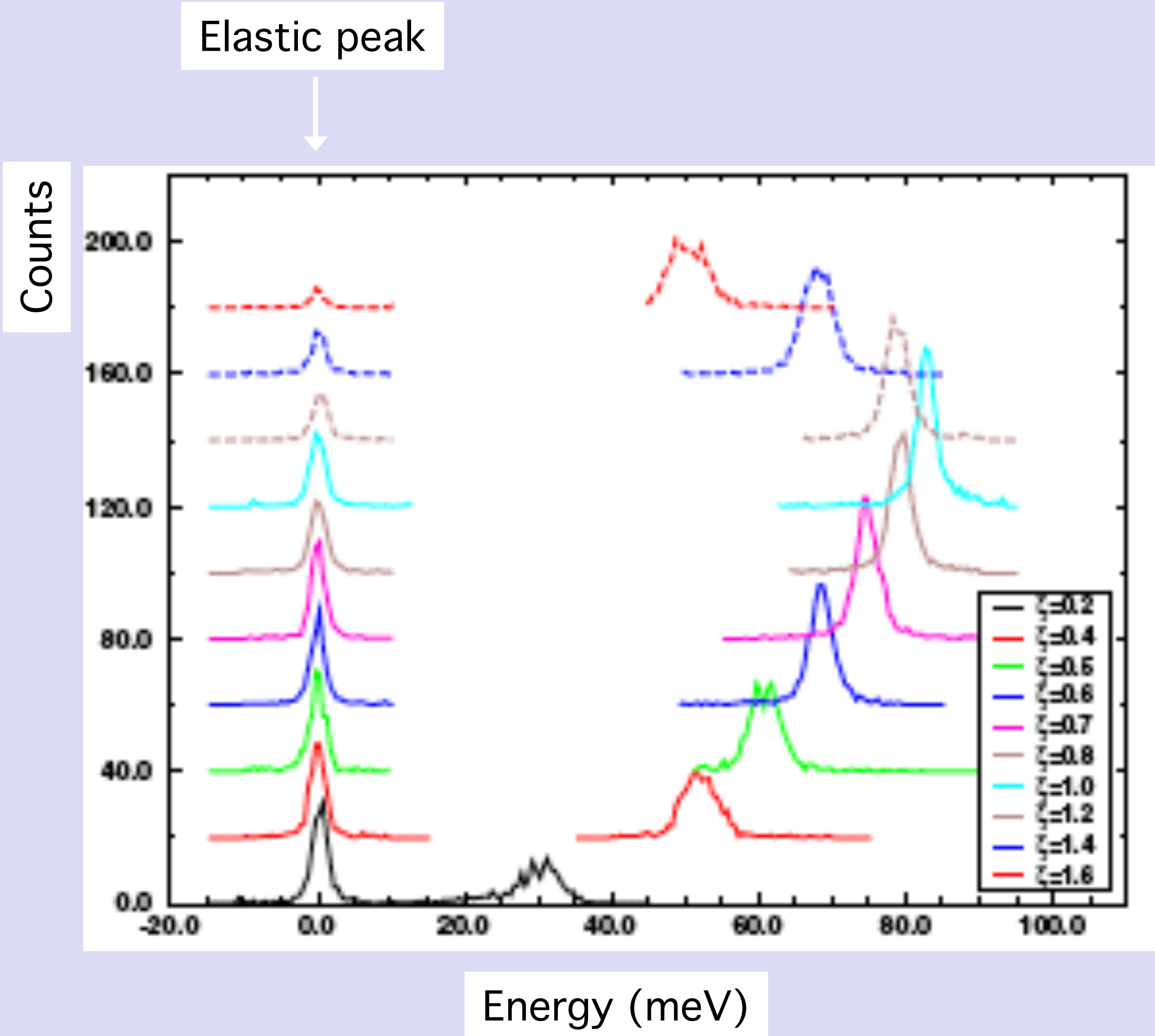
1 μrad divergence !

Monochromator

Channel-cut crystal

ω_{in} varied by rotating the crystal

Mesaurements

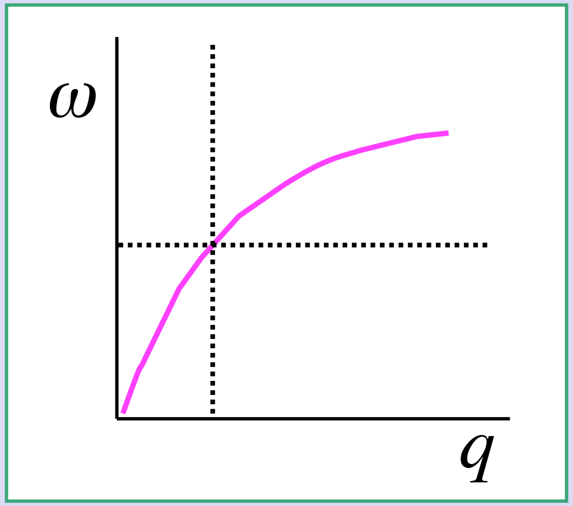


Beryllium

Energy scans
at different q values

$$(0,0,\zeta)$$

Longitudinal phonons



Dispersion curves

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