HERCULES School 2019 — Grenoble, FRANCE

Introduction to Inelastic Scattering

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Outline

- **1 General concepts**
  - **From elastic to inelastic scattering**
  - Conservation laws and consequences
- 2 Inelastic Neutron Scattering
  - Nuclear Interaction
  - Magnetic Interaction
- 3 Inelastic X-ray Scattering

Elastic Scattering

Sample

Elastic Scattering

Incident plane wave

$\vec{k}_i$

Sample

Scattered plane wave

$\vec{k}_f$

Elastic Scattering

Wave vector

$$\vec{q} = \vec{k}_f - \vec{k}_i$$

Incident plane wave

$$\vec{k}_i$$

Sample

Scattered plane wave

$$\vec{k}_f$$

$$\left|\vec{k}_f\right| = \left|\vec{k}_i\right|$$

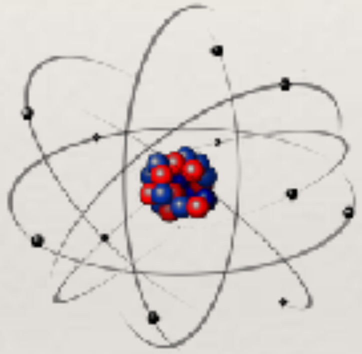
$$E_f = E_i$$

Elastic Scattering

X-rays

interact with :

e^- charge
e^- spin
e^- orbital momentum



Neutron

interact with :

nucleus
e^- spin
e^- orbital momentum

Why Inelastic Scattering ?

- Dynamical aspects are responsible for some properties (thermal conductivity etc…)
- Gives access to Hamiltonian parameters and why the ground state is stable

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Momentum conservation

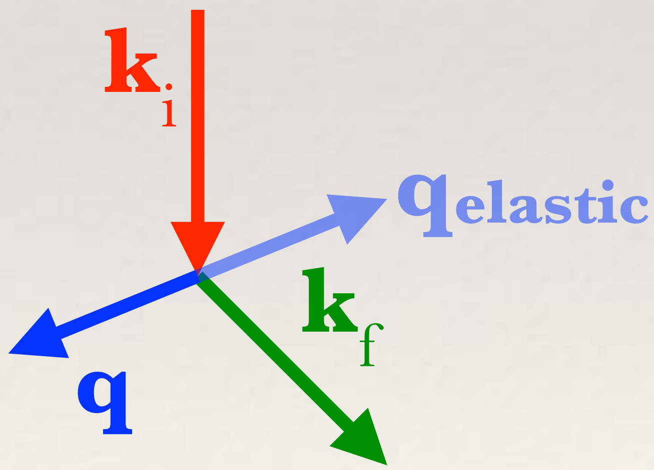
- For both neutron and X rays, the momentum writes :

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

- The wave vector (transferred momentum to the sample) thus writes

$$\vec{q} = \vec{k}_i - \vec{k}_f$$

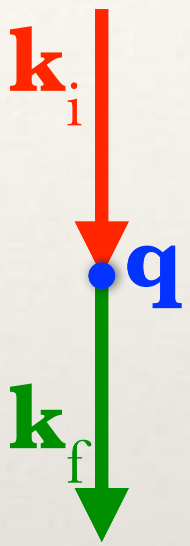
Note that $\vec{q}_{inelastic} = -\vec{q}_{elastic}$



Momentum conservation

- Minimum value of wave vector

$$\vec{q}_{min} = (k_i - k_f)\widetilde{k_i} \underset{\omega=0}{=} \vec{0}$$



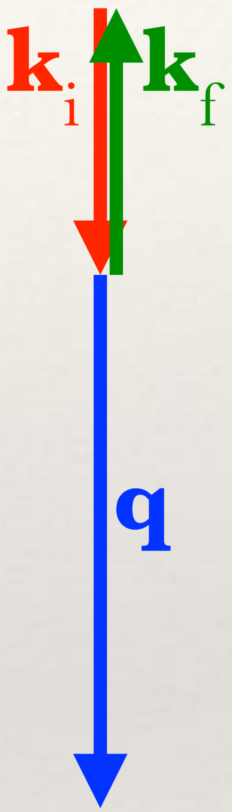
Momentum conservation

- Minimum value of wave vector

$$\vec{q}_{min} = (k_i - k_f)\widetilde{k_i} \underset{\omega=0}{=} \vec{0}$$

- Maximum value of wave vector

$$\vec{q}_{max} = (k_i + k_f)\widetilde{k_i} \underset{\omega=0}{=} 2\vec{k_i}$$



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- Visible photons (λ=500nm, ħω=2.5 eV) : $|\vec{k}_i| = 10^{-3}\mathring{A}^{-1}$
- X-rays photons (λ=14Å, ħω=900 eV) : $|\vec{k}_i| = 1\mathring{A}^{-1}$
- Neutrons (λ=2.36Å, ħω=15 meV) : $|\vec{k}_i| = 1\mathring{A}^{-1}$
- Typical Brillouin zone (a=5Å) : $|\vec{q}_x| = 1\mathring{A}^{-1}$

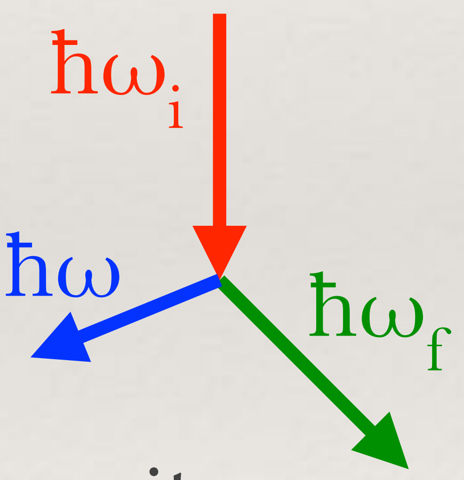
Energy conservation

- Energy for neutrons writes :

$$\hbar\omega_i = \frac{p_i^2}{2m} = \frac{\hbar^2 k_i^2}{2m}$$

- Energy transferred to the sample by a neutron thus writes :

$$\hbar\omega = \hbar\omega_i - \hbar\omega_f = \frac{\hbar^2}{2m}(k_i^2 - k_f^2)$$



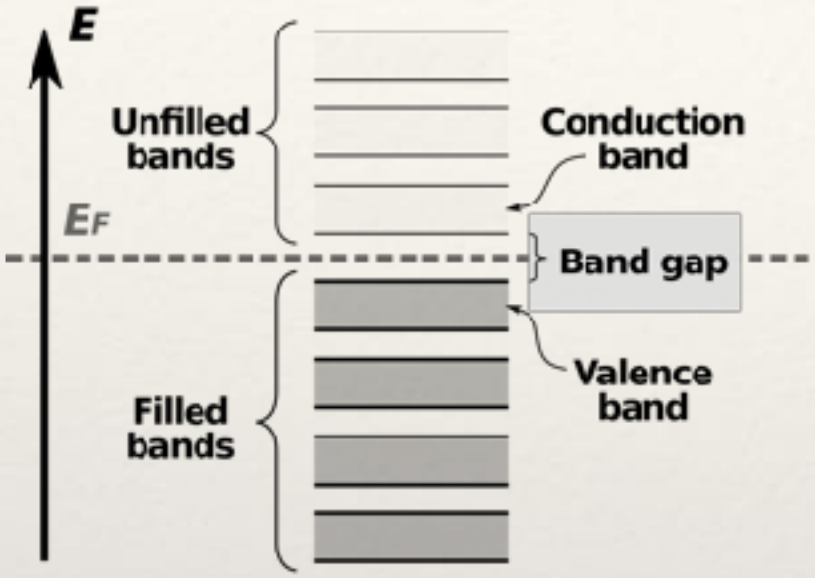
- Energy for photons writes :

$$\hbar\omega_i = p_i c = \hbar c k_i$$

- Energy transferred to the sample by a photon thus writes :

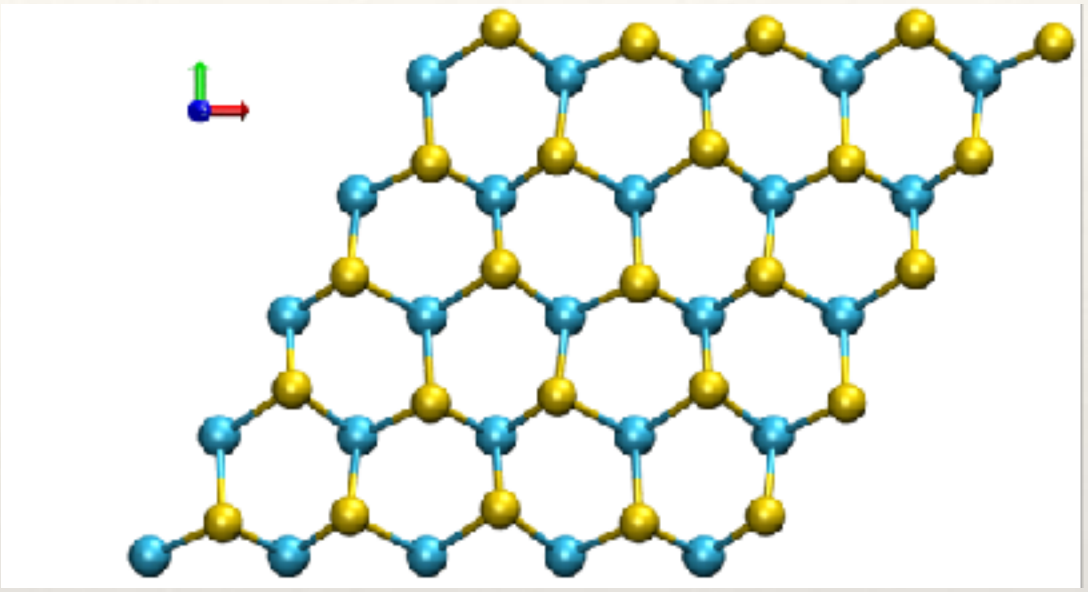
$$\hbar\omega = \hbar\omega_i - \hbar\omega_f = \hbar c(k_i - k_f)$$

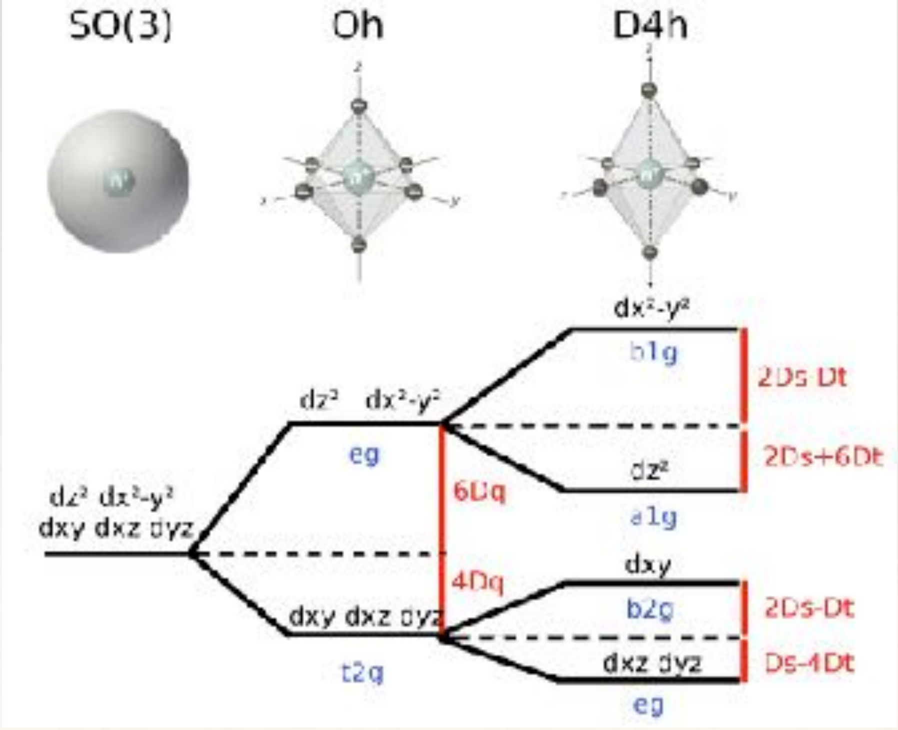
Energy conservation



e–h excitation

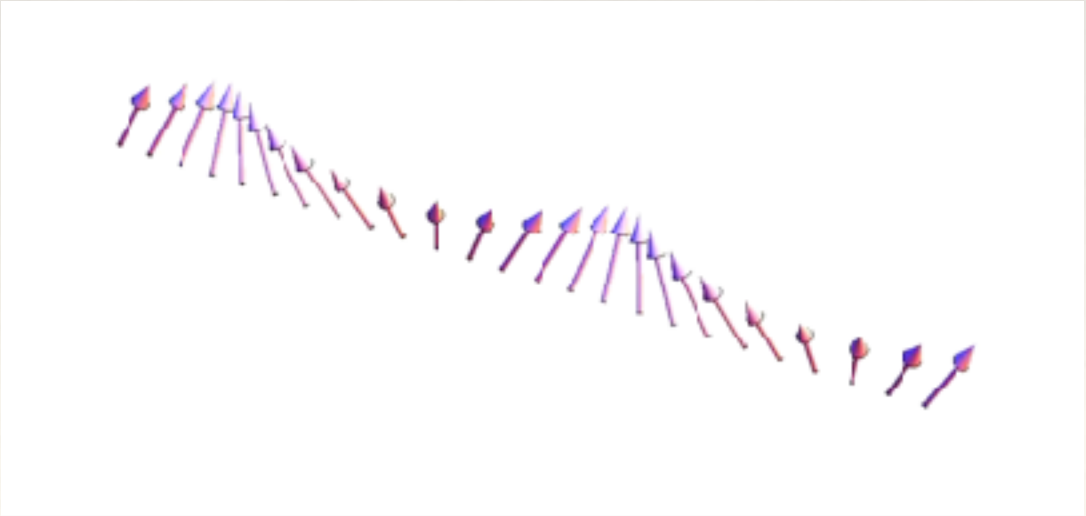
Phonon



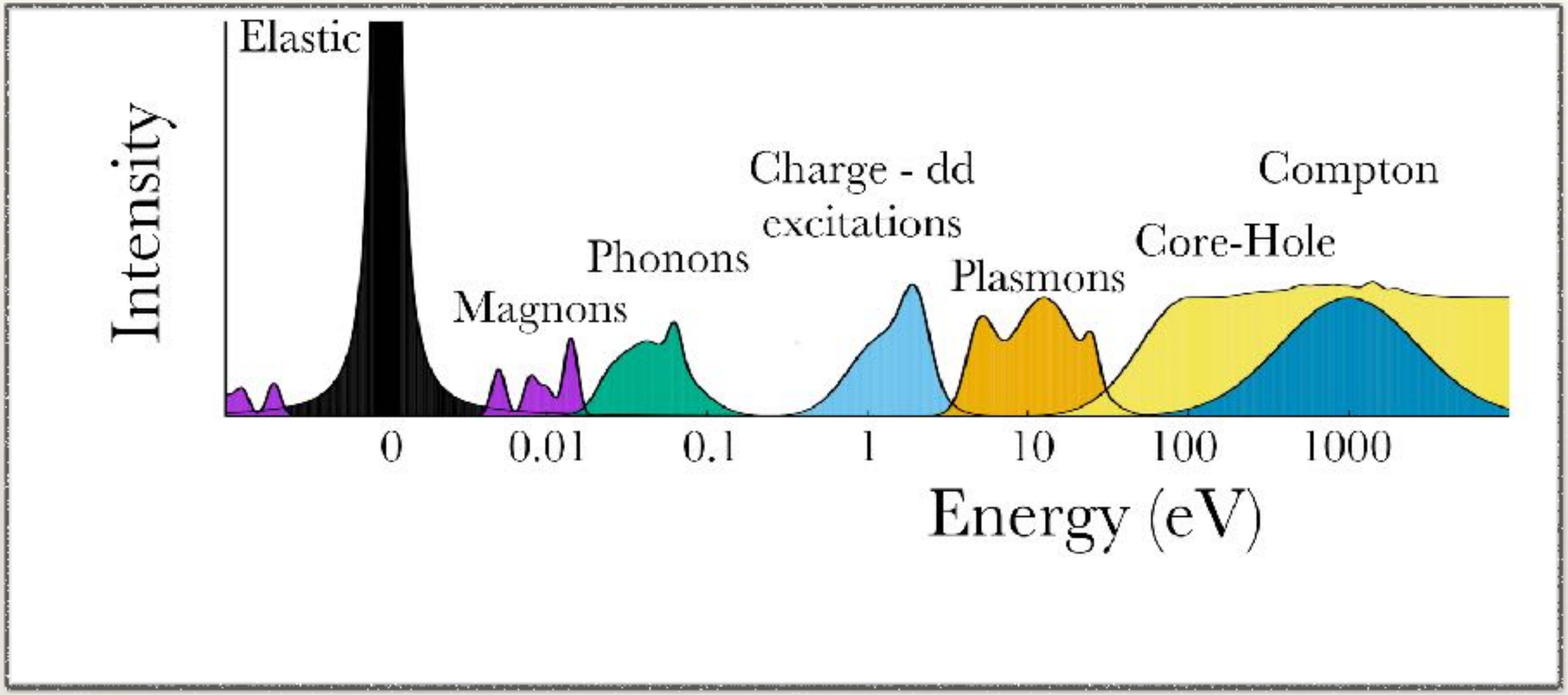


Crystal Field

Magnon



Energy conservation



Excitation	Crystal Field	Magnon	Phonon	*d-d* & *e*-*h*	Plasmon	Core hole
Energy	~ 1 meV	~ 10 meV	10-100 meV	~1 eV	~ 10 eV	0.1 - 100 keV

Energy conservation

Technique	Brillouin	Raman	Neutron Scattering	Infrared	IXS	RIXS
Probe	Photon (Visible)	Photon (Visible)	Neutron	Photon	Photon (X-ray)	Photon (X-ray)
Particule Energy	~1 eV	~1 eV	1 - 150 meV	1 - 100 meV	~10 keV	0.5 - 100 keV
Transfered Energy	0.01 - 1 meV	1 - 1000 meV	0.1 - 100 meV	1 - 100 meV	1 - 400 meV	-

Excitation	Crystal Field	Magnon	Phonon	*d-d* & e^--*h*	Plasmon	Core hole
Energy	~ 1 meV	~ 10 meV	10-100 meV	~1 eV	~ 10 eV	0.1 - 100 keV

Energy & Momentum

- For local excitations such as Crystal Field or Ising-like excitations, the energy does not depend on the transferred momentum :

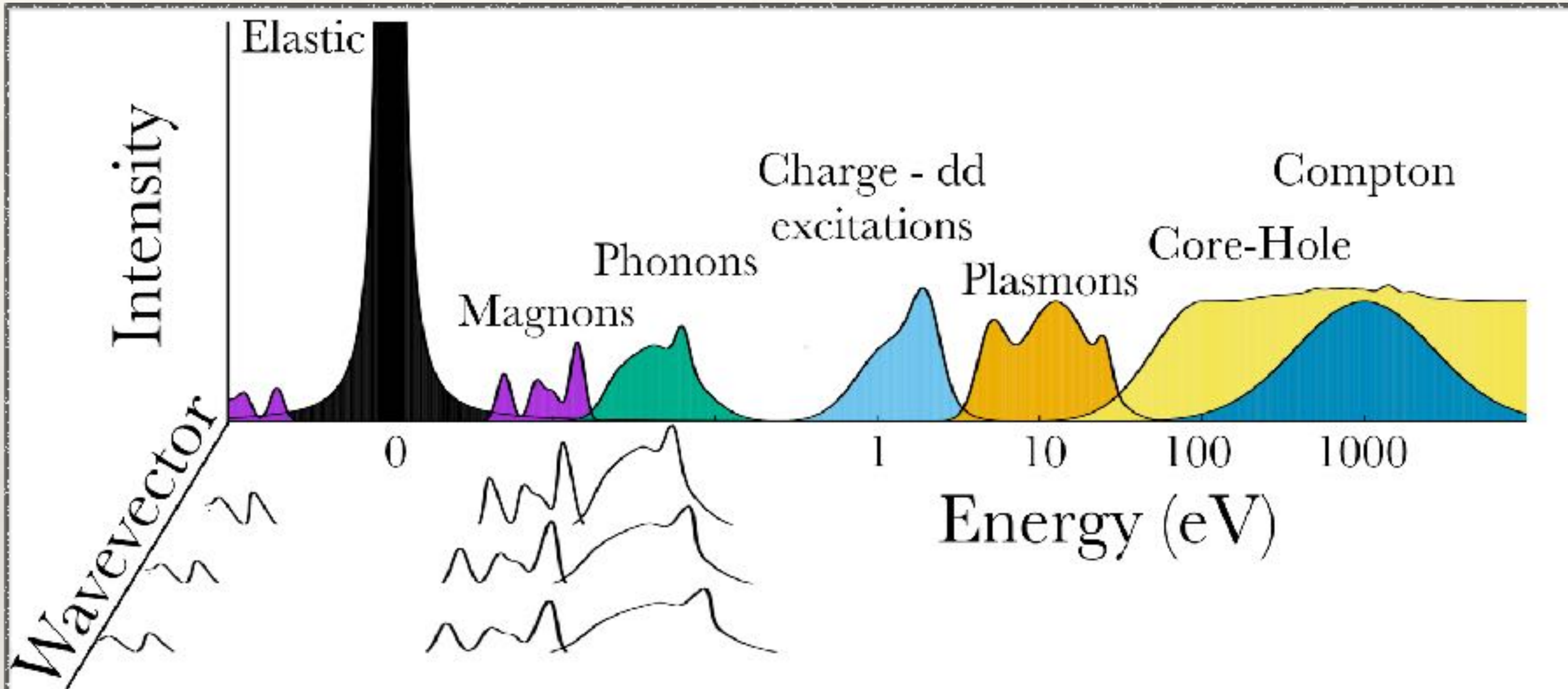
$$\omega(\vec{q}) = \omega_0$$

- However, some excitations has a momentum-dependent energy. Both parameters are no longer independent : they are connected through the dispersion relation :

$$\omega(\vec{q})$$

- This is the case for collective excitations such as magnons, phonons …

Energy & Momentum



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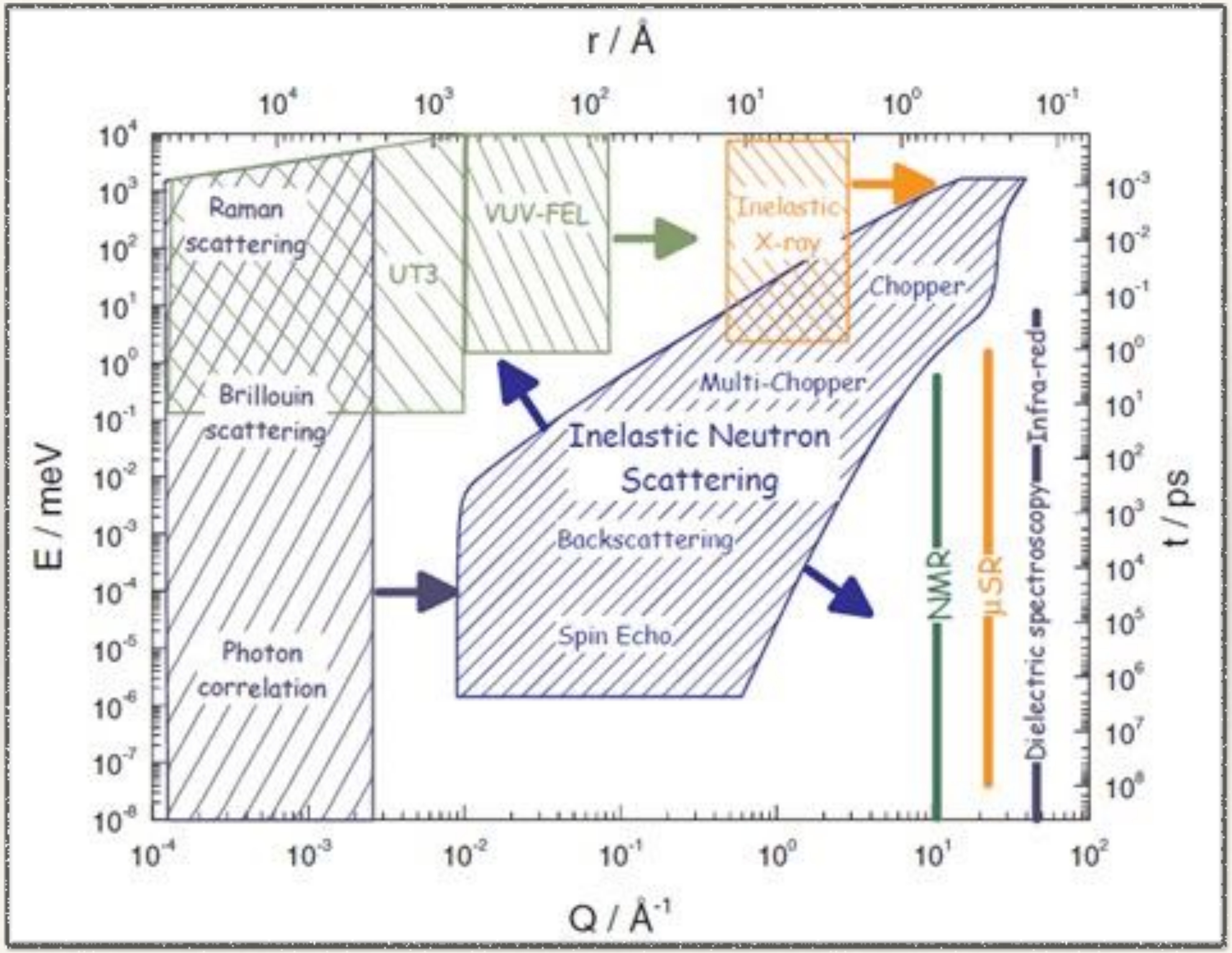
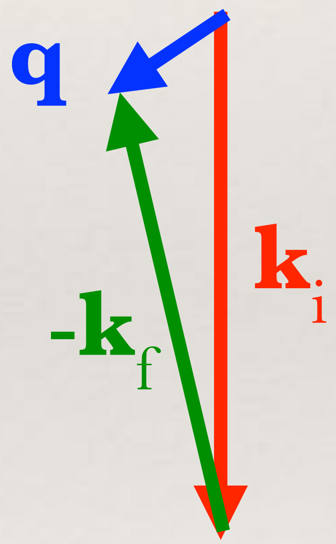
Energy & Momentum



Energy & Momentum

- The combination of momentum and energy conservation results in a restriction of the ω-**q** space reachable, known as the kinematic limit.



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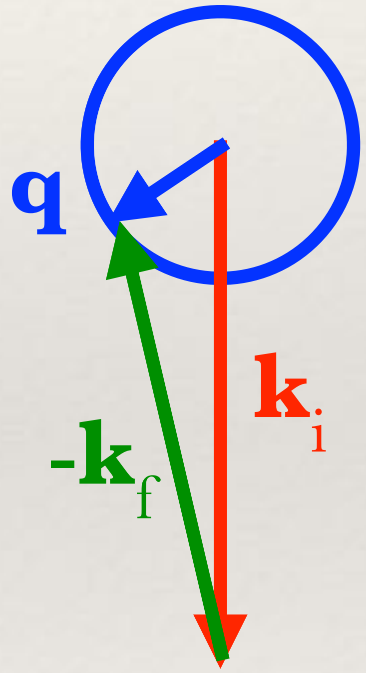

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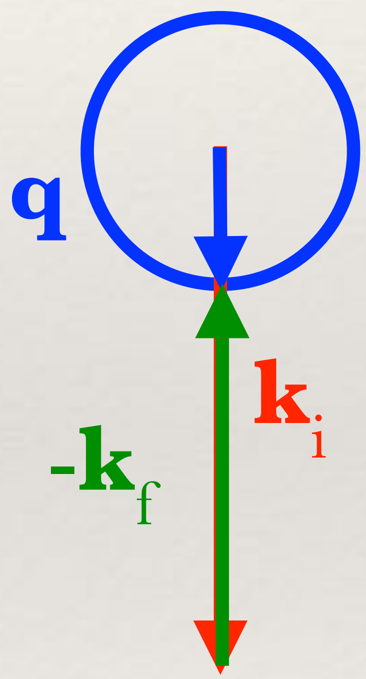

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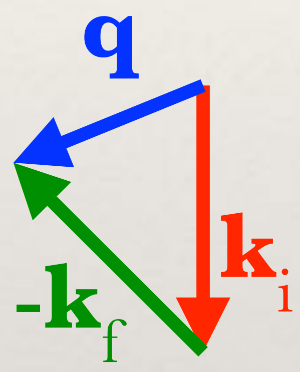

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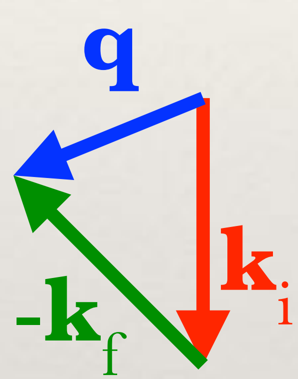
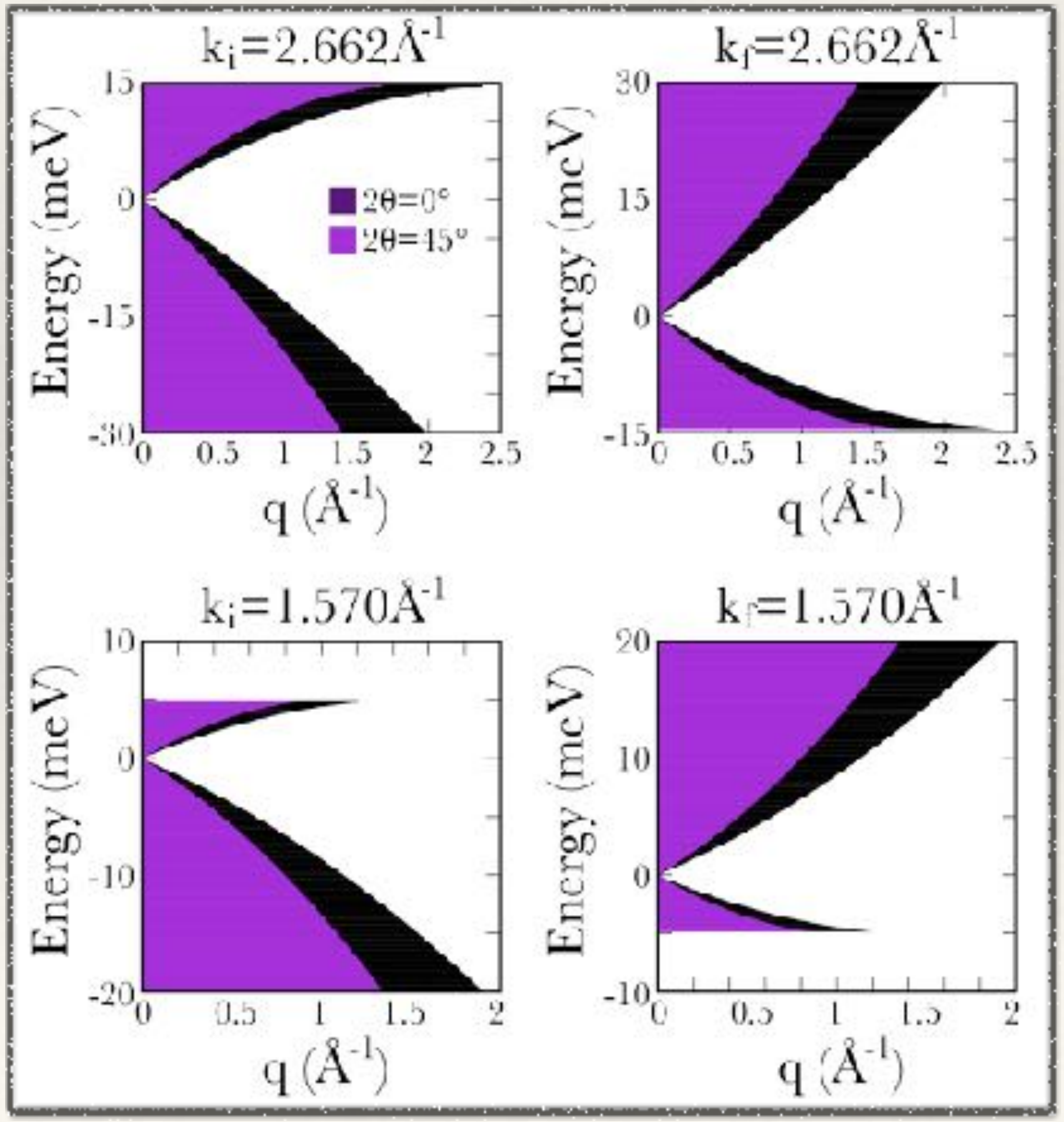
$$\vec{q} = \vec{k}_i - \vec{k}_f$$

$$\omega = \frac{\hbar^2}{2m}(k_i^2 - k_f^2)$$

$$q = \sqrt{2k_i^2 - \frac{2m\omega}{\hbar} - 2k_i\sqrt{k_i^2 - \frac{2m\omega}{\hbar}}cos(2\theta)}$$





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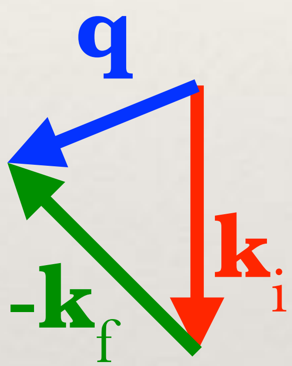

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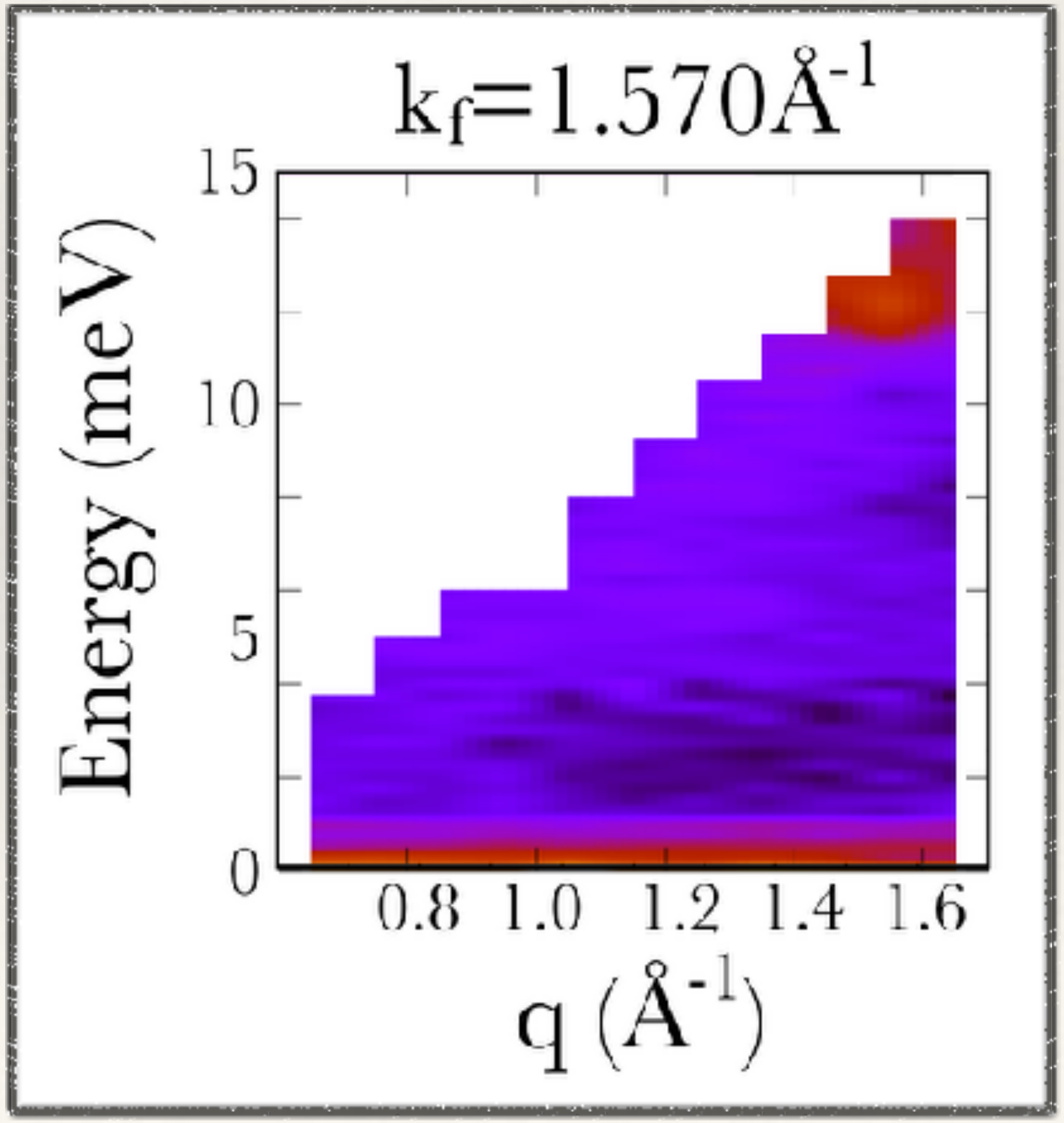

Energy & Momentum

- Kinematic limit for X-rays :

$$\vec{q} = \vec{k}_i - \vec{k}_f$$

$$\omega = \hbar c(k_i - k_f)$$

$$q = \sqrt{\frac{\omega^2}{c^2} + 2k_i^2(1 - cos(2\theta)) - \frac{2k_i\omega}{c}(1 + cos(2\theta))}$$

- Since $\omega << ck_i \Rightarrow q \approx \sqrt{1 - cos(2\theta)}k_i$, kinematic limit is equivalent to momentum conservation

Spin Angular Momentum

- Neutron spin angular momentum :

$$S_z = \pm \frac{\hbar}{2}$$

- Restricts accessible excitations to :

$$\Delta S = 0 \quad \text{and} \quad \Delta S = 1$$

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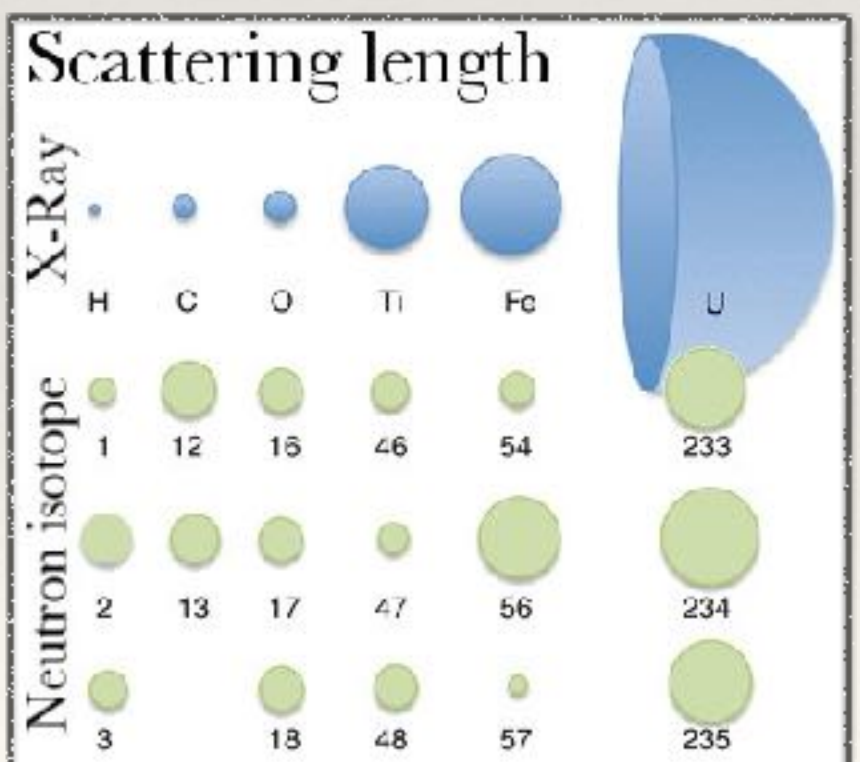
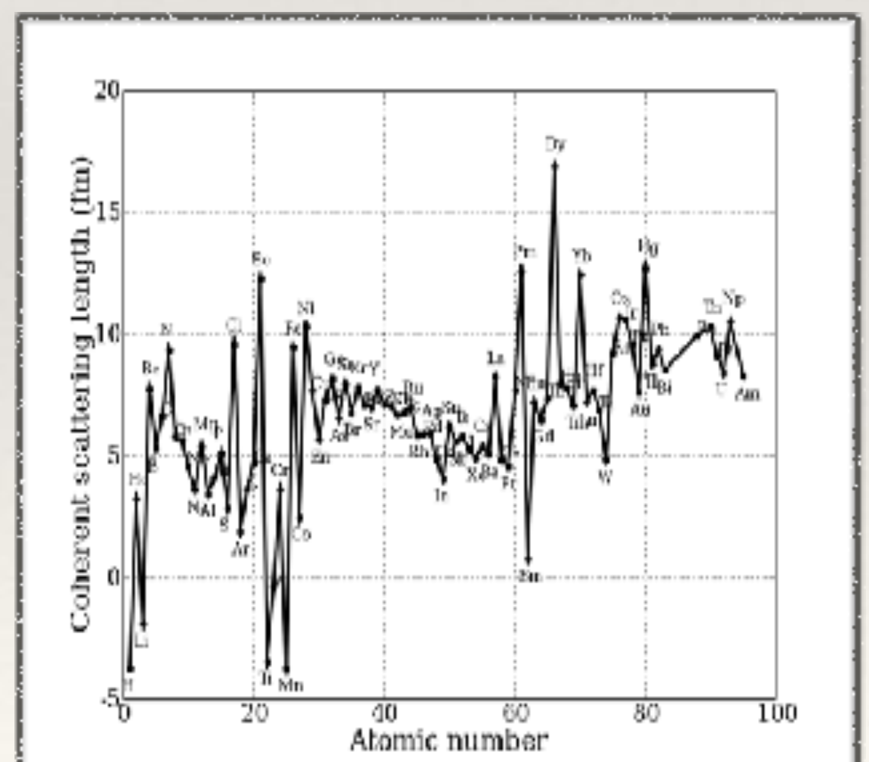
Inelastic Neutron Scattering

- Interaction neutron-nucleus : $\mathcal{V}(\vec{r}) = \frac{2\pi\hbar^2}{m_n} b\delta(\vec{r} - \vec{R})$
- m_n : neutron mass
- b : neutron scattering length of a nucleus : can be negative, complex and is isotope sensitive.





Inelastic Neutron Scattering

- Elastic cross section is proportional to structure factor

$$\frac{\partial\sigma}{\partial\Omega} = \frac{k_f}{k_i}\left|F(\vec{Q})\right|^2 \qquad F(\vec{Q}) = \sum_j b_j e^{-i\vec{Q}.\vec{r_j}}$$

- For inelastic cross section, one has to consider moving atoms :

$$\vec{R}_a(t) = \vec{R}_c + \vec{r}_a + \vec{u}_a(t)$$

- So cross section writes :

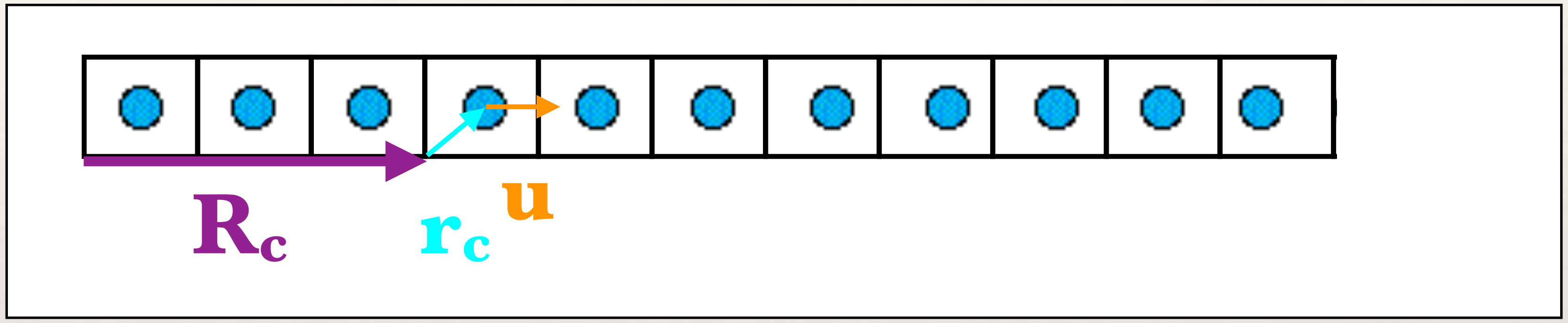
$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i} S(\vec{Q},\omega)$$

$$S(\vec{Q},\omega) = \sum_{a_1,a_2} b_{a_1} b_{a_2} \int_{-\infty}^{+\infty} \langle e^{i\vec{Q}.(\vec{R}_{a_1}(0)-\vec{R}_{a_2}(t))}\rangle e^{-i\omega t} dt$$

Inelastic Neutron Scattering

- Let's consider a collective displacement p in a crystal with only one atom a :

$$\vec{R}_a(t) = \vec{R}_c + \vec{r}_a + \vec{u}_a(t)$$



- Atomic displacement of atom a for this phonon mode p writes :

$$\vec{u}_{a,p}(t) = \sqrt{\frac{\hbar}{m_a \omega_p(\vec{q})}} e^{(i\vec{Q}.\vec{r}_a - \omega_p t)} \vec{\tilde{u}}_{a,p}$$

Inelastic Neutron Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = N\frac{(2\pi)^3}{v_0}\sum_{\vec{G}\in RS}\delta(\vec{Q}-\vec{G})\left|\sum_a b_a e^{-W_a} e^{i\vec{Q}.\vec{r}_a}\right|^2$$

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}b_a e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$

$$\times\left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q}))+n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

Inelastic Neutron Scattering

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Elastic cross section

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}b_a e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$
$$\times\left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q}))+n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

Inelastic cross section

Inelastic Neutron Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = N\frac{(2\pi)^3}{v_0}\sum_{\vec{G}\in RS}\delta(\vec{Q}-\vec{G})\left|\sum_a b_a e^{-W_a} e^{i\vec{Q}.\vec{r}_a}\right|^2$$

Elastic Structure Factor

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}b_a e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$

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Inelastic Structure Factor

Inelastic Neutron Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = N\frac{(2\pi)^3}{v_0}\sum_{\vec{G}\in RS}\delta(\vec{Q}-\vec{G})\left|\sum_a b_a \boxed{e^{-W_a}} e^{i\vec{Q}.\vec{r}_a}\right|^2$$

Debye-Waller Factor

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}b_a \boxed{e^{-W_a}} e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$

$$\times\left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q}))+n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

Inelastic Neutron Scattering

$$\left.\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right|_{inel} = \frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}b_a e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$
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Energy conservation term

Inelastic Neutron Scattering

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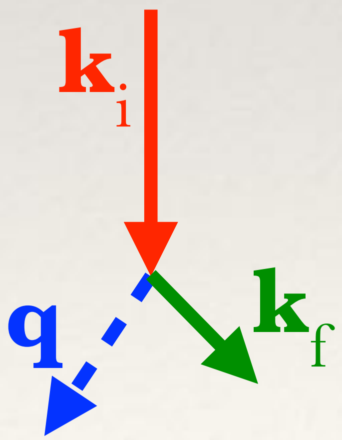
Energy conservation : creation process



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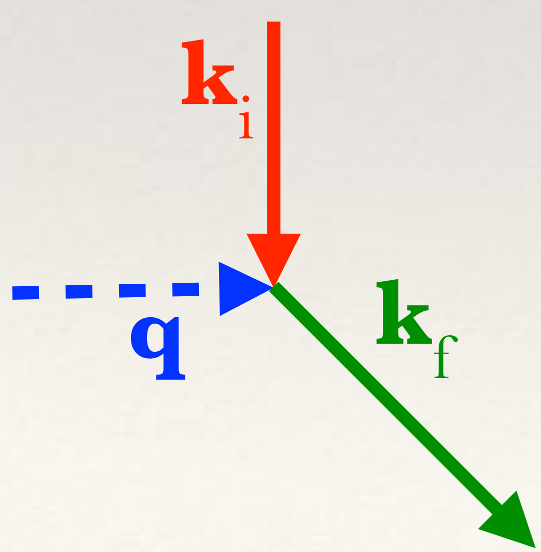
$$\times\left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q}))+n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

Energy conservation : annihilation process



Inelastic Neutron Scattering

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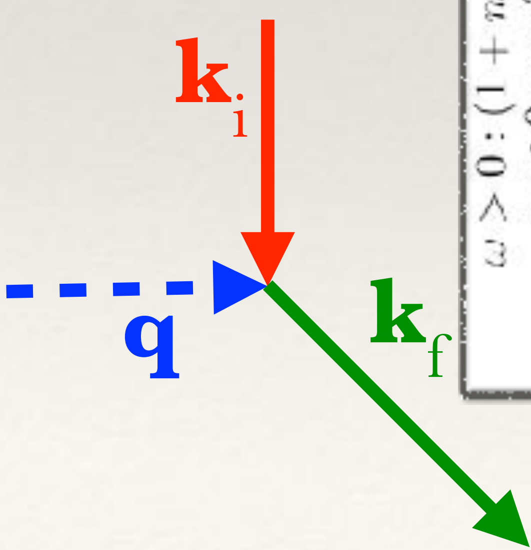
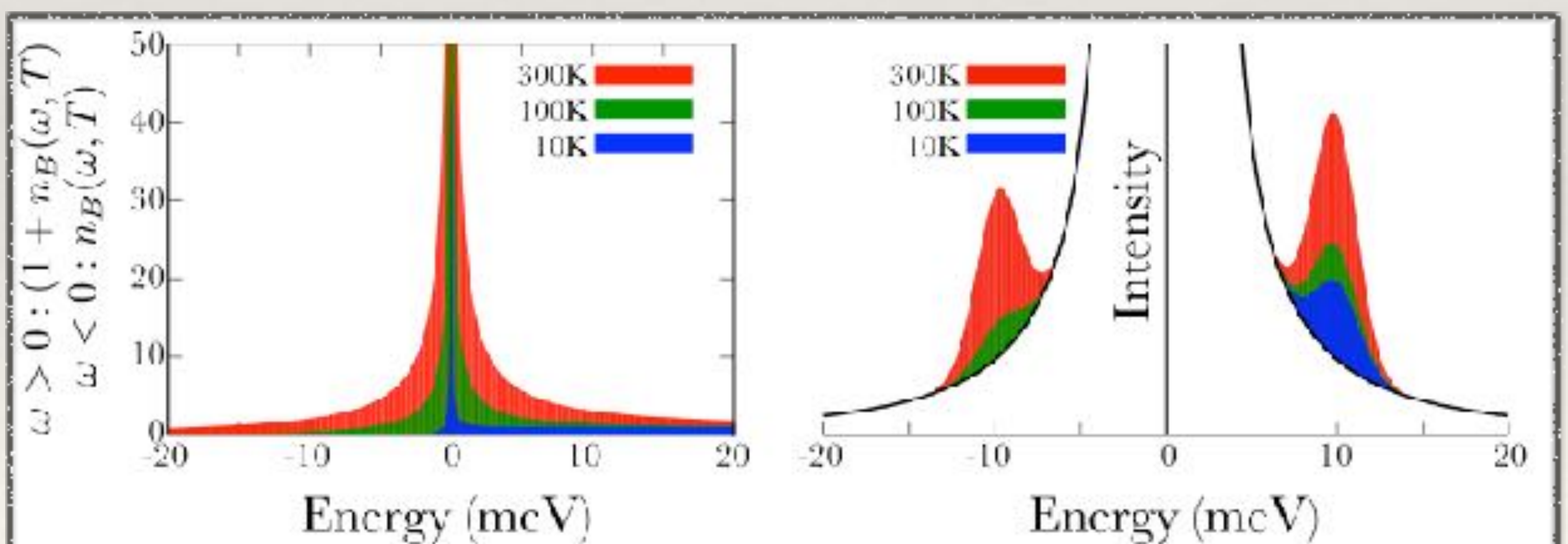
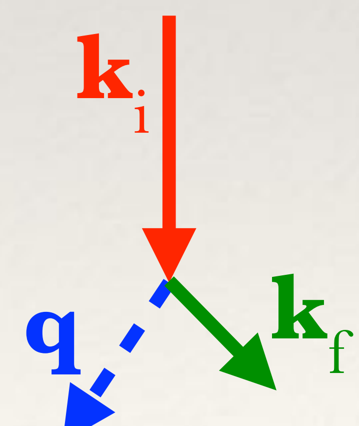
Detailed Balance Factor

$$n_B(\omega,T) = \frac{1}{e^{\frac{\hbar\omega}{k_B T}}-1}$$







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Phononic term

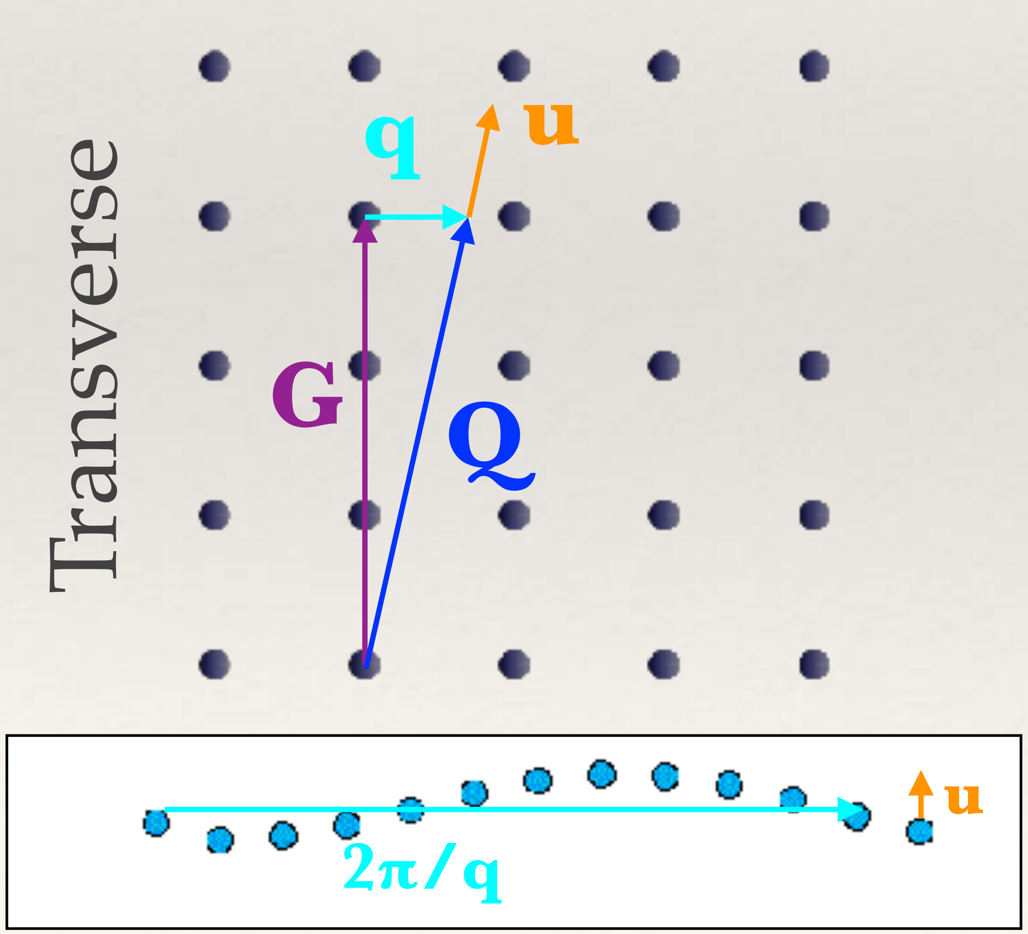
Inelastic Neutron Scattering

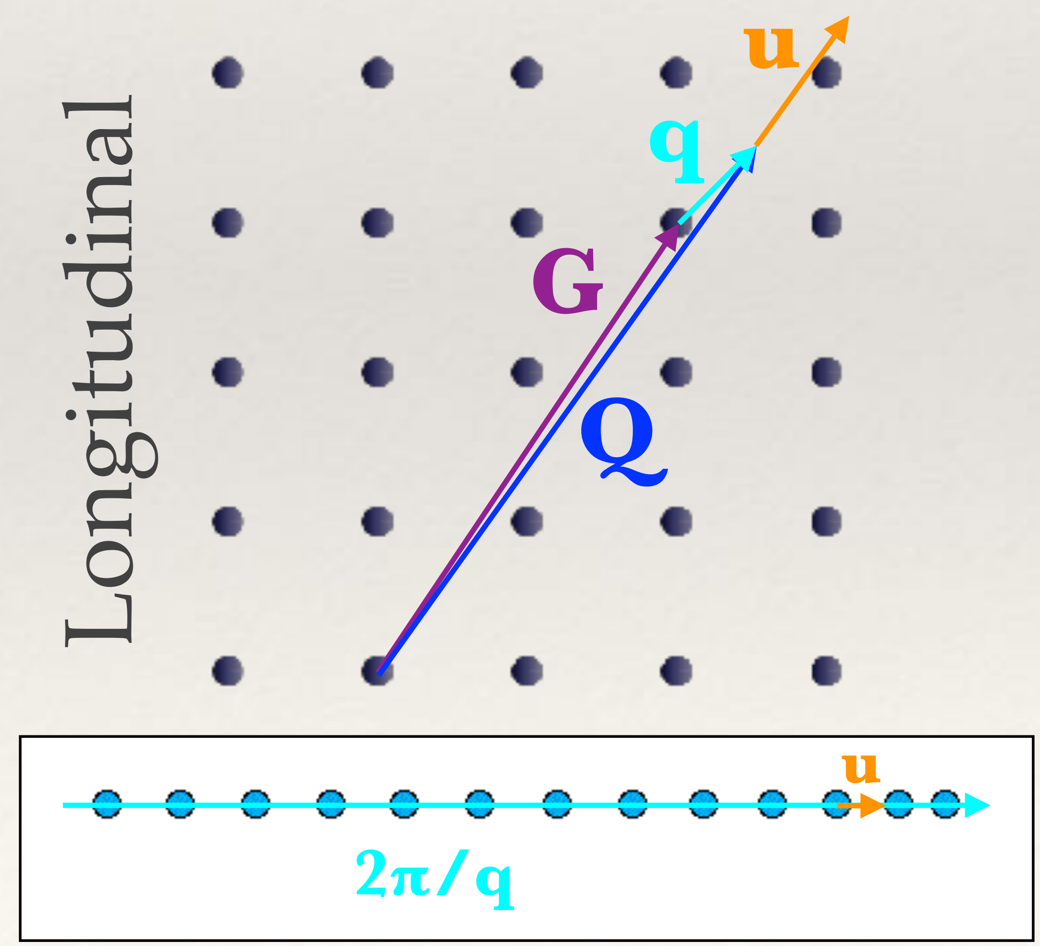
$$\left.\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right|_{inel} = \frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}b_a e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$
$$\times\left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q}))+n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

- Sensitive to displacement along $\vec{Q}$
- Proportional to Q^2

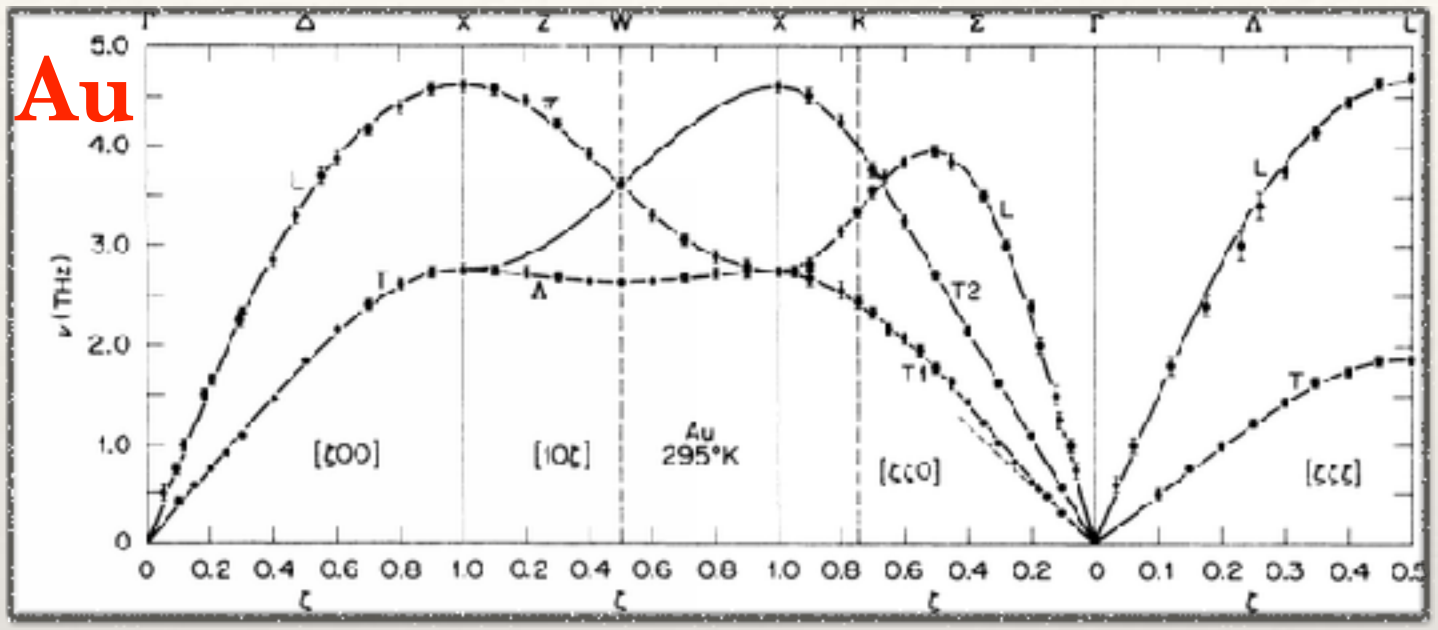
Inelastic Neutron Scattering

$$\left.\frac{\partial^2\sigma}{\partial\Omega\partial\omega}\right|_{inel} = \frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}b_a e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$
$$\times\left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q}))+n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

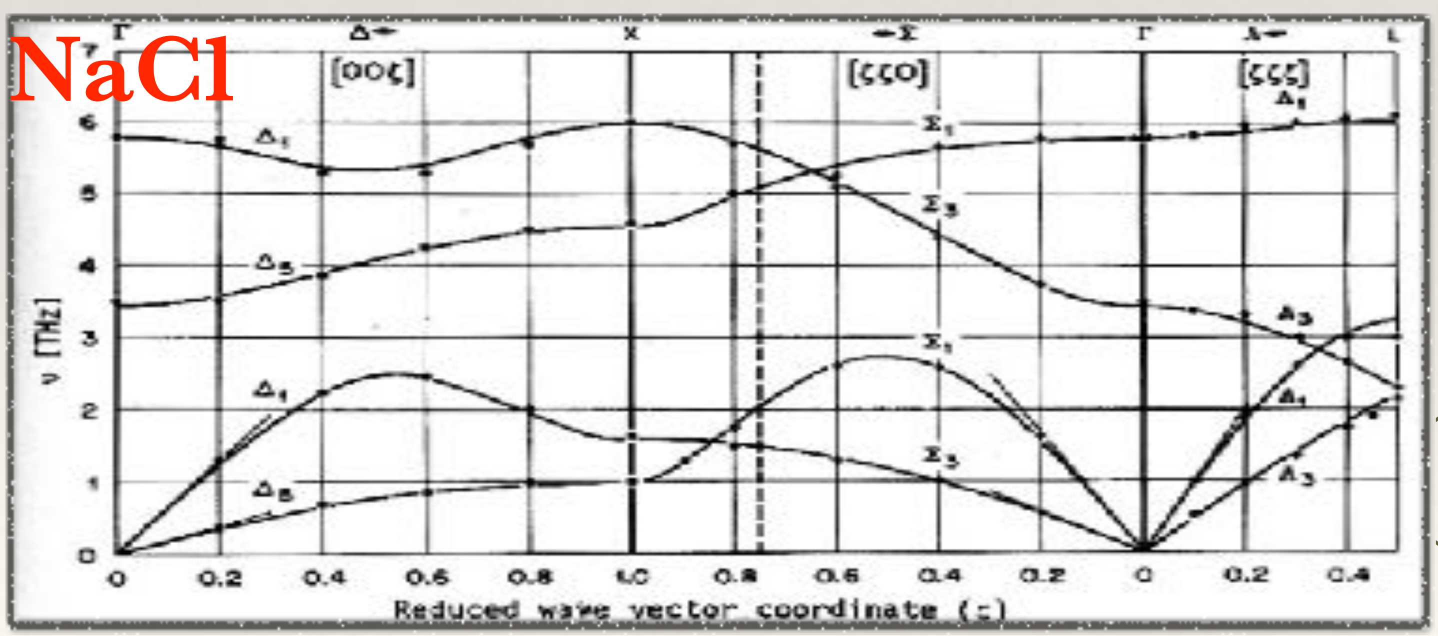




Inelastic Neutron Scattering



PRB 8, 3496 (1973)



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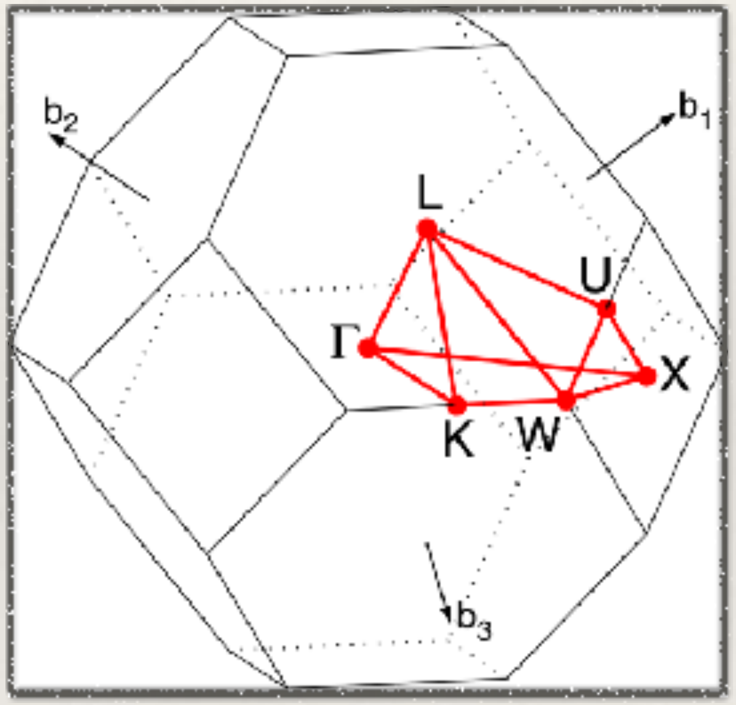


Outline

- 1 General concepts
  From elastic to inelastic scattering
  Conservation laws and consequences
- **2 Inelastic Neutron Scattering**
  Nuclear Interaction
  Magnetic Interaction
- 3 Inelastic X-ray Scattering

Inelastic Neutron Scattering

- Interaction neutron-magnetic moment :

$$\mathcal{V}(\vec{r}) = -\vec{\mu}_n.\frac{\mu_0}{4\pi}\left(r\vec{o}t\left(\frac{\vec{\mu_e}\wedge\vec{r}}{r^3}\right) - \frac{2\mu_B}{\hbar}\frac{\vec{p}\wedge\vec{r}}{r^3}\right)$$

- $\vec{\mu_e} = 2\mu_B\vec{S}$: electron magnetic moment operator
- $\vec{\mu_n} = -\gamma\mu_N\vec{\sigma}$: neutron magnetic moment operator

$$\mathcal{V}(\vec{r}) = -\vec{\mu}_n.r\vec{o}t(r\vec{o}t\left(\frac{\mu_e^S + \mu_e^L}{r}\right))$$

Inelastic Neutron Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_e)^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G}) \left| \sum_a r_e f_a(\vec{Q}) S_{\perp,a} e^{-W_a} e^{i\vec{Q}.\vec{r}_a} \right|^2 \delta(\omega)$$

Elastic cross section

$$+ \frac{k_f}{k_i}(\gamma r_e)^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G}) \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \frac{Q^\alpha Q^\beta}{Q^2} \right)$$

$$\times \sum_{a_1,a_2} f_{a_1}(\vec{Q}) f_{a_2}(\vec{Q}) e^{i\vec{Q}.(\vec{r}_{a_1}-\vec{r}_{a_2})} e^{-W_{a1}-W_{a2}} \int_{-\infty}^{+\infty} \langle S^\alpha_{a1}(0) S^\beta_{a2}(t) \rangle e^{-i\omega t} dt$$

Inelastic cross section

Inelastic Neutron Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_e)^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G}) \left| \sum_a r_a f_a(\vec{Q}) S_{\perp,a} e^{-W_a} e^{i\vec{Q}.\vec{r}_a} \right|^2 \delta(\omega)$$

$$+ \frac{k_f}{k_i}(\gamma r_e)^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G}) \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \frac{Q^\alpha Q^\beta}{Q^2}\right)$$

$$\times \sum_{a_1,a_2} f_{a_1}(\vec{Q}) f_{a_2}(\vec{Q}) e^{i\vec{Q}.(\vec{r}_{a_1}-\vec{r}_{a_2})} e^{-W_{a1}-W_{a2}} \int_{-\infty}^{+\infty} \langle S^\alpha_{a1}(0) S^\beta_{a2}(t)\rangle e^{-i\omega t} dt$$

Magnetic form factor

Inelastic Neutron Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_e)^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G}) \left| \sum_a r_e f_a(\vec{Q}) S_{\perp,a} e^{-W_a} e^{i\vec{Q}.\vec{r}_a} \right|^2 \delta(\omega)$$

$$+ \frac{k_f}{k_i}(\gamma r_e)^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G}) \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \frac{Q^\alpha Q^\beta}{Q^2} \right)$$

Geometrical factor

$$\times \sum_{a_1,a_2} f_{a_1}(\vec{Q}) f_{a_2}(\vec{Q}) e^{i\vec{Q}.(\vec{r}_{a_1}-\vec{r}_{a_2})} e^{-W_{a1}-W_{a2}} \int_{-\infty}^{+\infty} \langle S^\alpha_{a1}(0) S^\beta_{a2}(t) \rangle e^{-i\omega t} dt$$

Inelastic Neutron Scattering

- For a ferromagnet, the cross section writes :

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_0)^2 S^2 \left(1 - \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G})\delta(\omega)$$

$$+ \frac{k_f}{k_i}(\gamma r_0)^2 S \left(1 + \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G})$$

$$\times \left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q})) + n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

Inelastic Neutron Scattering

- For a ferromagnet, the cross section writes :

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_0)^2 S^2 \left(1 - \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G})\delta(\omega)$$

$$+ \frac{k_f}{k_i}(\gamma r_0)^2 S \left(1 + \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G})$$

$$\times \left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q})) + n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

- Elastic intensity is sensitive to the magnetic moment perpendicular to $\vec{Q}$

Inelastic Neutron Scattering

- For a ferromagnet, the cross section writes :

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_0)^2 S^2 \left(1 - \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G})\delta(\omega)$$

$$+ \frac{k_f}{k_i}(\gamma r_0)^2 S \left(1 + \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G})$$

$$\times \left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q})) + n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

- Elastic intensity is sensitive to the magnetic moment perpendicular to $\vec{Q}$
- Elastic intensity is proportional to the square of the moment amplitude

Inelastic Neutron Scattering

- For a ferromagnet, the cross section writes :

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_0)^2 S^2 \left(1 - \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G})\delta(\omega)$$

$$+ \frac{k_f}{k_i}(\gamma r_0)^2 S \boxed{\left(1 + \left(\frac{Q^z}{Q}\right)^2\right)} \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G})$$

$$\times \left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q})) + n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

- Inelastic intensity is sensitive to the magnetic moment parallel to $\vec{Q}$

Inelastic Neutron Scattering

- For a ferromagnet, the cross section writes :

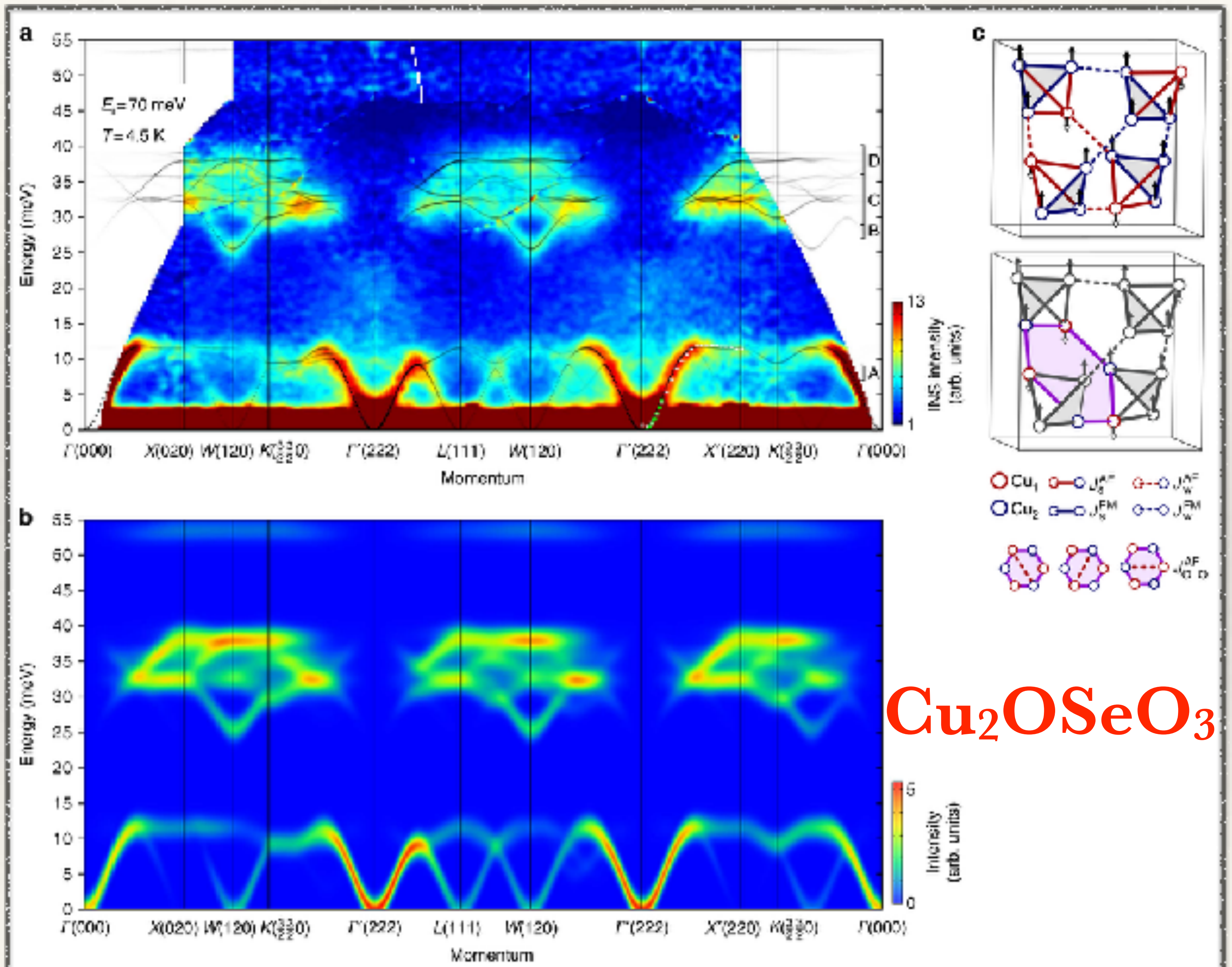
$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i}(\gamma r_0)^2 S^2 \left(1 - \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G})\delta(\omega)$$

$$+ \frac{k_f}{k_i}(\gamma r_0)^2 S \left(1 + \left(\frac{Q^z}{Q}\right)^2\right) \left|f(\vec{Q})e^{-W}\right|^2 \sum_{\vec{G},\vec{q}} \delta(\vec{Q}-\vec{q}-\vec{G})$$

$$\times \left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q})) + n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

- Inelastic intensity is sensitive to the magnetic moment parallel to $\vec{Q}$
- Inelastic intensity is linear in moment amplitude

Inelastic Neutron Scattering



Cu_2OSeO_3

Nature Com. 7, 10725 (2016)

Inelastic Neutron Scattering

Discriminating between phonon and magnon

Phonon	Magnon
Intensity proportional to $\mathbf{Q}^2$	Intensity decreases with **Q** (magnetic form factor)
Always present	Appears in ordered phase $T<T_C$

And Polarized Inelastic Neutron Scattering…

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Inelastic X-ray Scattering

- Interaction X-ray-electron :

$$\mathcal{V}(\vec{r}) = \frac{q}{m_e c}\vec{p}.\vec{A}(\vec{r}) + \frac{q^2}{m_e c^2}\vec{A}^2$$

- m_e : electron mass

Inelastic X-ray Scattering

- Elastic cross section is proportional to structure factor

$$\frac{\partial \sigma}{\partial \Omega} = \frac{k_f}{k_i} r_e^2 \left|\vec{\epsilon}_i . \vec{\epsilon}_f\right|^2 \left|F(\vec{Q})\right|^2 \qquad F(\vec{Q}) = \sum_j f_j(\vec{Q}) e^{-i\vec{Q}.\vec{r_j}}$$

- For inelastic cross section, one has to consider moving atoms :

$$\vec{R}_a(t) = \vec{R}_c + \vec{r}_a + \vec{u}_a(t)$$

- So cross section writes :

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} = \frac{k_f}{k_i} r_e^2 |\vec{\epsilon}_1 . \vec{\epsilon}_2|^2 S(\vec{Q}, \omega)$$

Atomic form factor

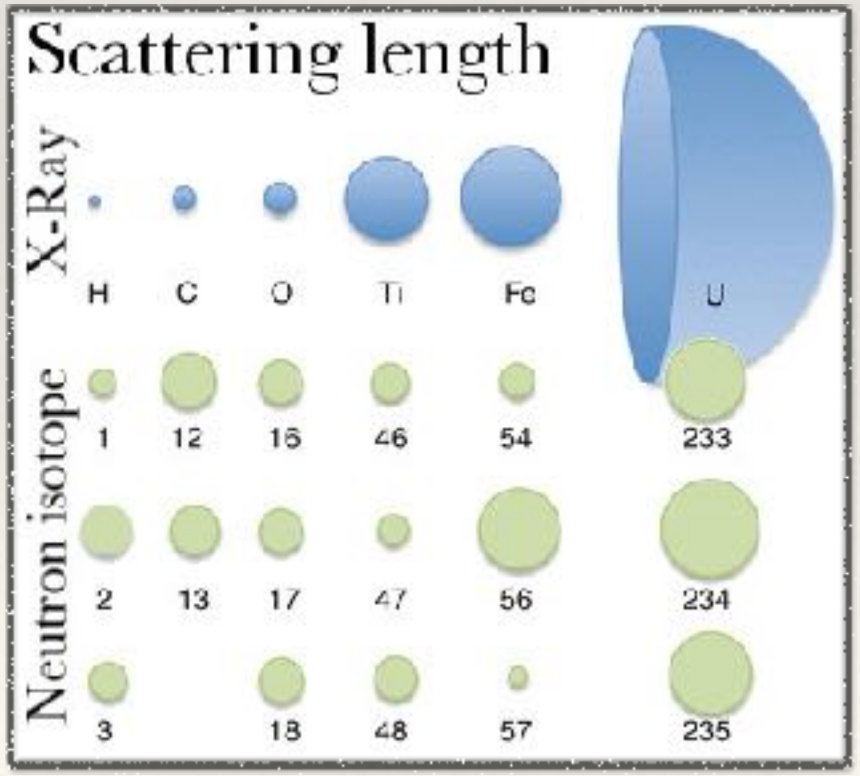
$$S(\vec{Q}, \omega) = \sum_{a_1, a_2} f_{a_1}(\vec{Q}) f_{a_2}(\vec{Q}) \int_{-\infty}^{+\infty} \langle e^{i\vec{Q}.\vec{R}_{a_1}(0)} e^{-i\vec{Q}.\vec{R}_{a_2}(t)} \rangle e^{-i\omega t} dt$$

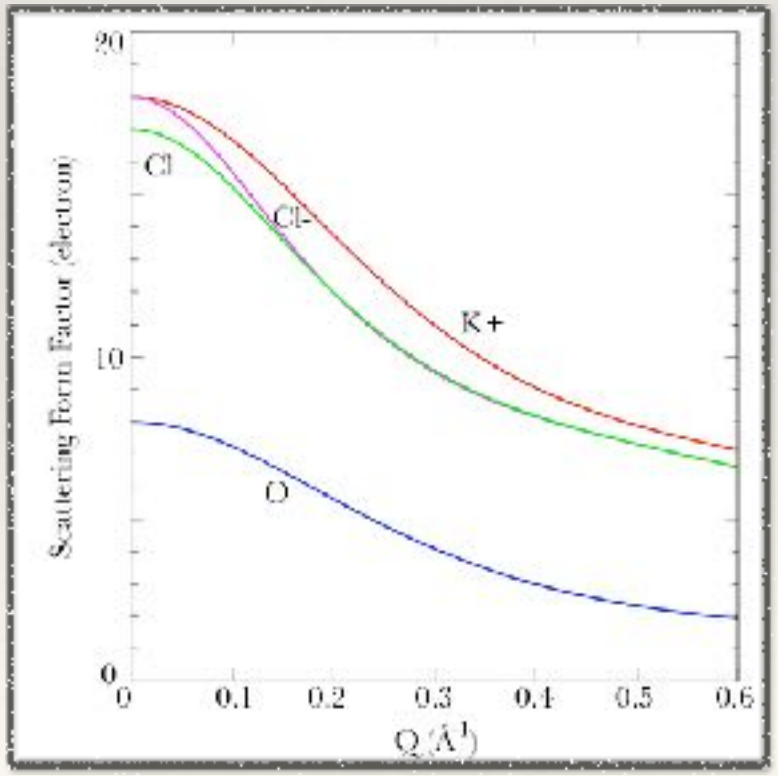
Inelastic X-ray Scattering

Atomic form factor

$$f(\vec{Q}) = \int \rho(\vec{r}) e^{i\vec{Q}.\vec{r}} d^3\vec{r}$$

$$f(\vec{Q} = \vec{0}) = \mathcal{Z}$$





Inelastic X-ray Scattering

- Elastic cross section is proportional to structure factor

$$\frac{\partial\sigma}{\partial\Omega} = \frac{k_f}{k_i} r_e^2 \, |\vec{\epsilon}_i . \vec{\epsilon}_f|^2 \left| F(\vec{Q}) \right|^2 \qquad F(\vec{Q}) = \sum_j f_j(\vec{Q}) e^{-i\vec{Q}.\vec{r_j}}$$

- For inelastic cross section, one has to consider moving atoms :

$$\vec{R}_a(t) = \vec{R}_c + \vec{r}_a + \vec{u}_a(t)$$

- So cross section writes :

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = \frac{k_f}{k_i} r_e^2 |\vec{\epsilon}_1 . \vec{\epsilon}_2|^2 S(\vec{Q},\omega)$$

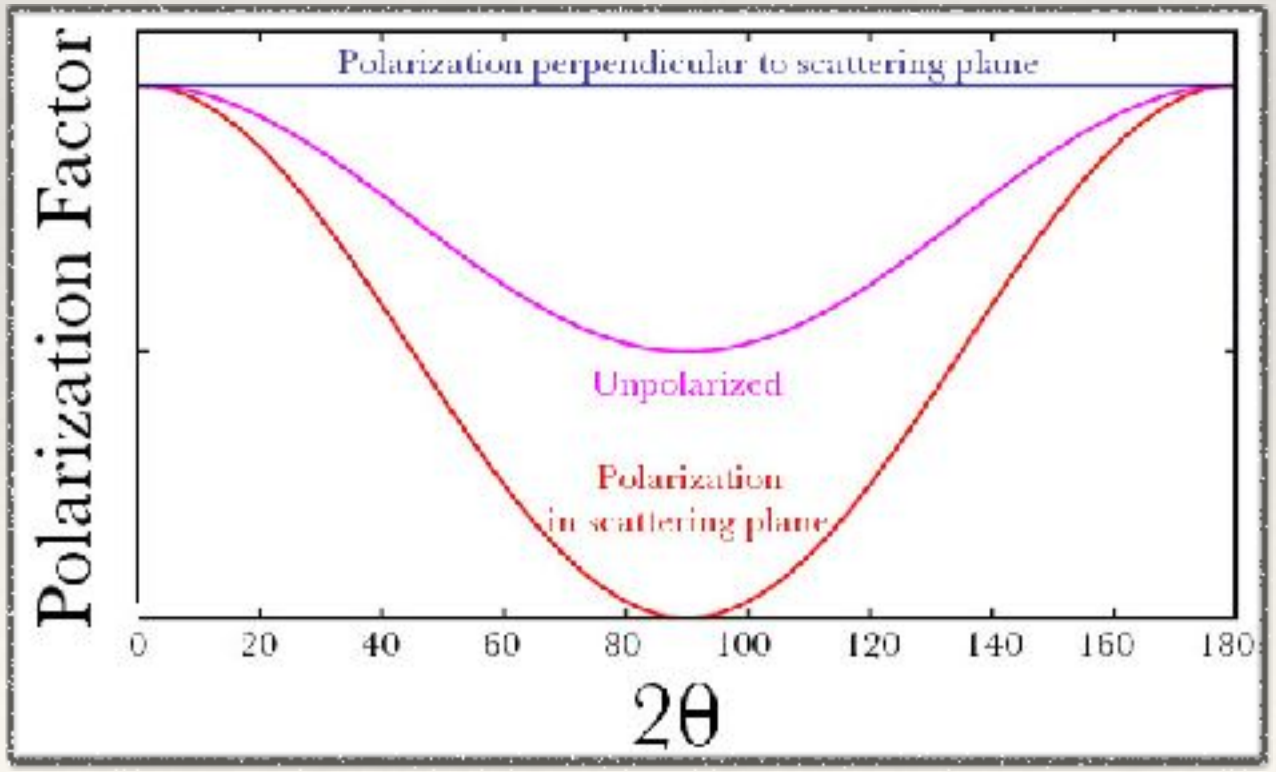
Polarization factor

$$S(\vec{Q},\omega) = \sum_{a_1,a_2} f_{a_1}(\vec{Q}) f_{a_2}(\vec{Q}) \int_{-\infty}^{+\infty} \langle e^{i\vec{Q}.\vec{R}_{a_1}(0)} e^{-i\vec{Q}.\vec{R}_{a_2}(t)} \rangle e^{-i\omega t} dt$$

Inelastic X-ray Scattering

Polarization factor

- Polarization in the scattering plane : $|\vec{\epsilon}_i.\vec{\epsilon}_f|^2 = cos(2\theta)$
- Polarization perpendicular to the scattering plane : $|\vec{\epsilon}_i.\vec{\epsilon}_f|^2 = 1$
- Unpolarized beam : $|\vec{\epsilon}_i.\vec{\epsilon}_f|^2 = \dfrac{1 + cos^2(2\theta)}{2}$



Inelastic X-ray Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = N\frac{(2\pi)^3}{v_0} r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G}) \left|\sum_a f_a(\vec{Q}) e^{-W_a} e^{i\vec{Q}.\vec{r}_a}\right|^2$$

Elastic cross section

$$+ \frac{k_f}{k_i}\frac{(2\pi)^3}{v_0} r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2 \sum_{\vec{q}\in BZ} \delta(\vec{Q}-\vec{q}-\vec{G}) \sum_p \left|\sum_a \sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}} f_a(\vec{Q}) e^{-W_a} e^{i\vec{Q}.\vec{r}_a} (\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$

$$\times \left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q})) + n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

$$+ \frac{k_f}{k_i}\frac{(2\pi)^3}{v_0} r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2$$

$$\times \sum_{\vec{q},\vec{q}'\in BZ} \delta(\vec{Q}-\vec{q}-\vec{q}'-\vec{G}) \frac{1}{2} \sum_{p,p'} \left|\sum_a \frac{\hbar}{m_a\sqrt{\omega_p(\vec{q})\omega_{p'}(\vec{q}')}} f_a(\vec{Q}) e^{-W_a} e^{i\vec{Q}.\vec{r}_a} (\vec{Q}.\vec{\tilde{u}}_{a,p})(\vec{Q}.\vec{\tilde{u}}_{a,p'})\right|^2$$

$$\times \Big[(1+n_B(\omega_p(\vec{q}),T))(1+n_B(\omega_p'(\vec{q}'),T))\delta(\omega-\omega_p(\vec{q})-\omega_{p'}(\vec{q}'))$$

$$+ 2n_B(\omega_p(\vec{q}),T)(1+n_B(\omega_p'(\vec{q}'),T))\delta(\omega+\omega_p(\vec{q}))-\omega_{p'}(\vec{q}'))$$

$$+ n_B(\omega_p(\vec{q}),T)n_B(\omega_p'(\vec{q}'),T)\delta(\omega+\omega_p(\vec{q}))+\omega_{p'}(\vec{q}'))\Big]$$

Inelastic X-ray Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = N\frac{(2\pi)^3}{v_0} r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2 \sum_{\vec{G}\in RS} \delta(\vec{Q}-\vec{G}) \left|\sum_a f_a(\vec{Q}) e^{-W_a} e^{i\vec{Q}.\vec{r}_a}\right|^2$$

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0} r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2 \sum_{\vec{q}\in BZ} \delta(\vec{Q}-\vec{q}-\vec{G}) \sum_p \left|\sum_a \sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}} f_a(\vec{Q}) e^{-W_a} e^{i\vec{Q}.\vec{r}_a} (\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$

$$\times \left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q})) + n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0} r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2$$

1 phonon inelastic cross section

$$\times \sum_{\vec{q},\vec{q}'\in BZ} \delta(\vec{Q}-\vec{q}-\vec{q}'-\vec{G}) \frac{1}{2} \sum_{p,p'} \left|\sum_a \frac{\hbar}{m_a\sqrt{\omega_p(\vec{q})\omega_{p'}(\vec{q}')}} f_a(\vec{Q}) e^{-W_a} e^{i\vec{Q}.\vec{r}_a} (\vec{Q}.\vec{\tilde{u}}_{a,p})(\vec{Q}.\vec{\tilde{u}}_{a,p'})\right|^2$$

$$\times \Big[(1+n_B(\omega_p(\vec{q}),T))(1+n_B(\omega_p'(\vec{q}'),T))\delta(\omega-\omega_p(\vec{q})-\omega_{p'}(\vec{q}'))$$

$$+2n_B(\omega_p(\vec{q}),T)(1+n_B(\omega_p'(\vec{q}'),T))\delta(\omega+\omega_p(\vec{q}))-\omega_{p'}(\vec{q}'))$$

$$+n_B(\omega_p(\vec{q}),T)n_B(\omega_p'(\vec{q}'),T)\delta(\omega+\omega_p(\vec{q}))+\omega_{p'}(\vec{q}'))\Big]$$

Inelastic X-ray Scattering

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} = N\frac{(2\pi)^3}{v_0}r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2\sum_{\vec{G}\in RS}\delta(\vec{Q}-\vec{G})\left|\sum_a f_a(\vec{Q})e^{-W_a}e^{i\vec{Q}.\vec{r}_a}\right|^2$$

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2\sum_{\vec{q}\in BZ}\delta(\vec{Q}-\vec{q}-\vec{G})\sum_p\left|\sum_a\sqrt{\frac{\hbar}{m_a\omega_p(\vec{q})}}f_a(\vec{Q})e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})\right|^2$$

$$\times\left[(1+n_B(\omega_p(\vec{q}),T))\delta(\omega-\omega_p(\vec{q}))+n_B(\omega_p(\vec{q}),T)\delta(\omega+\omega_p(\vec{q}))\right]$$

2 phonons inelastic cross section

$$+\frac{k_f}{k_i}\frac{(2\pi)^3}{v_0}r_e^2\,|\vec{\epsilon}_i.\vec{\epsilon}_f|^2$$

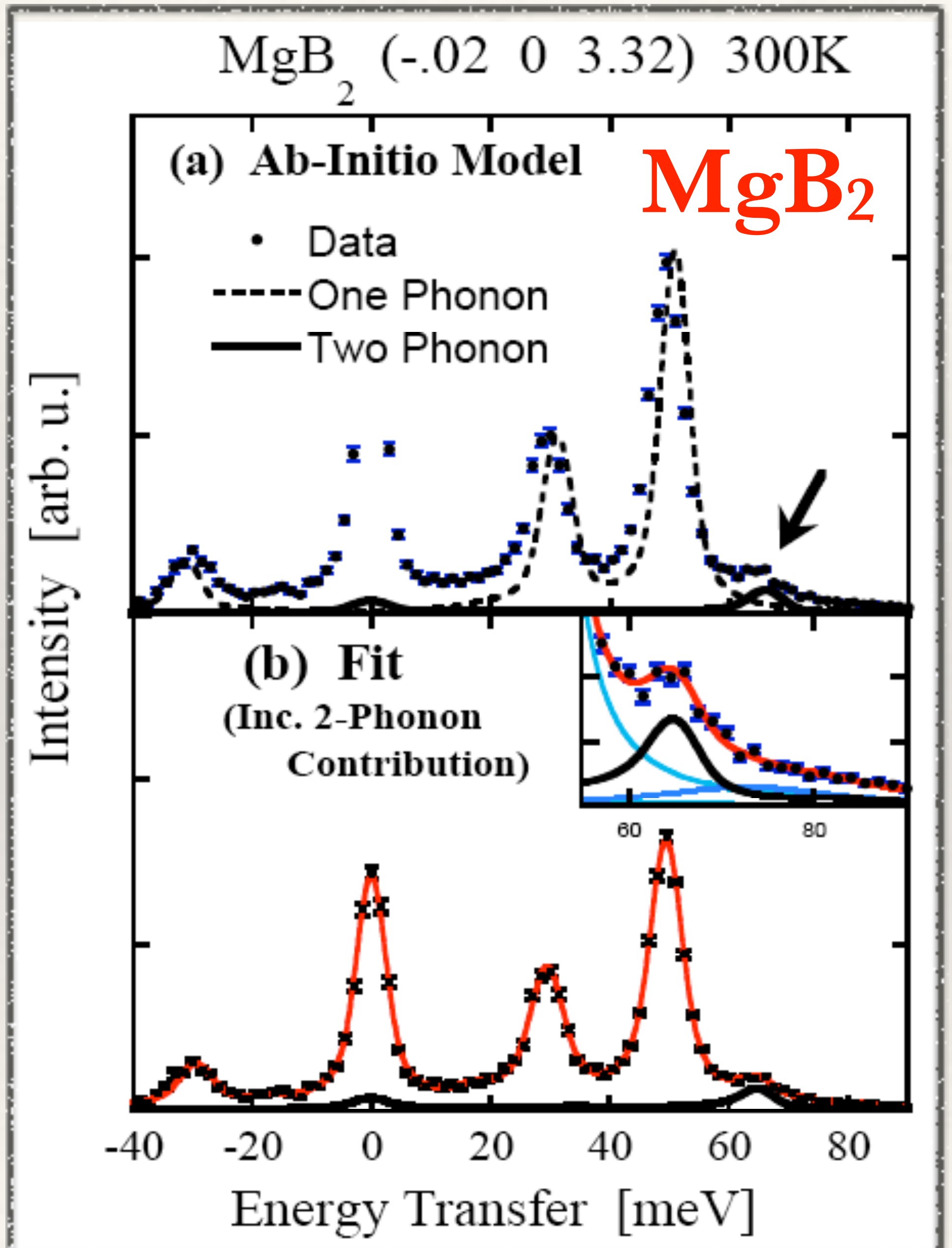
$$\times\sum_{\vec{q},\vec{q}'\in BZ}\delta(\vec{Q}-\vec{q}-\vec{q}'-\vec{G})\frac{1}{2}\sum_{p,p'}\left|\sum_a\frac{\hbar}{m_a\sqrt{\omega_p(\vec{q})\omega_{p'}(\vec{q}')}}f_a(\vec{Q})e^{-W_a}e^{i\vec{Q}.\vec{r}_a}(\vec{Q}.\vec{\tilde{u}}_{a,p})(\vec{Q}.\vec{\tilde{u}}_{a,p'})\right|^2$$

$$\times\Big[(1+n_B(\omega_p(\vec{q}),T))(1+n_B(\omega_p'(\vec{q}'),T))\delta(\omega-\omega_p(\vec{q})-\omega_{p'}(\vec{q}'))$$

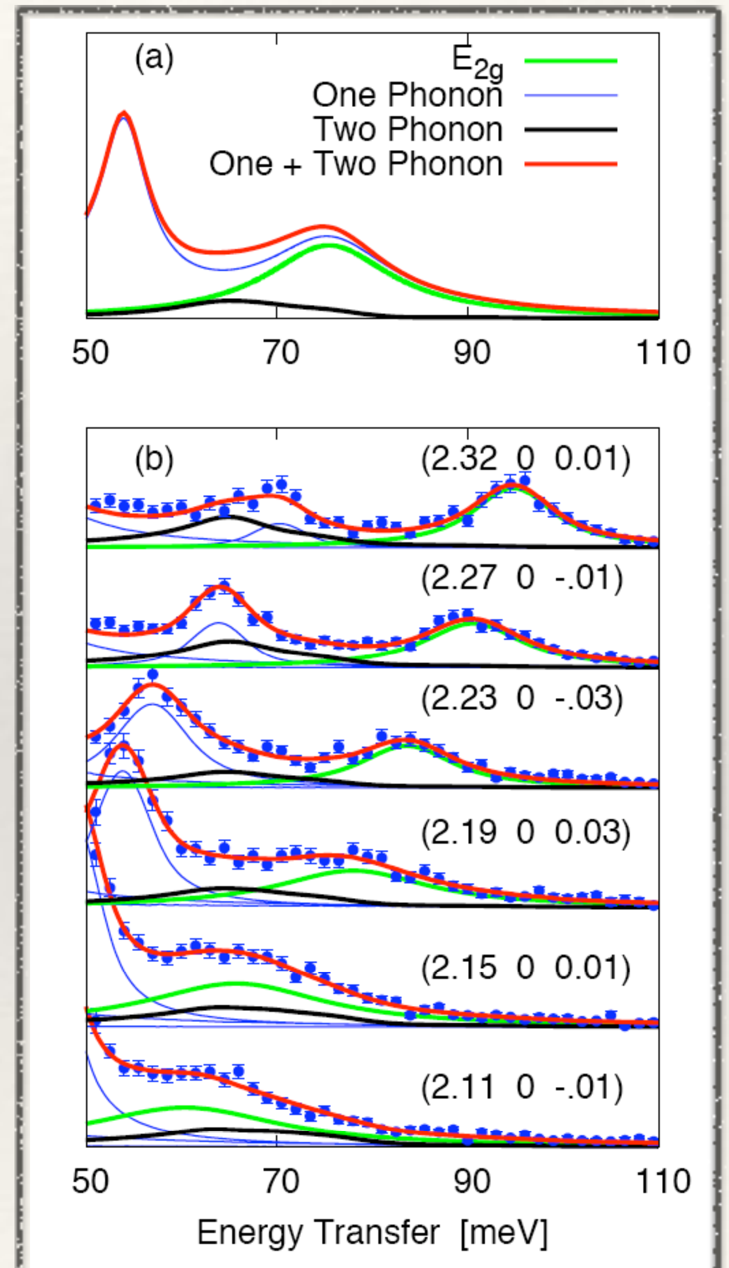
$$+2n_B(\omega_p(\vec{q}),T)(1+n_B(\omega_p'(\vec{q}'),T))\delta(\omega+\omega_p(\vec{q}))-\omega_{p'}(\vec{q}'))$$

$$+n_B(\omega_p(\vec{q}),T)n_B(\omega_p'(\vec{q}'),T)\delta(\omega+\omega_p(\vec{q}))+\omega_{p'}(\vec{q}'))\Big]$$

Inelastic X-ray Scattering



Phys. Rev. B, 75 020505(R) (2007)



Inelastic X-ray Scattering

INS	IXS
Strong ω-**Q** correlation : Kinematic limit	No ω-**Q** correlation : No kinematic limitation
No polarization factor	Polarization factor : $\|\vec{\epsilon_i}.\vec{\epsilon_f}\|^2$.
Intensity ~ b^2	Intensity ~ Z^2
Incoherent Scattering	No incoherent Scattering
Bulk measurement	Strong absorption ~ $\lambda^3 Z^4$
Large beam ~ cm	Small beam ~ 100 μm
Resolution down to 0.1 meV	Resolution ~ 1 meV

The end…