

# Inelastic neutron scattering



Rob McQueeney  
*Ames Laboratory*  
*Iowa State University*

IOWA STATE  
UNIVERSITY

# Outline

## I. Interaction of the neutron

- A. Nuclear
- B. Magnetic

## II. General inelastic scattering

## III. Nuclear inelastic scattering

- A. Correlation functions
- B. Examples

## IV. Magnetic inelastic scattering

- A. Correlation functions
- B. Examples

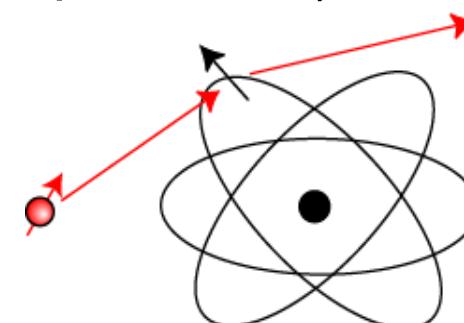
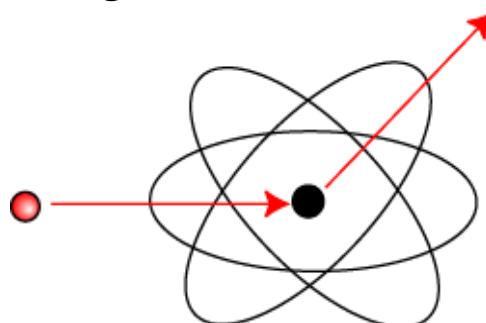
# Neutron interaction with matter

- Properties of the neutron

- Mass  $m_n = 1.675 \times 10^{-27}$  kg
- Charge 0
- Spin-1/2, magnetic moment  $\mu_n = -1.913 \mu_N$

- Neutrons interact with...

- Nucleus
  - Crystal structure/excitations (eg. phonons)
- Unpaired  $e^-$  via dipole scattering
  - Magnetic structure/excitations (eg. spin waves)



# Wavelength-energy relations

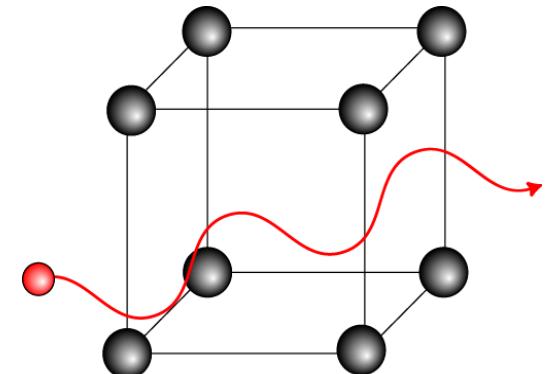
- **Neutron as a wave ...**

- Energy (E), velocity (v), wavenumber (k), wavelength ( $\lambda$ )

$$k = \frac{m_n v}{\hbar} = \frac{2\pi}{\lambda}$$

$$E = \frac{\hbar^2 k^2}{2m_n} = \frac{\hbar^2}{2m_n} \left( \frac{2\pi}{\lambda} \right)^2 = \frac{81.81 \text{ meV} \cdot \text{\AA}^2}{\lambda^2}$$

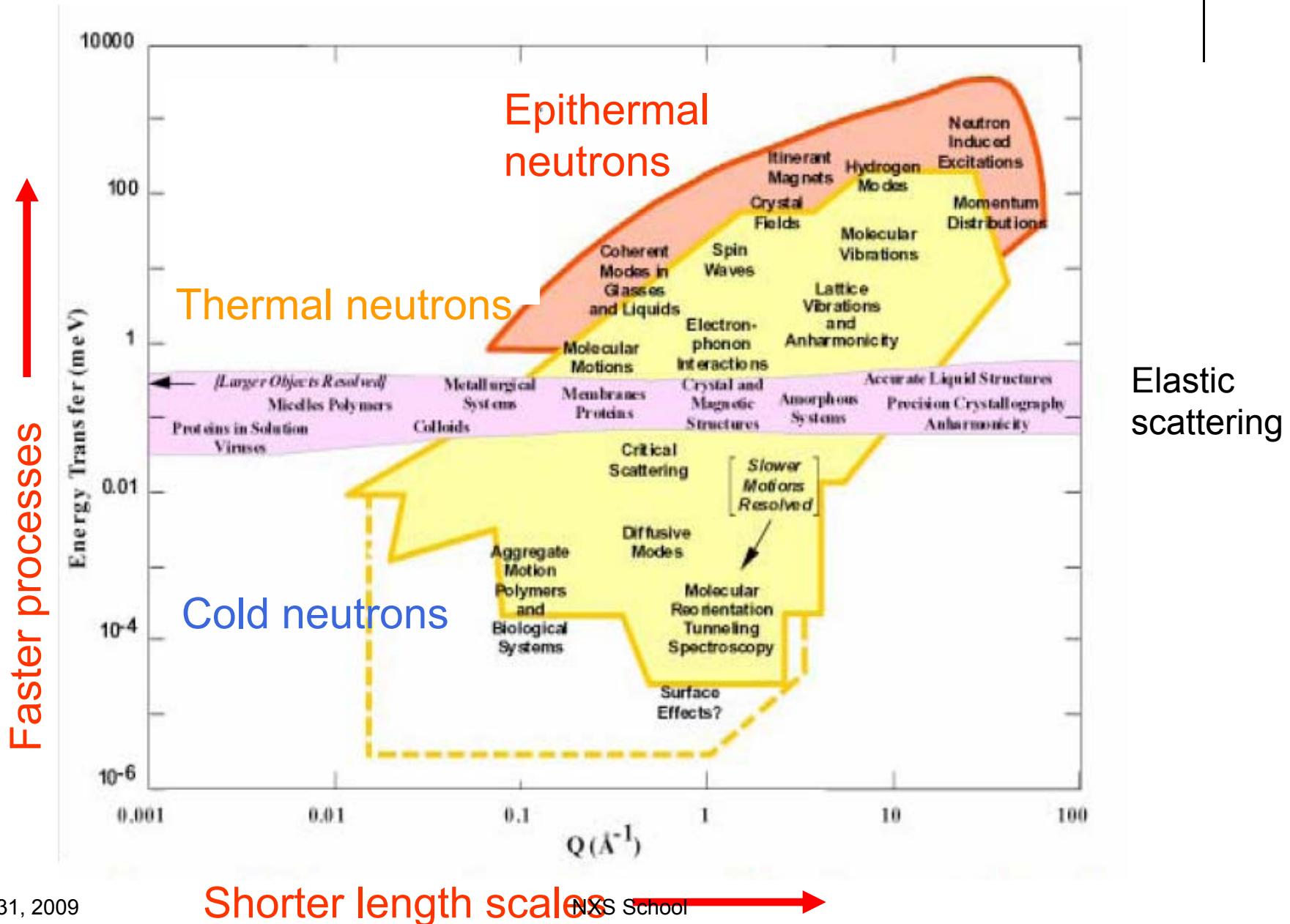
$$E = k_B T = (0.08617 \text{ meV} \cdot \text{K}^{-1}) T$$



$\lambda \sim$  interatomic spacing  $\rightarrow E \sim$  excitations in condensed matter

	Energy (meV)	Temperature (K)	Wavelength (Å)
Cold	0.1 – 10	1 – 120	4 – 30
Thermal	5 – 100	60 – 1000	1 – 4
Hot	100 – 500	1000 – 6000	0.4 – 1

# Dynamical (time) scales



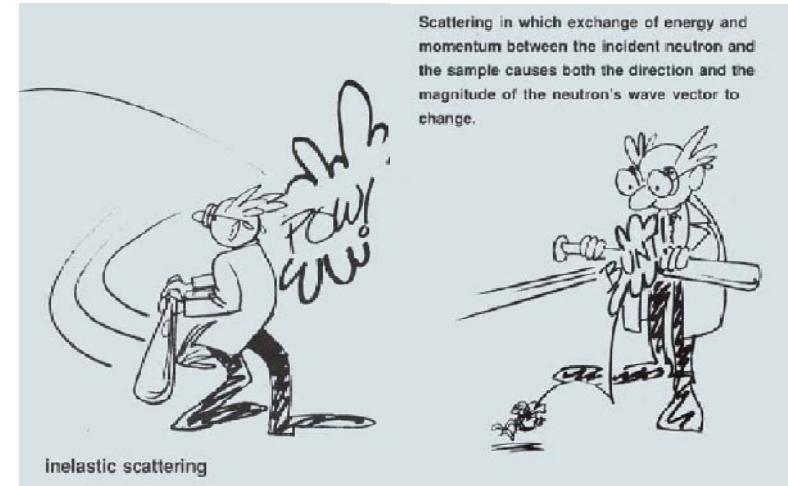
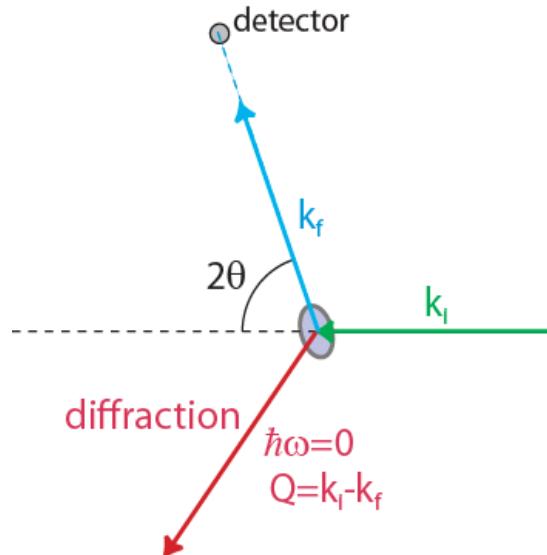
# Inelastic scattering

- Scattering process that changes the energy of the neutron

- Conservation of energy and momentum

$$\hbar\omega = E_i - E_f \quad \mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

- Scattering triangle



## Elastic scattering

$$\hbar\omega = 0$$

$$|\mathbf{k}_i| = |\mathbf{k}_f|$$

$$Q = 2k_i \sin \theta$$

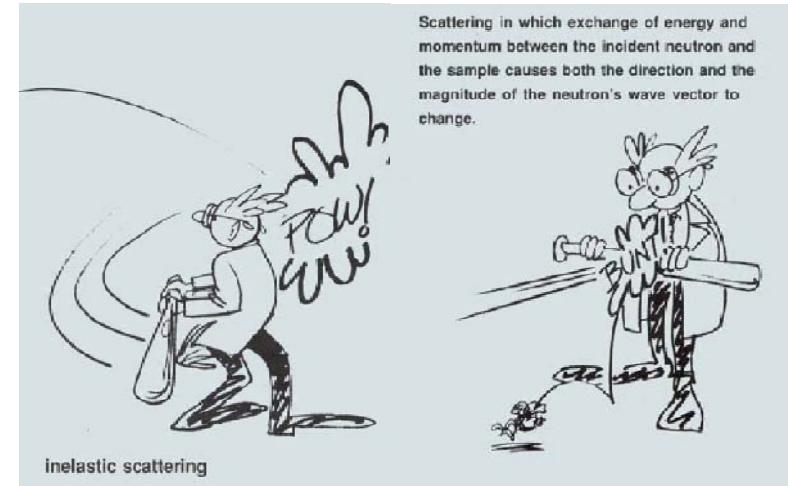
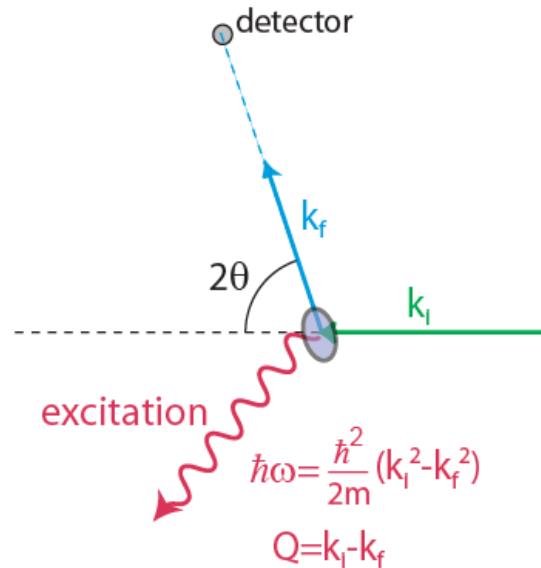
# Inelastic scattering

- Scattering process that changes the energy of the neutron

- Conservation of energy and momentum

$$\hbar\omega = E_i - E_f \quad \mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

- Scattering triangle



## Inelastic scattering

$$\hbar\omega > 0$$

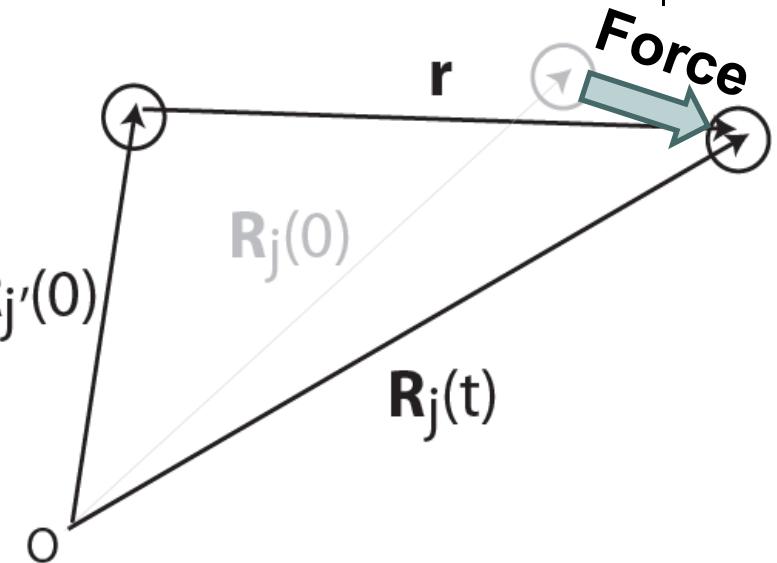
$$|\mathbf{k}_i| \neq |\mathbf{k}_f|$$

$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos 2\theta$$

# Nuclear correlation functions

## Pair correlation function

$$G(\mathbf{r}, t) = \frac{1}{N} \int \sum_{jj'} \delta(\mathbf{r}' - \mathbf{R}_{j'}(0)) \delta(\mathbf{r}' + \mathbf{r} - \mathbf{R}_j(t)) d\mathbf{r}'$$



## Intermediate function

$$I(\mathbf{Q}, t) = \int G(\mathbf{r}, t) e^{i\mathbf{Q} \cdot \mathbf{r}} d\mathbf{r} = \frac{1}{N} \sum_{jj'} \exp(-i\mathbf{Q} \cdot \mathbf{R}_{j'}(0)) \exp(i\mathbf{Q} \cdot \mathbf{R}_j(t))$$

## Scattering function

$$S(\mathbf{Q}, \omega) = \frac{1}{2\pi\hbar} \int I(\mathbf{Q}, t) e^{-i\omega t} dt$$



## Differential scattering cross-section

$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{\sigma_{scat}}{4\pi} \frac{k_f}{k_i} N S(\mathbf{Q}, \omega)$$

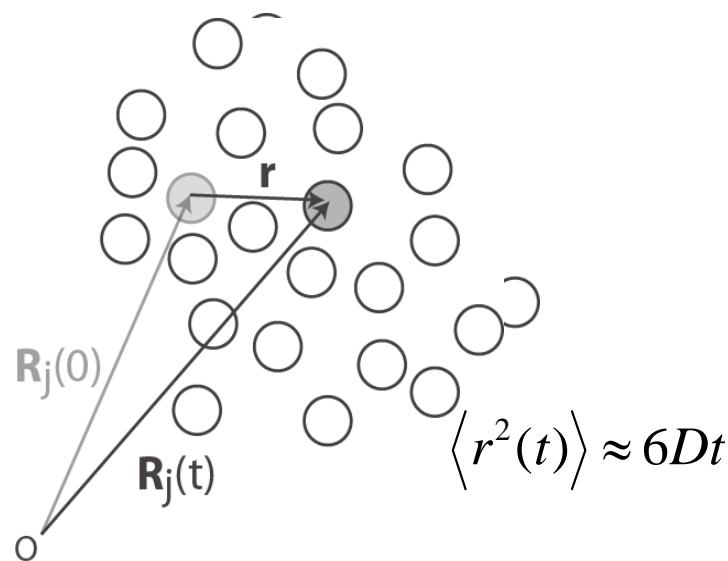
# Nuclear (lattice) excitations

Neutron scattering measures simultaneously the wavevector and energy of **collective excitations** → dispersion relation,  $\omega(\mathbf{q})$   
In addition, **local excitations** can of course be observed

- **Commonly studied excitations**
  - Phonons
  - Librations and vibrations in molecules
  - Diffusion
  - Collective modes in glasses and liquids
- **Excitations can tell us about**
  - Interatomic potentials & bonding
  - Phase transitions & critical phenomena (soft modes)
  - Fluid dynamics
  - Momentum distributions & superfluids (eg. He)
  - Interactions (eg. electron-phonon coupling)

# Atomic diffusion

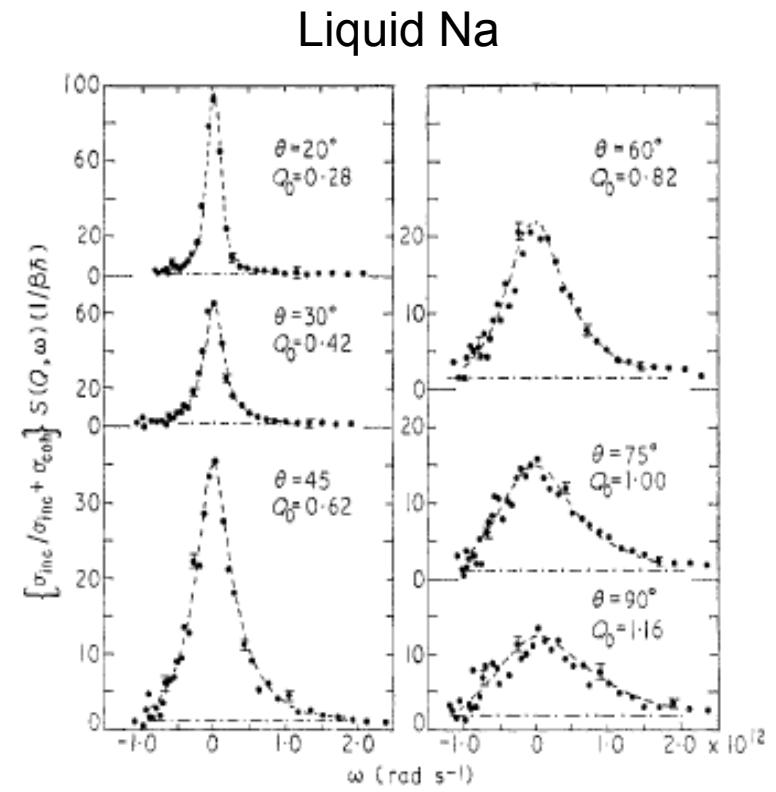
For long times compared to the collision time, atom diffuses



Auto-correlation function

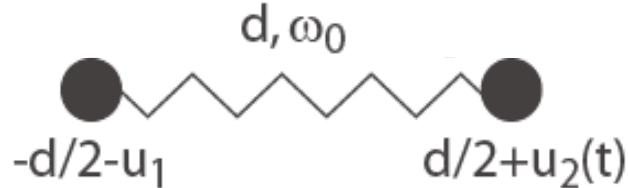
$$G_s(r,t) = \left\{ 6\pi \langle r^2(t) \rangle \right\}^{-3/2} \exp \left( -\frac{r^2}{6\langle r^2(t) \rangle} \right)$$

$$S(Q,\omega) = \frac{1}{\pi\hbar} \exp \left( \frac{\hbar\omega}{2k_B T} \right) \frac{DQ^2}{\omega^2 + (DQ^2)^2}$$



Cocking, J. Phys. C **2**, 2047 (1969)..

# Diatom



$$R_1(0) = -\frac{d}{2} - u(0)$$

$$R_2(t) = \frac{d}{2} + u(t)$$

$$u(t) = \sqrt{\frac{\hbar}{2M\omega_0}} [\hat{a}e^{-i\omega_0 t} + \hat{a}^+e^{i\omega_0 t}]$$

$$S(Q, \omega) = \frac{1}{2\pi\hbar N} \int_{-\infty}^{\infty} dt e^{-i\omega t} \sum_{jj'} \langle \exp(-iQR_{j'}(0)) \exp(iQR_j(t)) \rangle$$

$$S(Q, \omega) = \frac{1}{2\pi\hbar} e^{-Q^2 \langle u^2 \rangle} \int_{-\infty}^{\infty} dt e^{-i\omega t} [e^{Q^2 \langle u(0)u(t) \rangle} + \cos(Qd)e^{-Q^2 \langle u(0)u(t) \rangle}]$$

SHO correlation functions

$$\langle u^2 \rangle = \frac{\hbar}{2M\omega_0} \coth(\hbar\omega_0\beta)$$

$$\langle u(0)u(t) \rangle = \frac{\hbar}{2M\omega_0} \left[ \left( 1 + \frac{1}{e^{\hbar\omega_0\beta} - 1} \right) e^{i\omega_0 t} + \frac{1}{e^{\hbar\omega_0\beta} - 1} e^{-i\omega_0 t} \right] = \frac{\hbar}{2M\omega_0} \frac{\cosh\omega_0(it + \hbar\beta/2)}{\sinh(\hbar\omega_0\beta/2)}$$

$$e^{y \cosh x} = \sum_{n=-\infty}^{\infty} I_n(y) e^{nx}$$

$$y = \frac{\hbar Q^2}{2M\omega_0} \operatorname{csch}\left(\frac{1}{2}\hbar\omega_0\beta\right)$$

# Diatomeric molecule

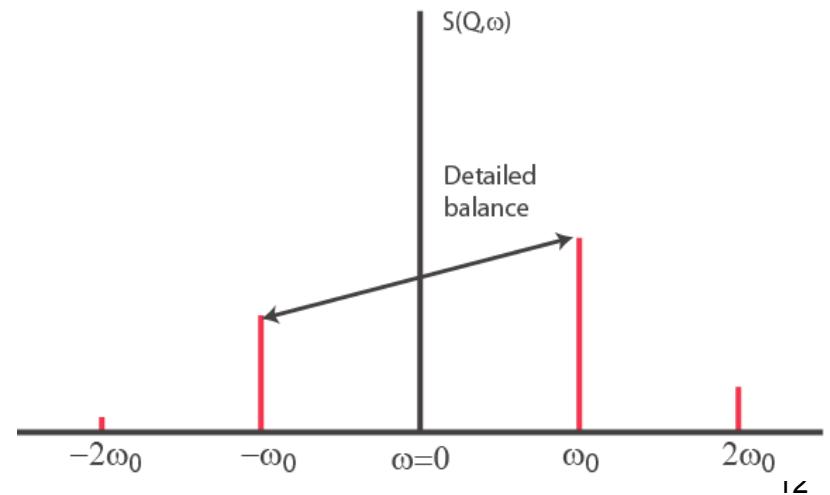
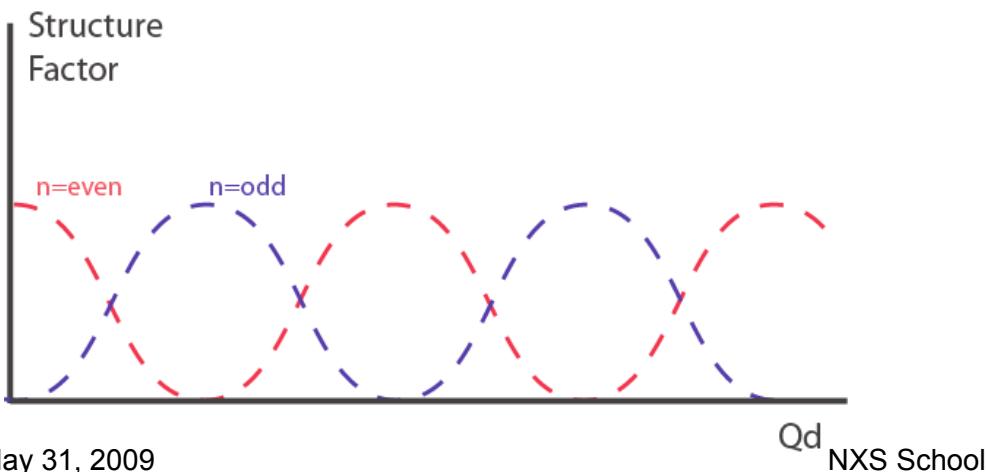
$$S(Q, \omega) = \frac{1}{\hbar} e^{-Q^2 \langle u^2 \rangle} e^{\hbar \omega \beta / 2} \sum_{n=-\infty}^{\infty} [1 + (-1)^n \cos(Qd)] I_n(y) \delta(\omega - n\omega_0)$$

Debye-Waller      Detailed balance      Structure factor      Form factor      Excitation energy

Small-amplitude approximation,  $y$  small

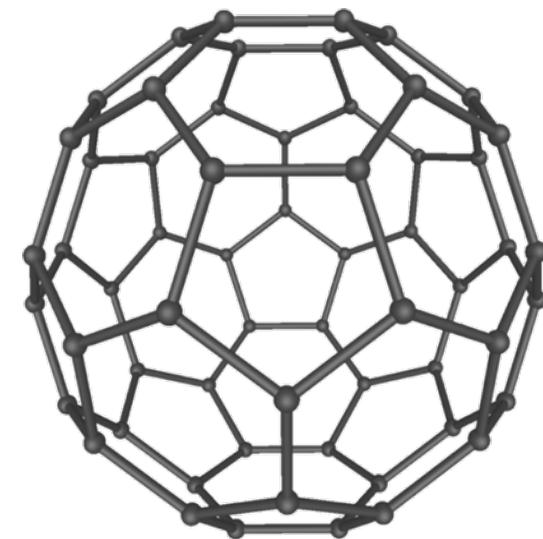
$$S(Q, \omega) \approx \frac{1}{\hbar} e^{-Q^2 \langle u^2 \rangle} \left\{ [1 + \cos(Qd)] \delta(\omega) + \frac{Q^2}{2M\omega_0} [1 - \cos(Qd)] \left[ \left( \frac{1}{2} \pm \frac{1}{2} + n(\omega_0) \right) \delta(\omega \mp m\omega_0) \right] + \dots \right\}$$

Elastic scattering      One quantum      Multi-quaanta

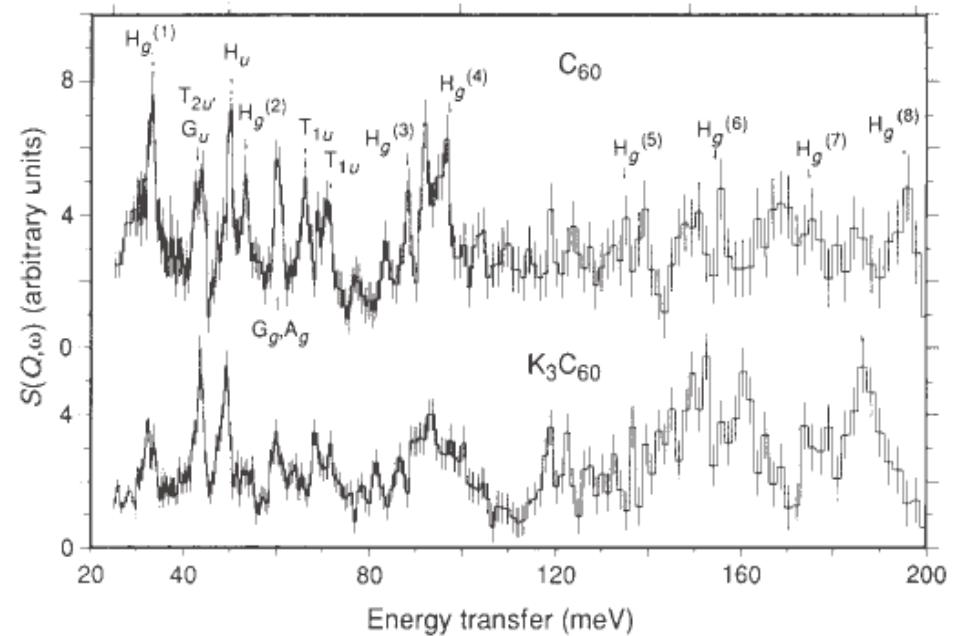


# Molecular vibrations

- Large molecule, many normal modes
- Harmonic vibrations can determine interatomic potentials



C<sub>60</sub> molecule



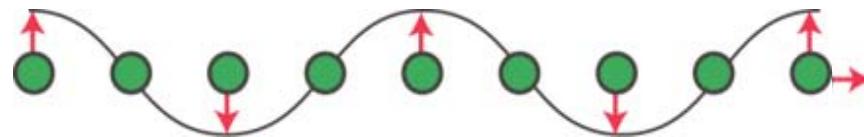
Prassides *et al.*, *Nature* **354**, 462 (1991).

# Phonons

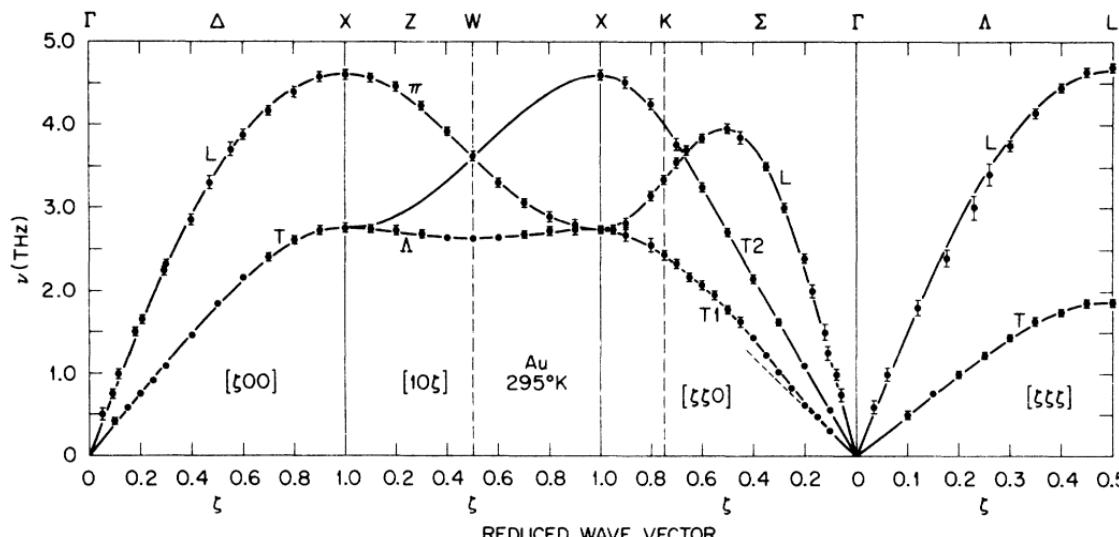
- Normal modes in periodic crystal → wavevector

$$\mathbf{u}(l,t) = \frac{1}{\sqrt{NM}} \sum_{j\mathbf{q}} \epsilon_j(\mathbf{q}) \exp(i\mathbf{q} \cdot \mathbf{l}) \hat{B}(\mathbf{q}, t)$$

- Energy of phonon depends on  $\mathbf{q}$  and polarization



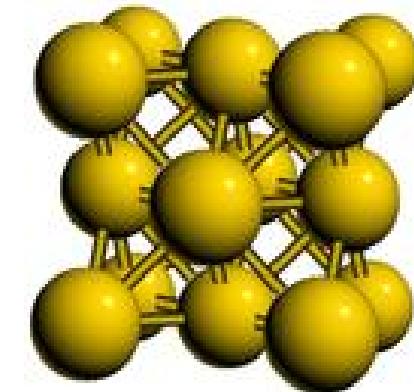
Longitudinal mode



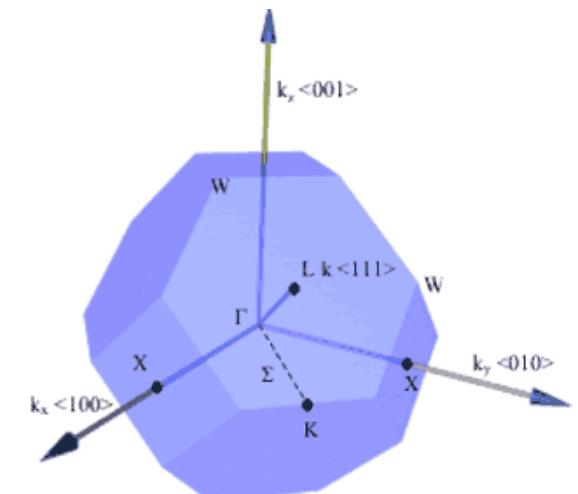
May 31, 2009

Lynn, et al., Phys. Rev. B 8, 3493 (1973).

NXS School



FCC structure



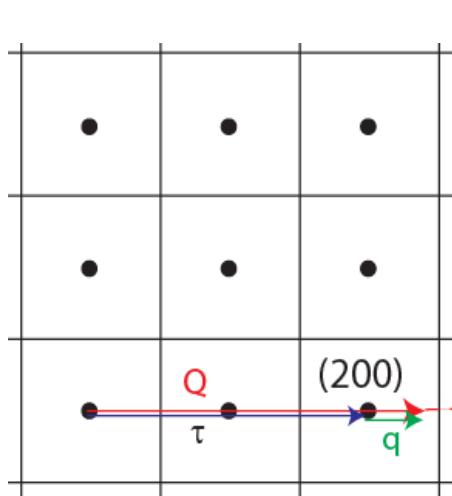
FCC Brillouin zone

14

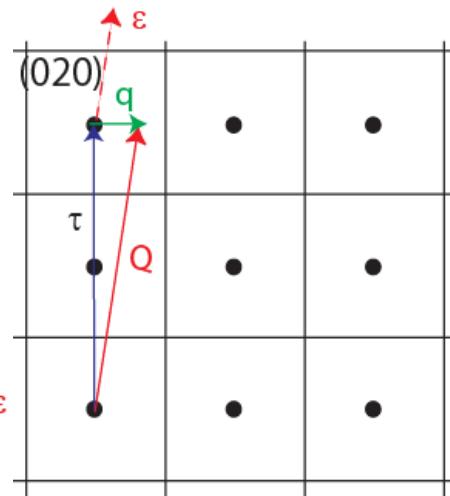
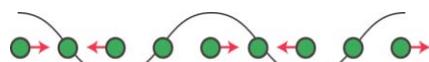
# Phonon intensities

$$S_{1+}(\mathbf{Q}, \omega) = \frac{1}{2NM} e^{-Q^2 \langle u^2 \rangle} \sum_{j\mathbf{q}} \frac{|\mathbf{Q} \cdot \boldsymbol{\varepsilon}_j(\mathbf{q})|^2}{\omega_j(\mathbf{q})} (1 + n(\omega)) \delta(\mathbf{Q} - \mathbf{q} - \boldsymbol{\tau}) \delta(\omega - \omega_j(\mathbf{q}))$$

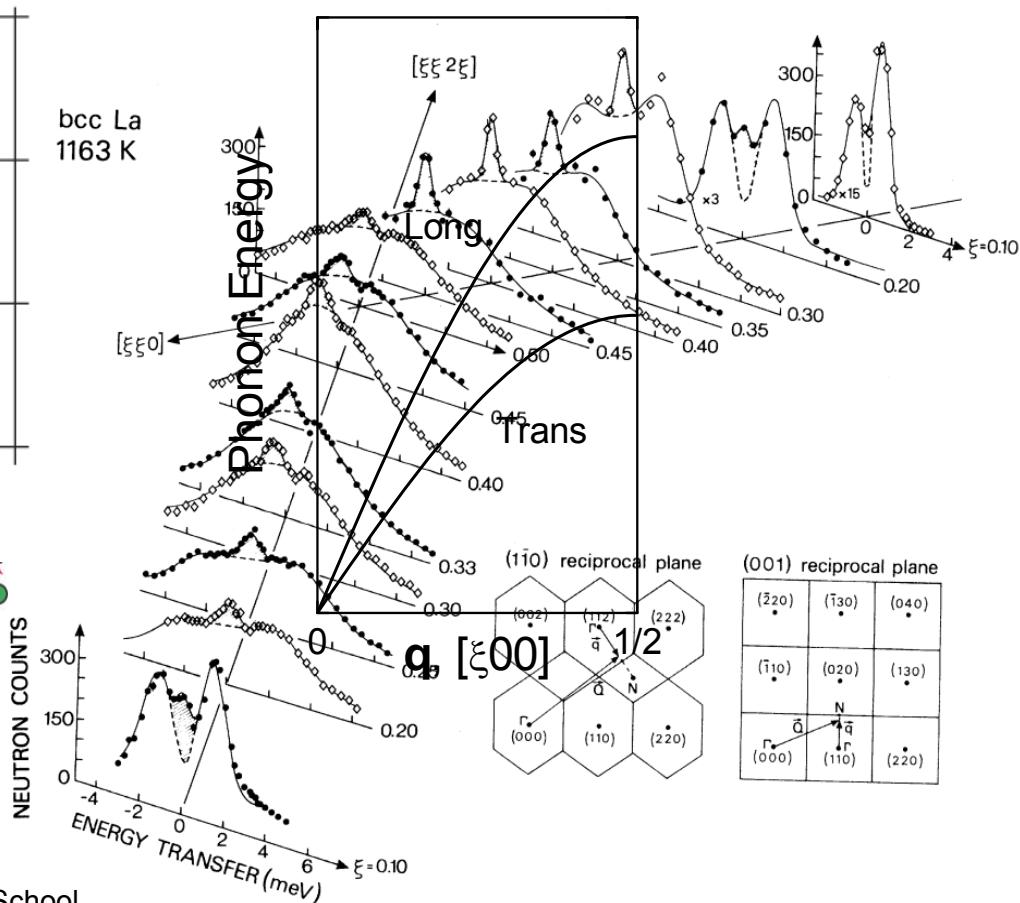
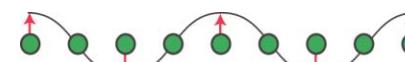
Structure (polarization) factor



## Longitudinal scan, $\mathbf{q} \parallel \boldsymbol{\varepsilon}$



Transverse scan,  $\mathbf{q} \perp \boldsymbol{\varepsilon}$

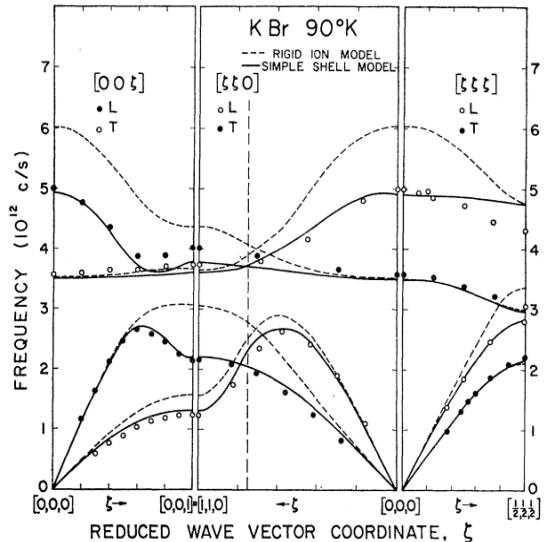


May 31, 2009

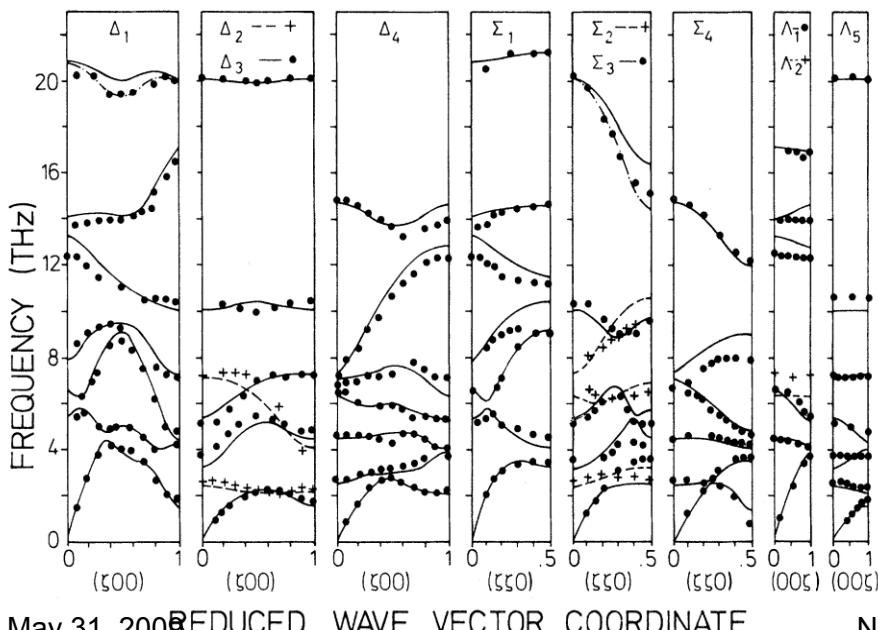
NXS School

Guthoff et al., Phys. Rev. B 47, 2563 (1993).

# More complicated structures

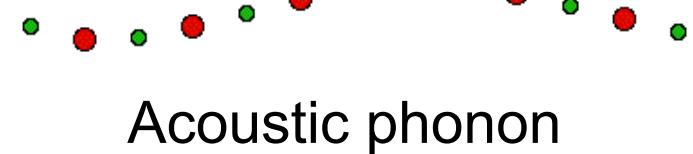


Woods, et al., Phys. Rev. **131**, 1025 (1963).

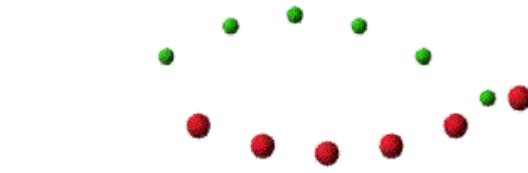


May 31, 2008 REDUCED WAVE VECTOR COORDINATE NXS School

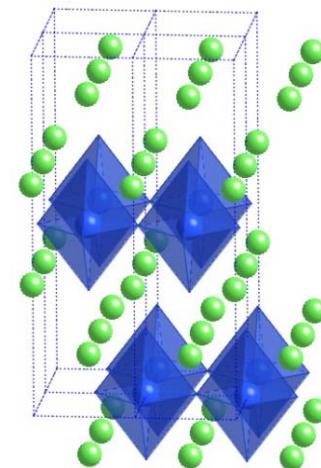
Chaplot, et al., Phys. Rev. B **52**, 7230(1995).



Acoustic phonon

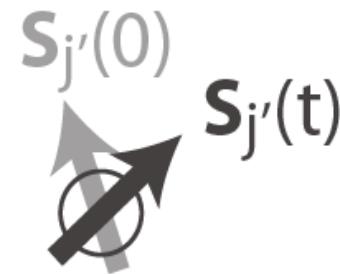


Optical phonon



$\text{La}_2\text{CuO}_4$

# Spin correlation functions



$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{k_f}{k_i} \left[ \frac{1}{2} \gamma_0 g F(Q) \right]^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \sum_{jj'} e^{i\mathbf{Q} \cdot (\mathbf{R}_{j'} - \mathbf{R}_j)} \frac{1}{2\pi\hbar} \int dt e^{-i\omega t} \langle S_j^\alpha(0) S_{j'}^\beta(t) \rangle$$

Scattering cross-section      Dipole interaction      Spin-spin correlation function

$$\left. \frac{d^2\sigma}{d\Omega dE_f} \right|_{inel} = \frac{k_f}{k_i} \left[ \frac{1}{2} \gamma_0 g F(Q) \right]^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \left( 1 - e^{h\omega/kT} \right)^{-1} \frac{1}{\pi(g\mu_B)^2} \text{Im} \{ \chi^{\alpha\beta}(\mathbf{Q}, \omega) \}$$

The cross-section is proportional to the magnetic susceptibility, i.e. it is the response of the system to spatially & time varying magnetic field

# Spin excitations

- **Spin excitations**
  - Spin waves in ordered magnets
  - Paramagnetic & quantum spin fluctuations
  - Crystal-field & spin-orbit excitations
- **Magnetic inelastic scattering can tell us about**
  - Exchange interactions
  - Single-ion and exchange anisotropy (determine Hamiltonian)
  - Phase transitions & critical phenomena
  - Quantum critical scaling of magnetic fluctuations
  - Other electronic energy scales (eg. CF & SO)
  - Interactions (eg. spin-phonon coupling)

# Paramagnetic scattering

$$\langle S_j^\alpha S_{j'}^\beta \rangle = 0 \quad (j \neq j')$$

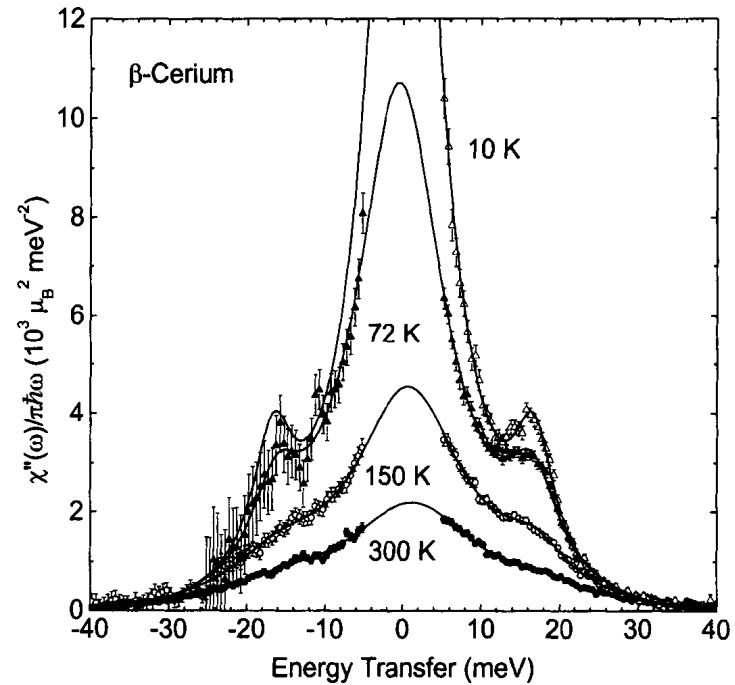
Single ion scattering

$$\langle S_j^z(0)S_j^z(t) \rangle = \langle (S_j^z)^2 \rangle e^{-\Gamma t} = \frac{1}{3} \langle (\mathbf{S}_j)^2 \rangle e^{-\Gamma t} = \frac{1}{3} S(S+1) e^{-\Gamma t}$$

$$\frac{\text{Im}\{\chi^{zz}(0,\omega)\}}{\pi\hbar\omega} = \frac{g^2 S(S+1) \mu_B^2}{3k_B T} \frac{1}{\pi} \frac{\Gamma}{\Gamma^2 + (\hbar\omega)^2}$$

- Inverse width,  $1/\Gamma$ , gives relaxation time
- Note crystal field excitation

$$\chi_0 = \int_{-\infty}^{\infty} \frac{\text{Im}\{\chi^{zz}(0,\omega)\}}{\pi\hbar\omega} d\omega = \frac{g^2 S(S+1) \mu_B^2}{3k_B T}$$



McQueeney *et al.*, *Phil. Mag. B* **81**, 675 (2001).

# Spin waves

$$H = - \sum_{\langle i,j \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

Heisenberg Hamiltonian

Linear spin wave theory

$$\begin{aligned} S^z &\approx S \\ S^\pm &= S^x \pm iS^y \end{aligned}$$

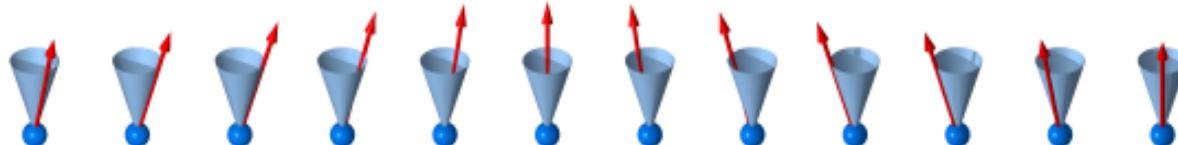
$$S_j^+(t) = \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{Q} \cdot \mathbf{R}_j} S_{\mathbf{q}}^+(t)$$

$$\langle S_j^\alpha(0) S_{j'}^\beta(t) \rangle = \langle S_j^-(0) S_{j'}^+(t) \rangle$$

For a simple ferromagnet

$$\langle S_{\mathbf{q}}^-(0) S_{\mathbf{q}}^+(t) \rangle = \frac{S}{2N} \left(1 - e^{-\hbar\omega/kT}\right)^{-1} e^{i\omega(\mathbf{q})t}$$

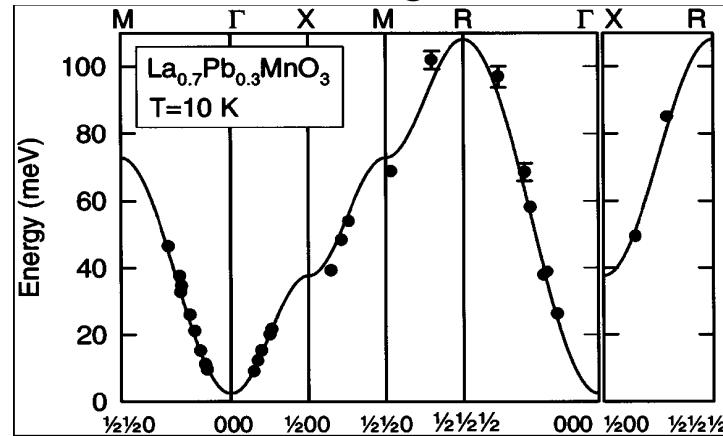
$$\frac{d^2\sigma}{d\Omega dE_f} = \frac{1}{2} \left(1 + \hat{Q}_z^2\right) \frac{k_f}{k_i} \left[ \frac{1}{2} g r_0 F(Q) \right]^2 \frac{S}{1 - e^{-\hbar\omega/kT}} \sum_{\mathbf{q}} \delta(\mathbf{Q} - \mathbf{q} - \boldsymbol{\tau}) \delta(\omega - \omega(\mathbf{q}))$$



Linear spin waves

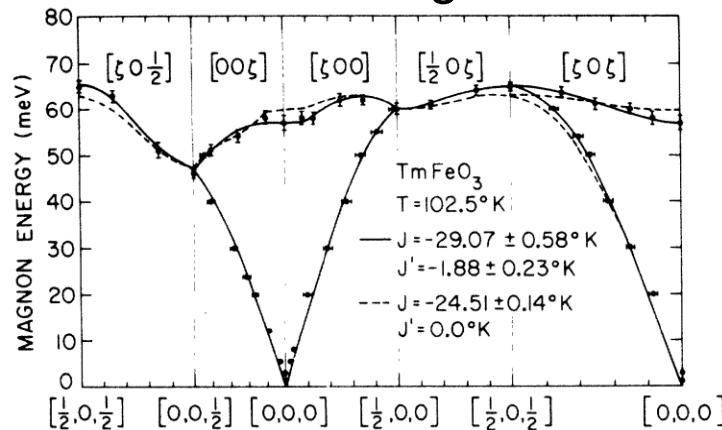
# Spin waves

## Ferromagnetic



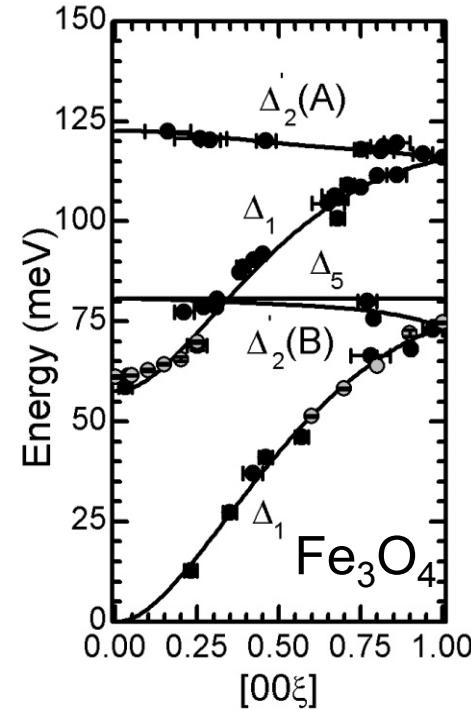
Perring *et al.*, Phys. Rev. Lett. **77**, 711 (1996).

## Antiferromagnetic



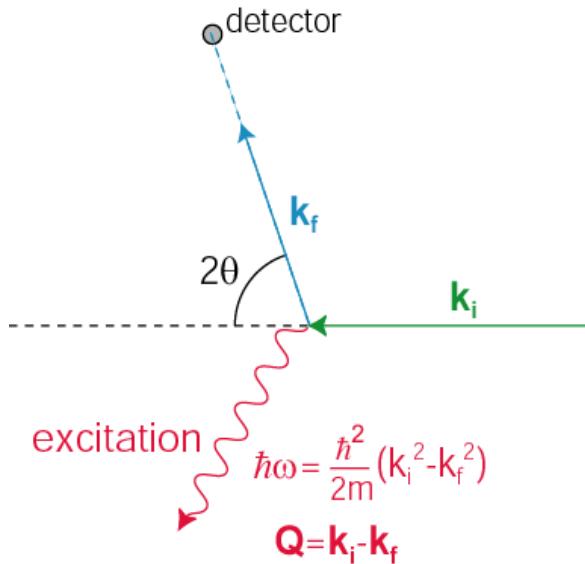
Shapiro *et al.*, Phys. Rev. B **10**, 2014 (1974).

## Ferrimagnetic

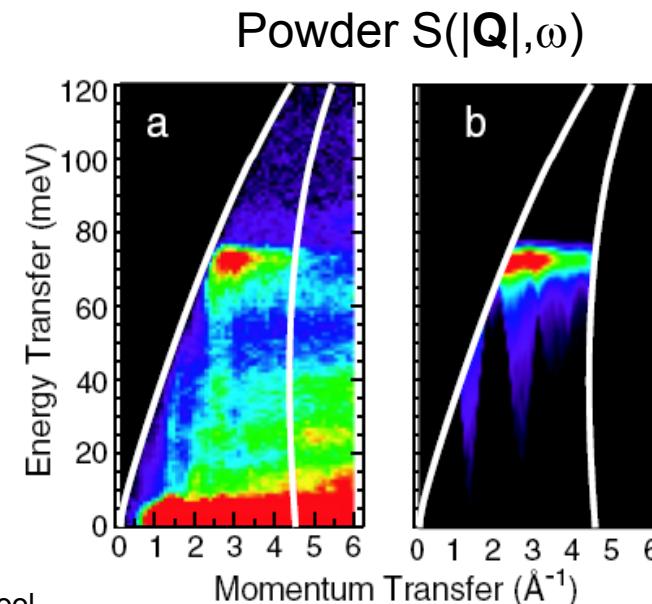
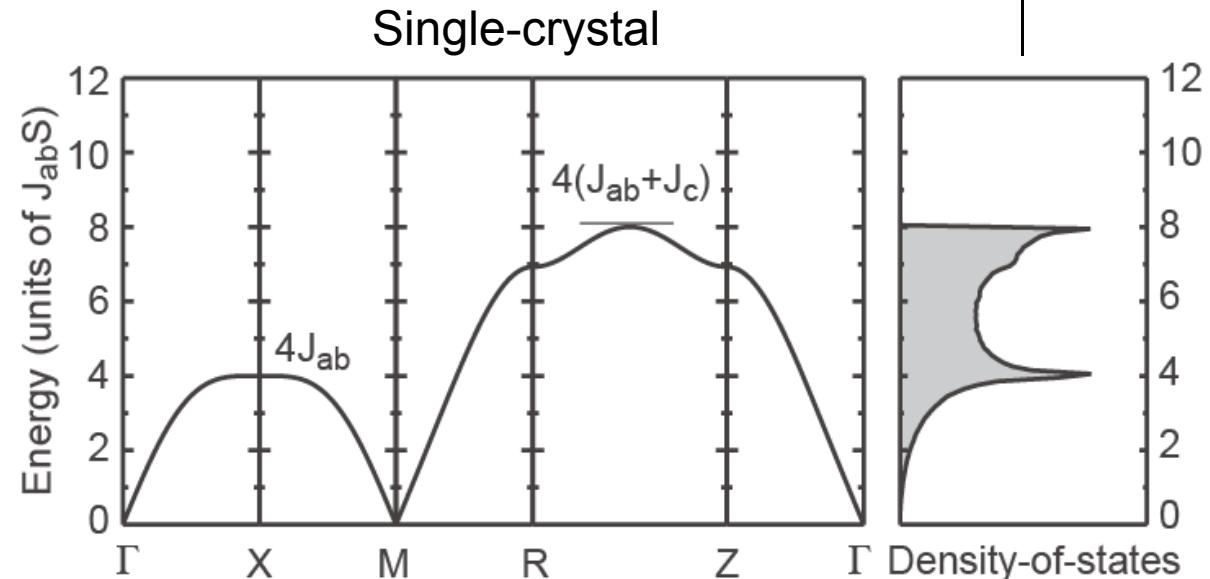


McQueeney *et al.*, Phys. Rev. Lett. **99**, 246401 (2007).

# Scattering experiments



Instrument and sample (powder or single-crystal) determine how  $(\mathbf{Q}, \omega)$  space is sampled



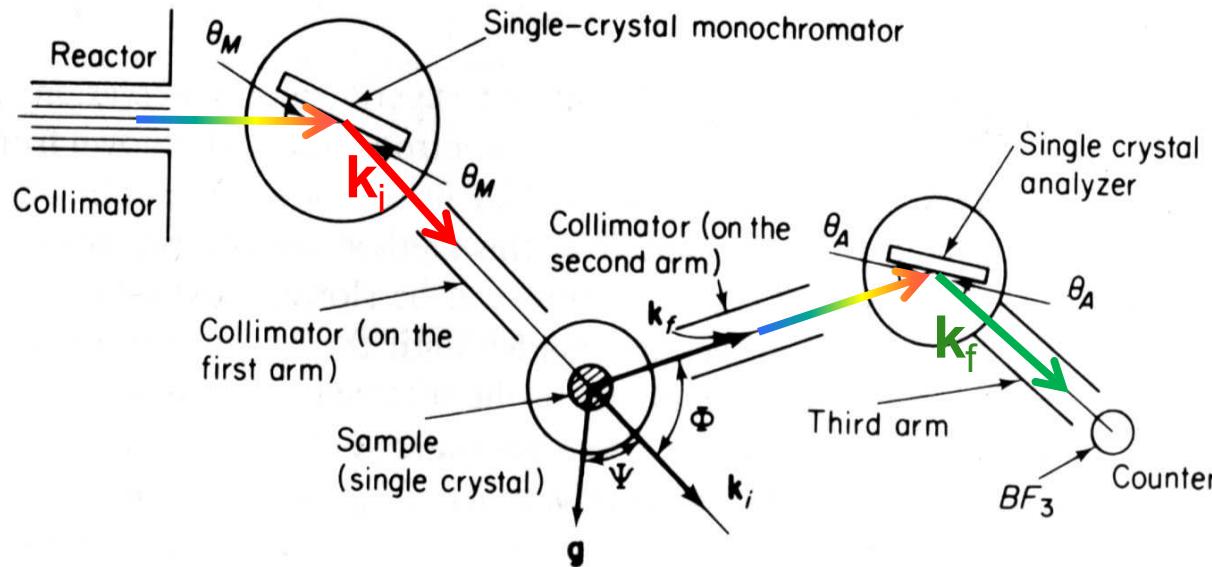
# Triple-axis instruments



High flux isotope reactor - ORNL

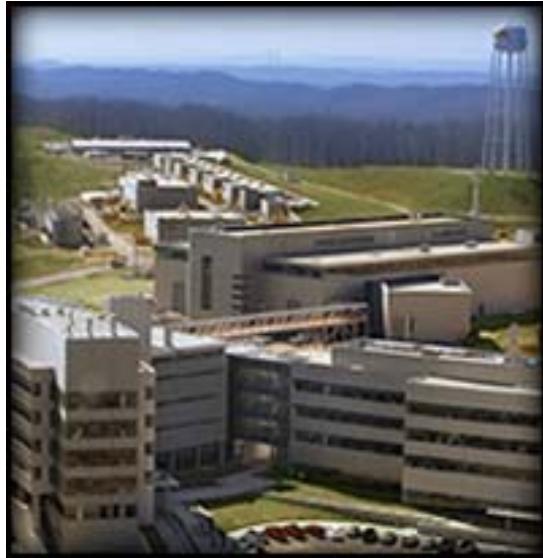


HB-1A 3-axis spectrometer



- Hardware flexibility
- Constant-Q (or E) scans
- Ideally suited for single-xtals

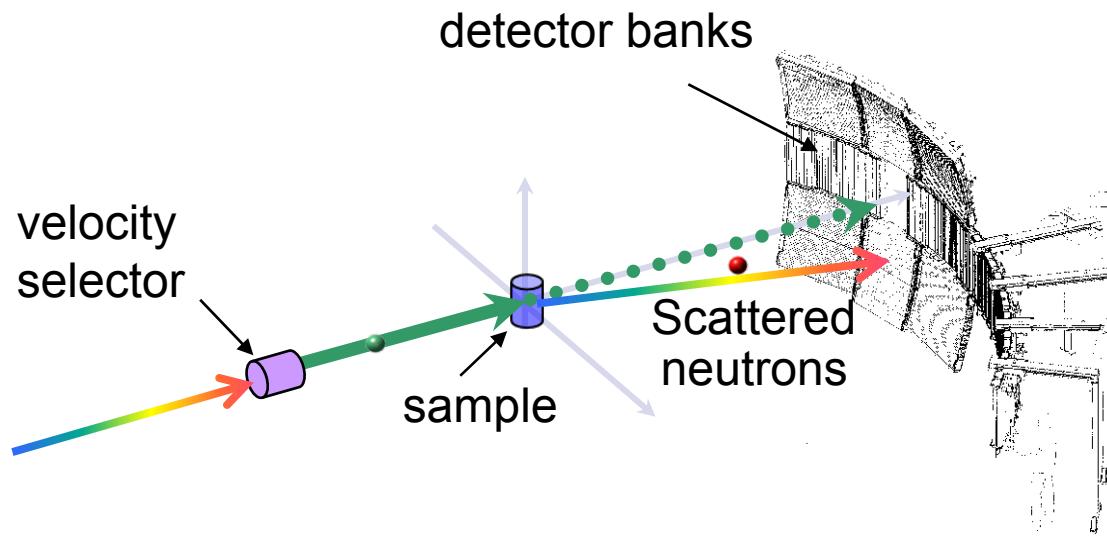
# Time-of-flight methods



Spallation neutron source

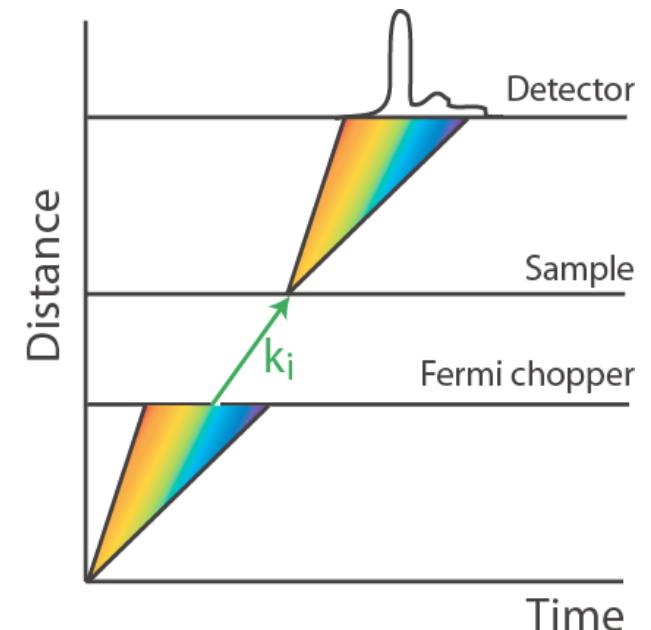


Pharos – Lujan Center



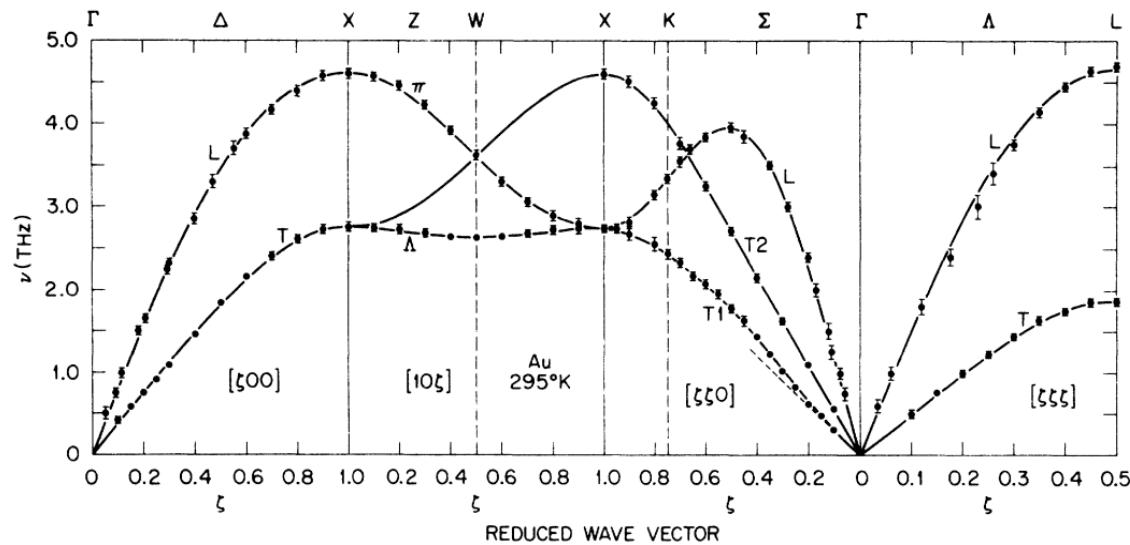
May 31, 2009

- Hardware inflexible
- Effective for powders
- Complicated  $Q, E$ -scans a challenge for single-xtals

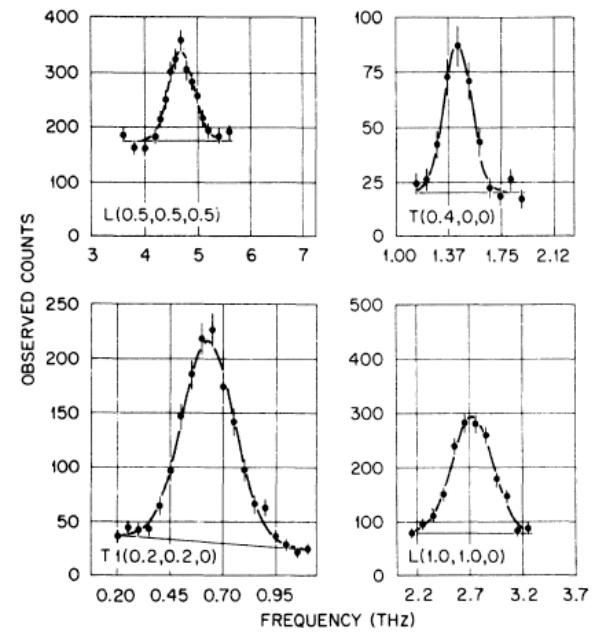


# INS data

- Intensities as a function of  $\mathbf{Q}$  and  $\omega$



Lynn, et al., *Phys. Rev. B* **8**, 3493 (1973).



# Reciprocal space

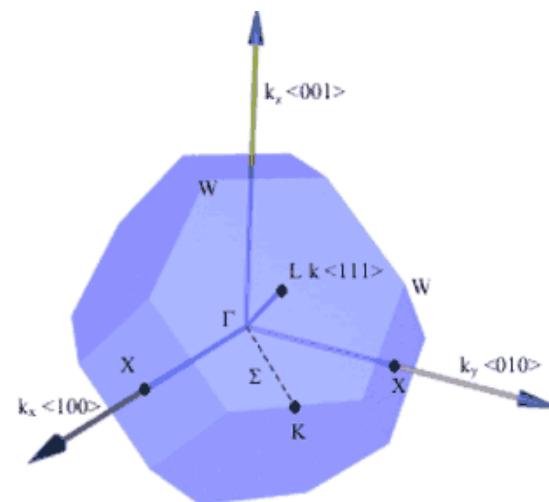
$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

$$\hbar\omega = E_i - E_f$$

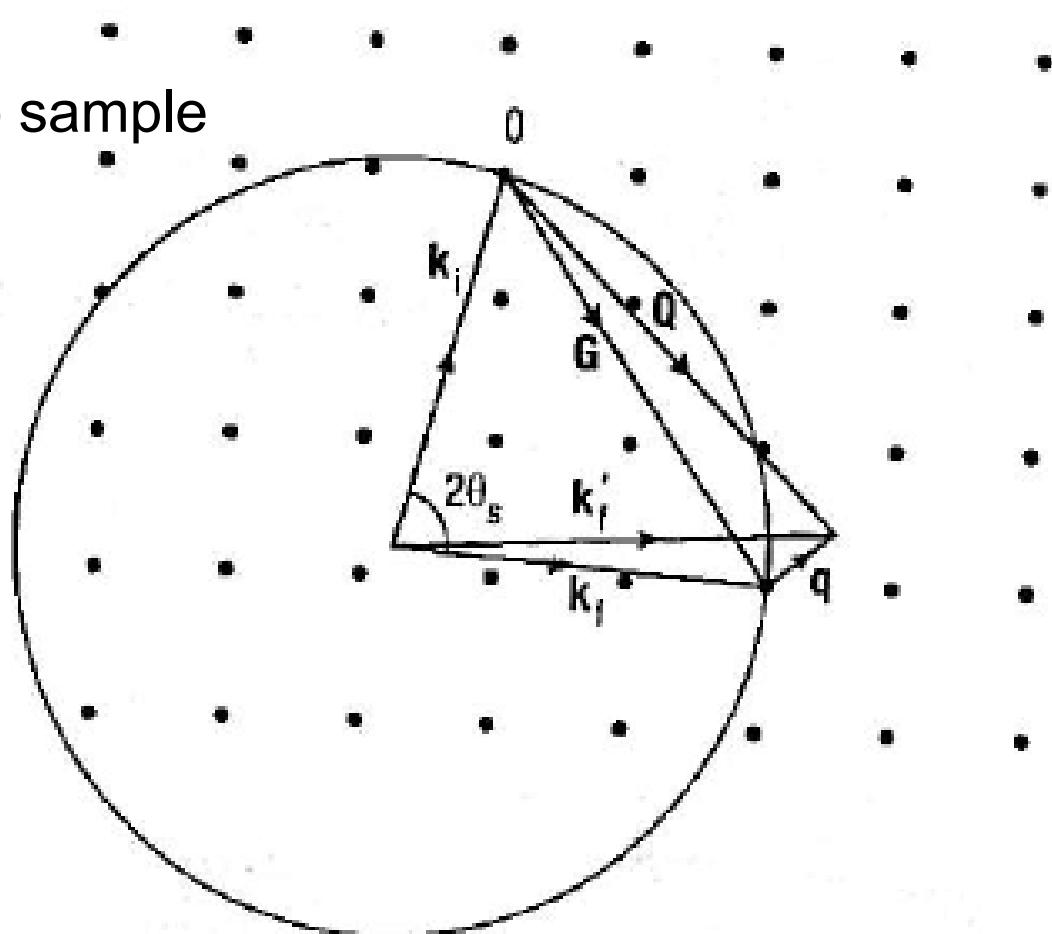
Momentum/energy transferred to sample

$$\mathbf{q} = \mathbf{Q} - \tau$$

Wavevector in 1<sup>st</sup>  
Brillouin zone



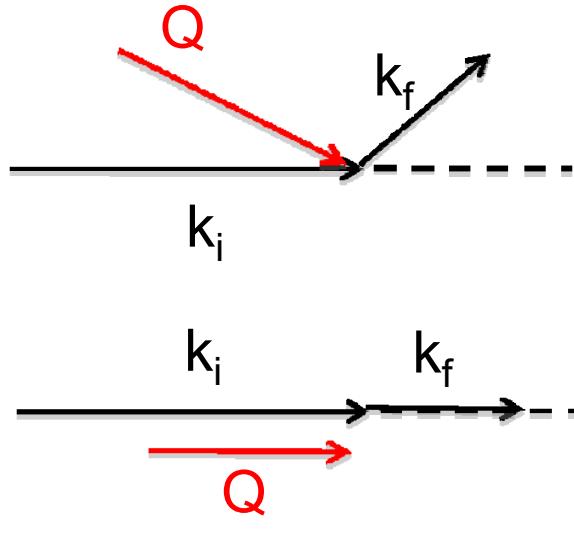
FCC Brillouin zone



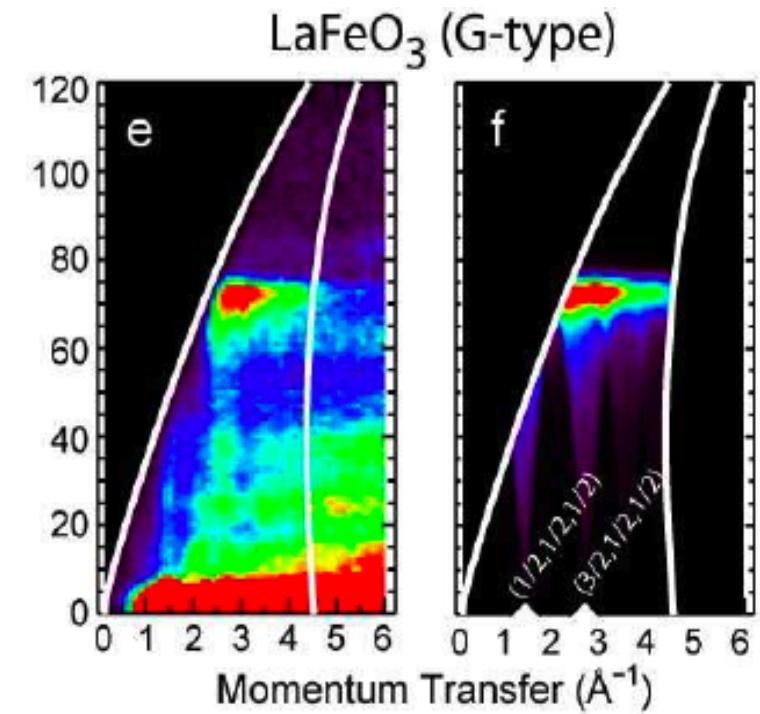
Scattering triangle

# Kinematic limitations

- Many combinations of  $k_i, k_f$  for same  $\mathbf{Q}, \omega$ 
  - Only certain configurations are used (eg.  $E_f$ -fixed)
- Cannot “close triangle” for certain  $\mathbf{Q}, \omega$  due to kinematics



Minimum accessible  $\mathbf{Q}$

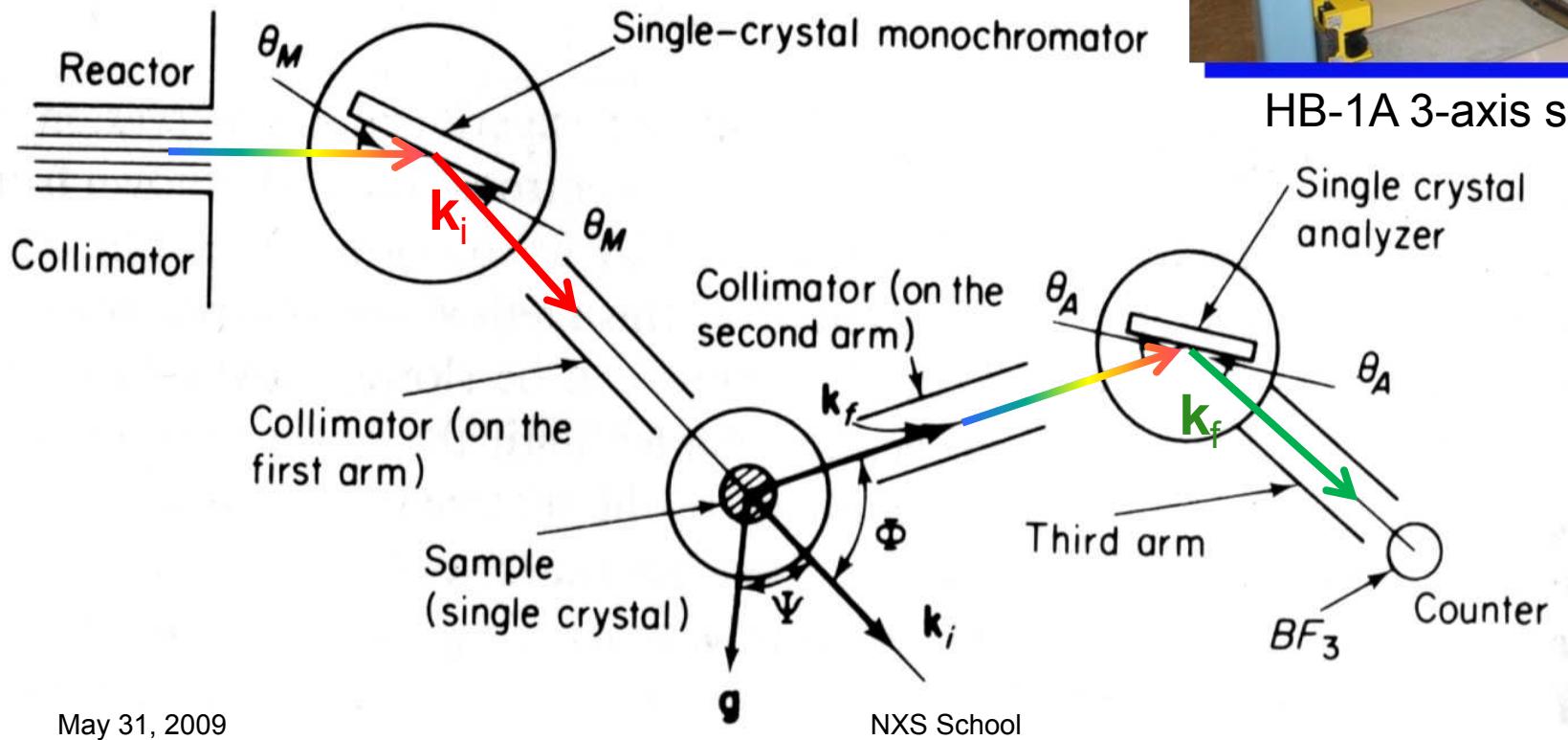


Kinematic limits,  $E_i = 160$  meV

# Triple-axis instruments

- Workhorse INS instrument

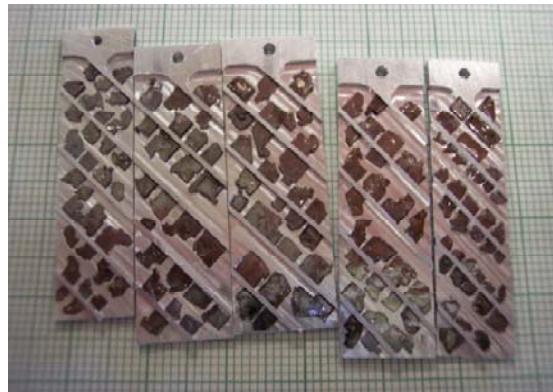
- $k_i, k_f$  defined by Bragg scattering
- Sample goniometer
- Detector
- Resolution/collimators



HB-1A 3-axis spectrometer

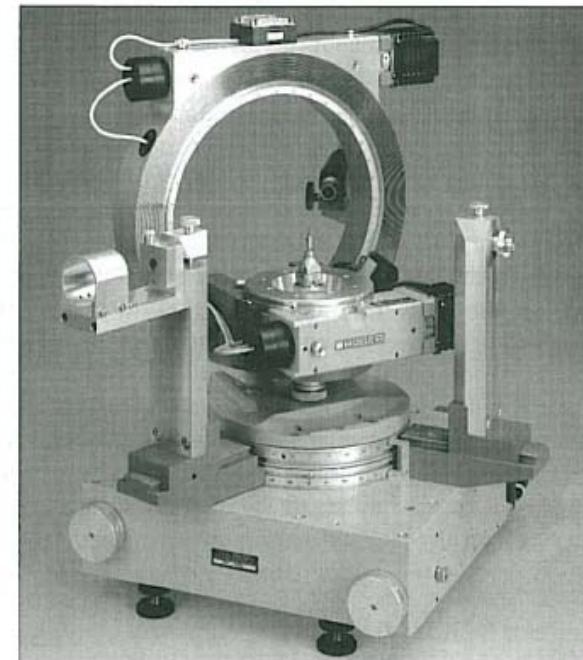
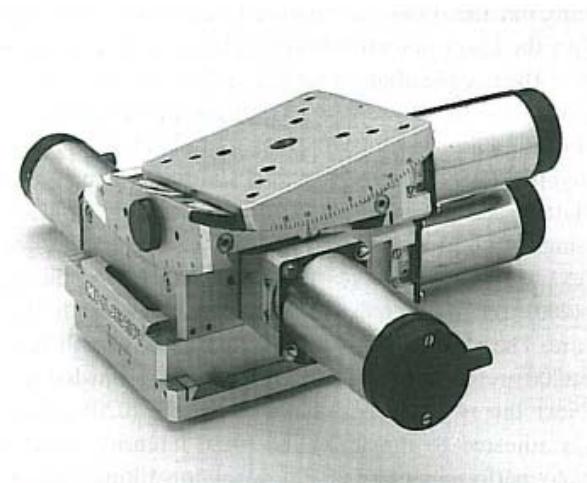
# Samples

- **Samples need to be BIG**
  - ~ gram or cc
  - Counting times are long (mins/pt)



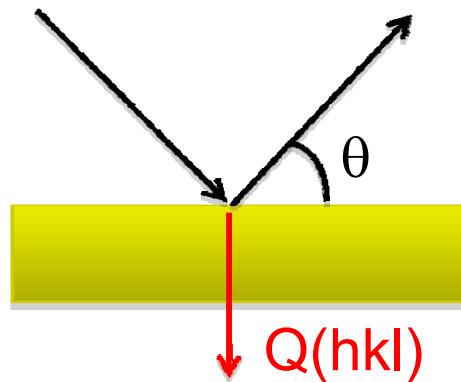
Co-aligned  $\text{CaFe}_2\text{As}_2$  crystals

- **Sample rotation**
- **Sample tilt**

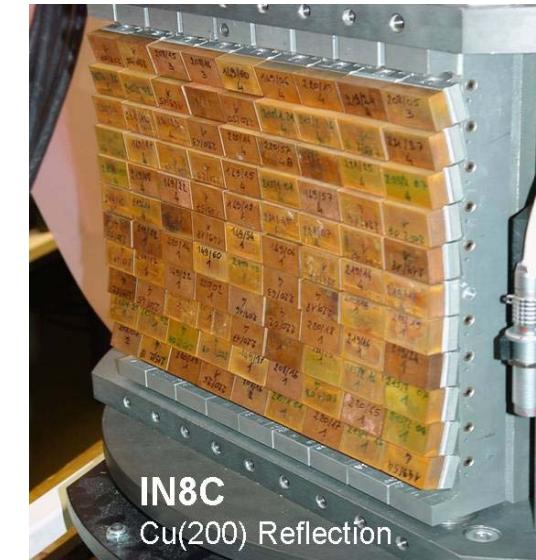


# Monochromators

- Selects the incident wavevector



$$Q(hkl) = \frac{2\pi}{d(hkl)} = 2k_i \sin \theta$$

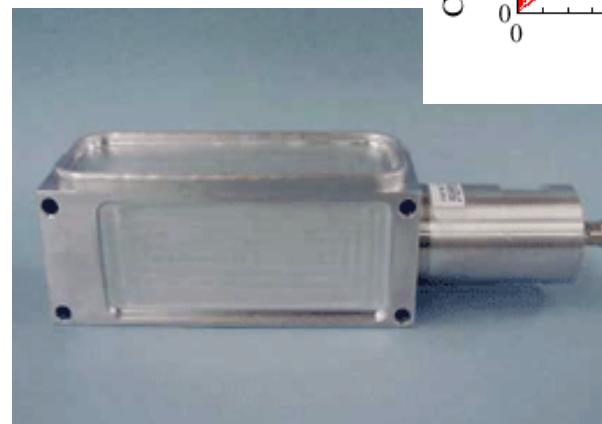
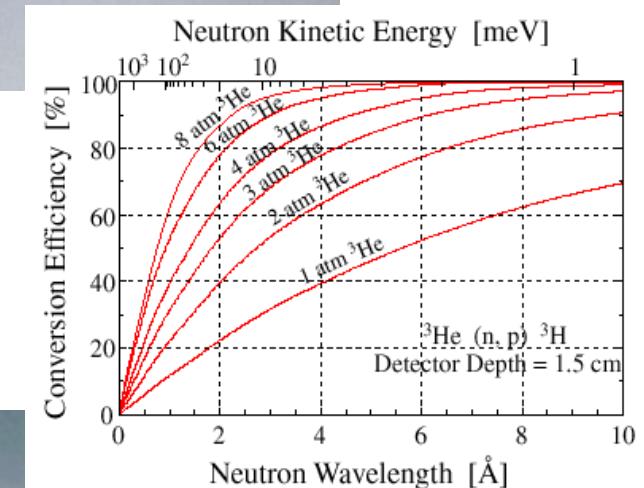


- Reflectivity
- focusing
- high-order contamination  
eg.  $\lambda/2$  PG(004)

Mono	d(hkl)	uses
PG(002)	3.353	General
Be(002)	1.790	High $k_i$
Si(111)	3.135	No $\lambda/2$

# Detectors

- **Gas Detectors**
- $n + {}^3\text{He} \rightarrow {}^3\text{H} + p + 0.764 \text{ MeV}$
- Ionization of gas
- $e^-$  drift to high voltage anode
- High efficiency
  
- **Beam monitors**
- Low efficiency detectors for measuring beam flux



# Other triple-axis stuff

- **Soller Collimators**

- Define beam divergence
- $Q, \omega$  resolution function

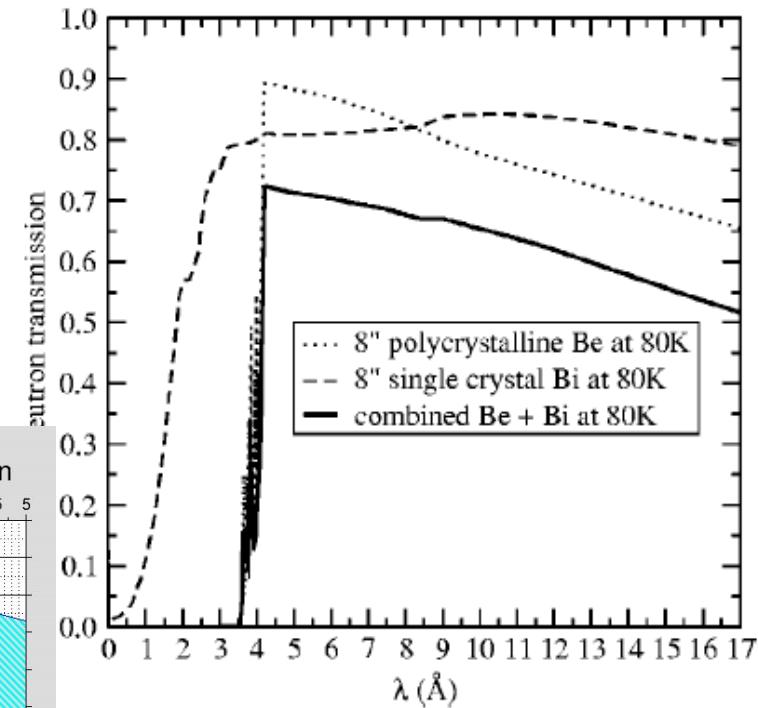
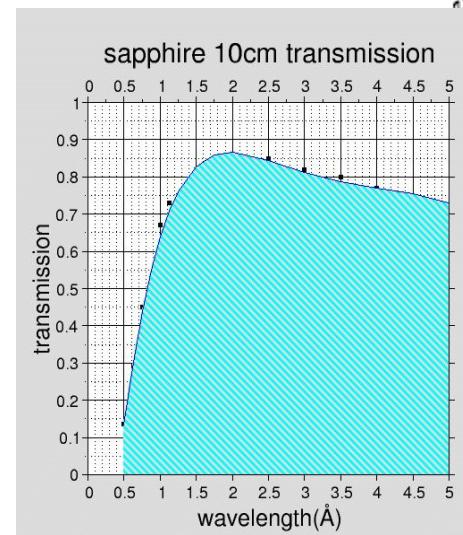


- **Filters**

- Xtal Sapphire: fast neutron background
- Poly Be: low-energy (5 meV) band pass
- PG: higher order contamination

- **Masks**

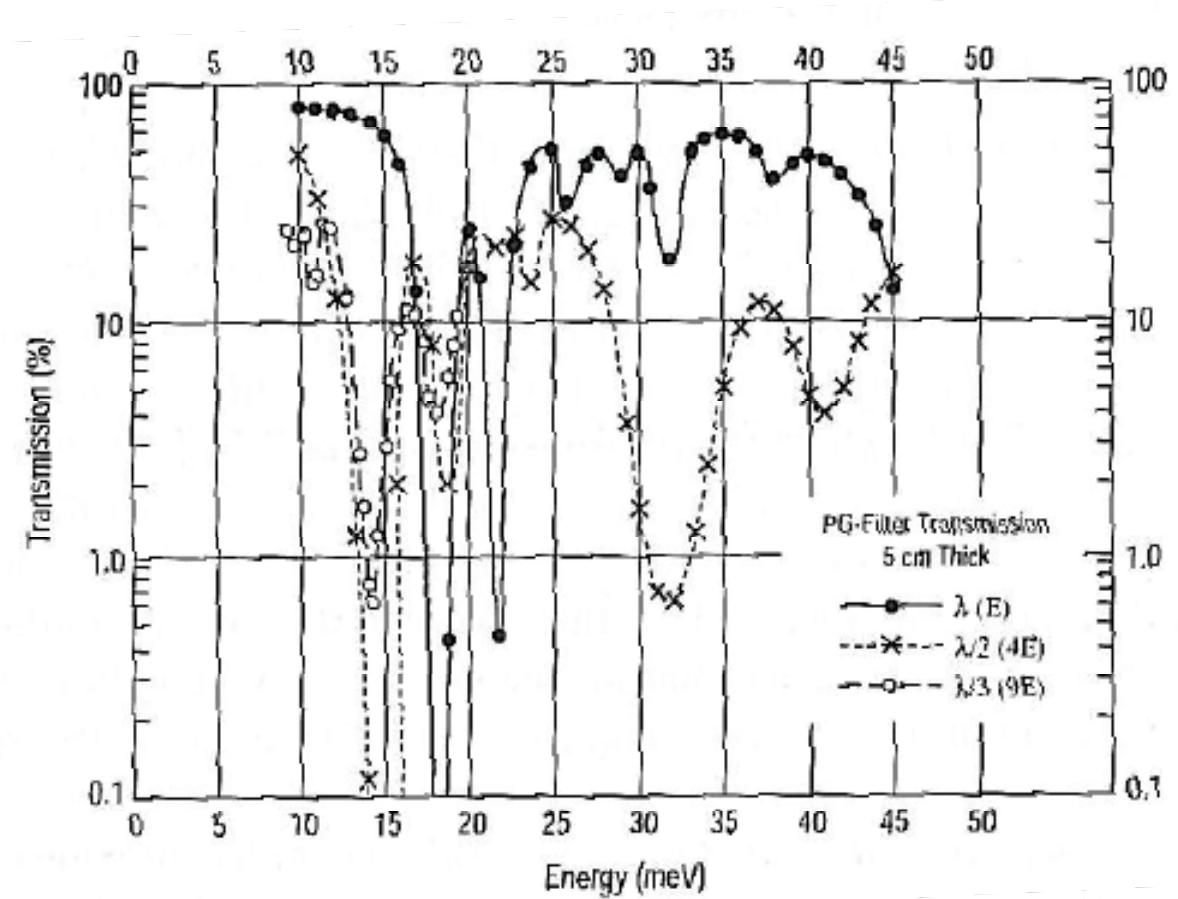
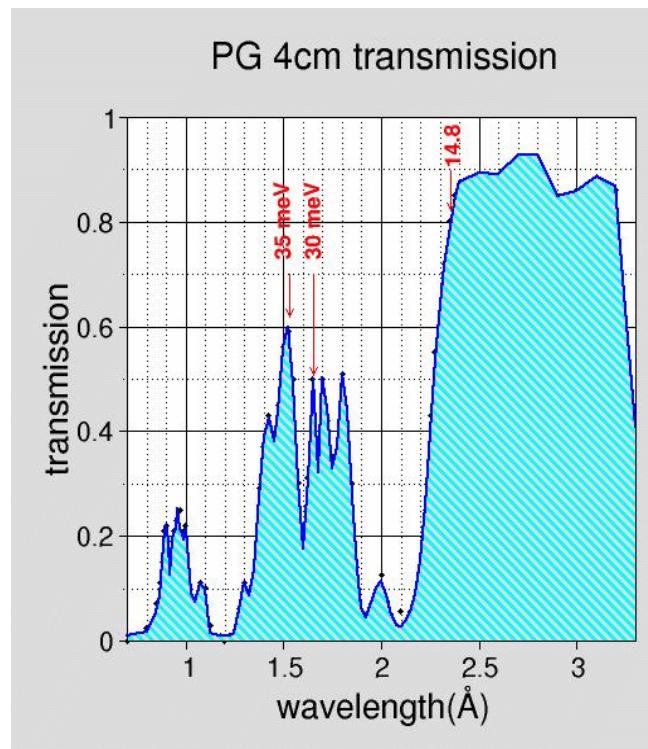
- Beam definition
- Background reduction



# PG filter

- Magic numbers

- Best filter for rejection of  $\lambda/2$  contamination
- $E_f = 13.7, 14.7, 30.5, 41$  meV



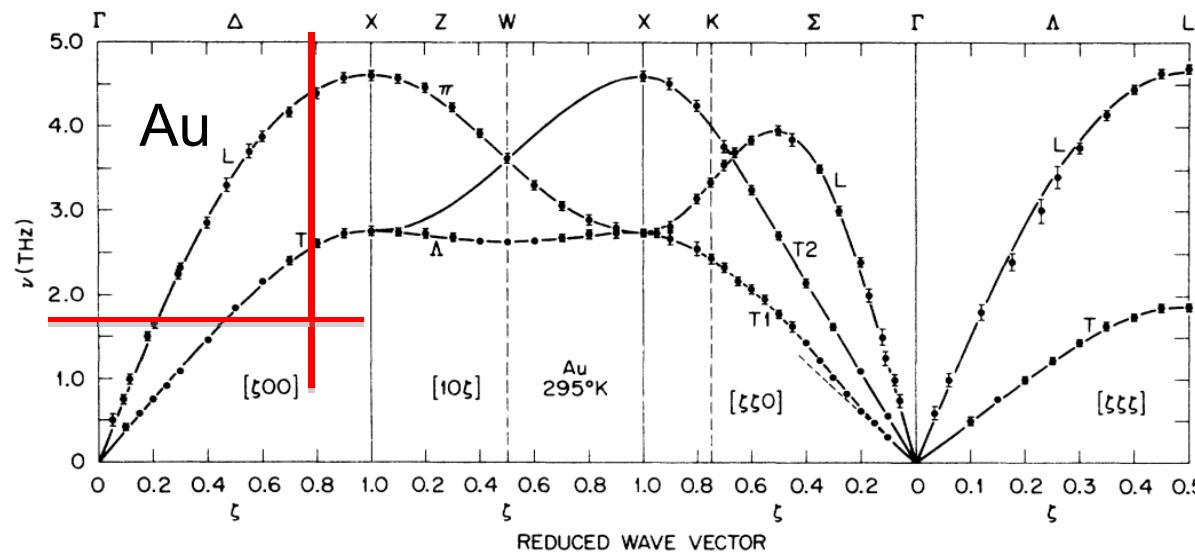
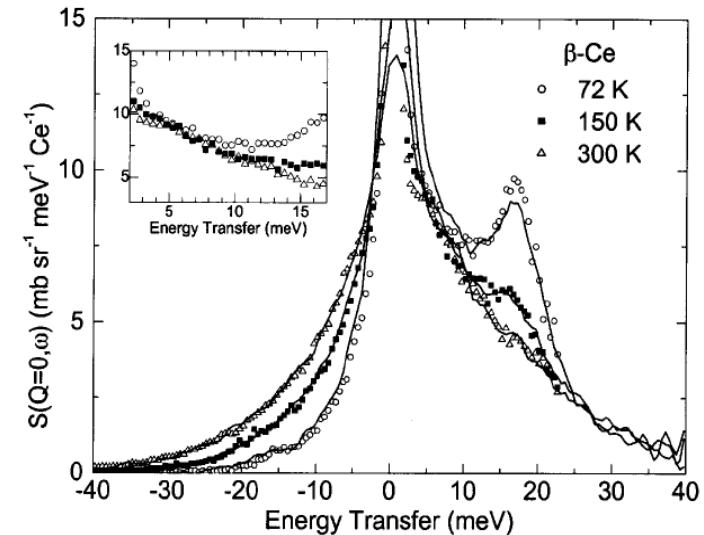
# Sample environment

- Temperature, field, pressure
- Heavy duty for large sample environment
  - CCR
  - He cryostats
  - SC magnets
  - ...

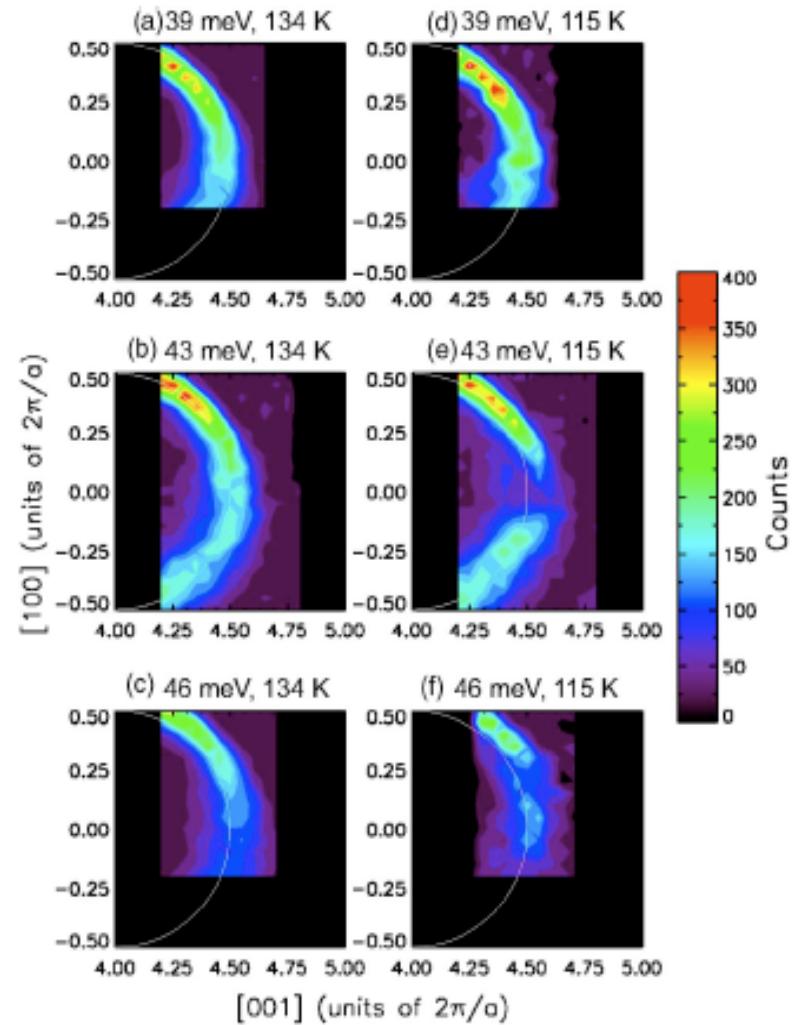
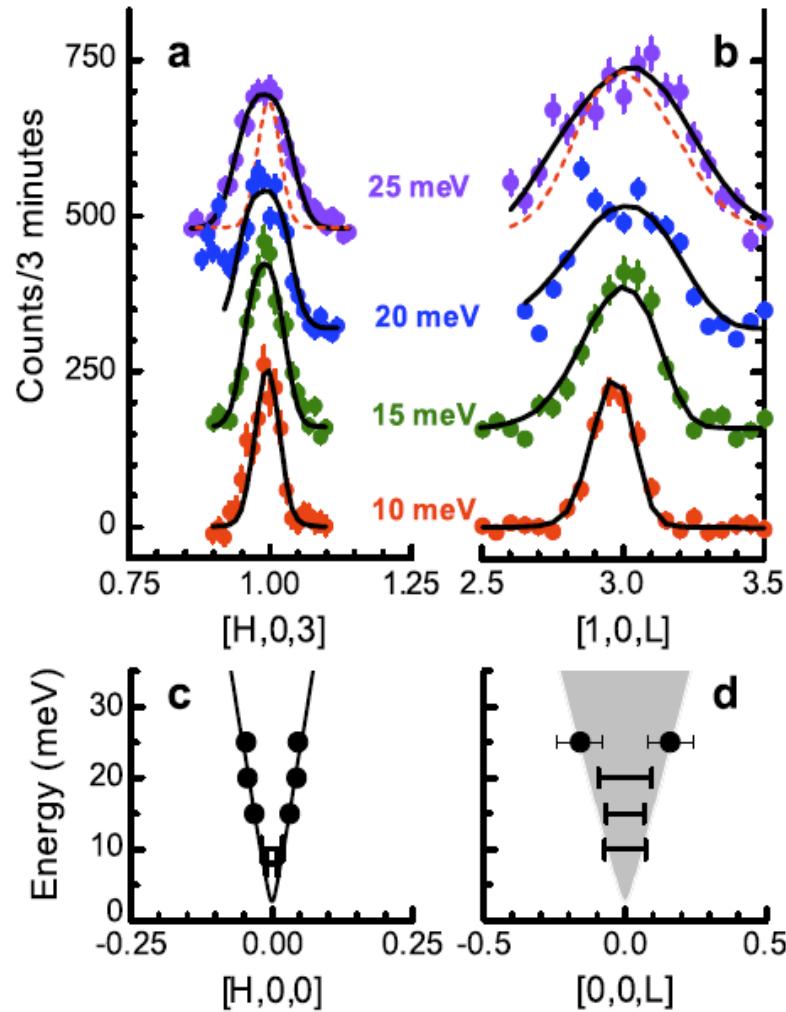


# Acquiring data

- Energy gain, energy loss
  - Detailed balance
- Constant-Q scans
  - Most common
- Constant- $\omega$  scans
  - Used for steep dispersions



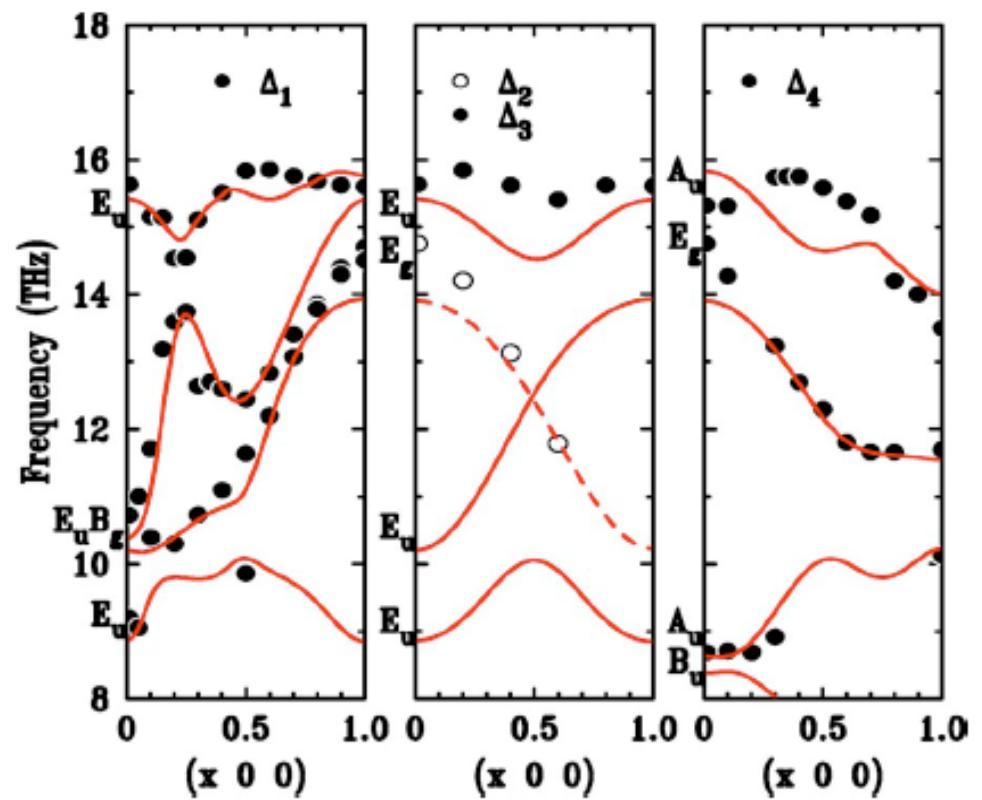
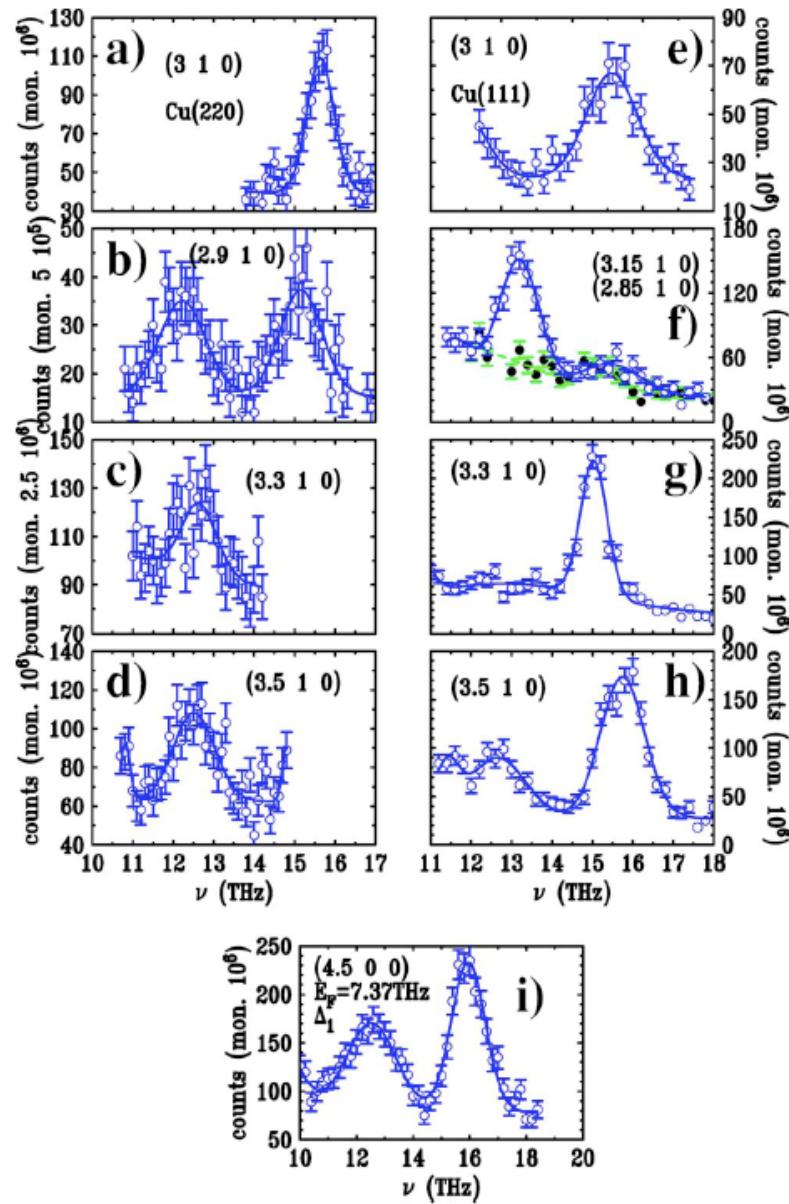
# Constant- $\omega$ scans



Steep AF spin waves in  $\text{CaFe}_2\text{As}_2$   
McQueeney et al, PRL 101, 227205 (2008)

Slice of spin wave cone in  $\text{Fe}_3\text{O}_4$   
McQueeney et al, PRB 73, 174409 (2006)

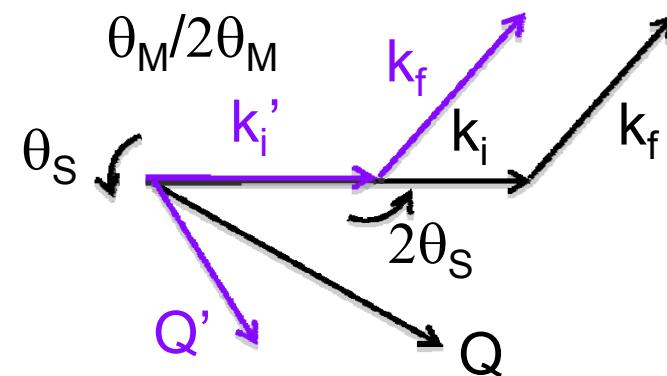
# Constant-Q scans



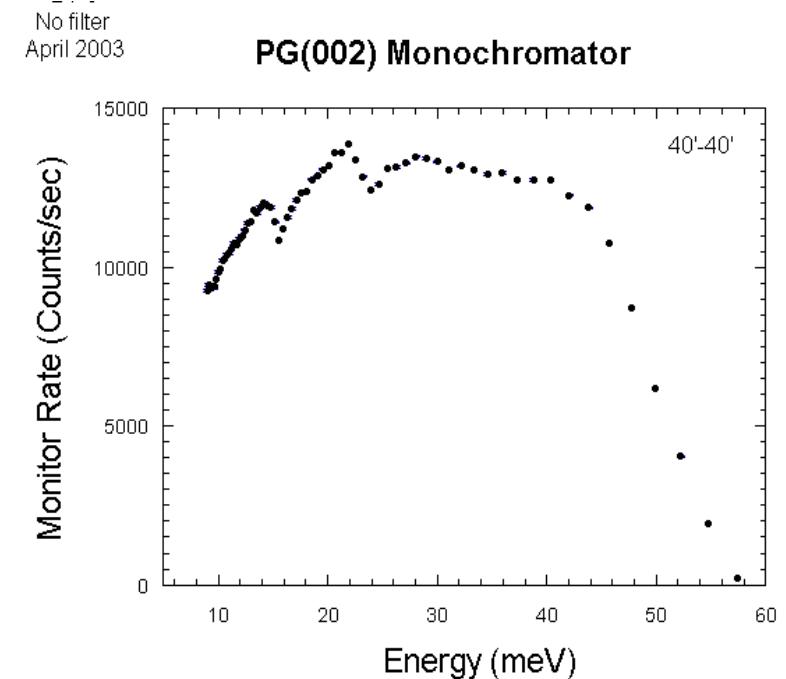
Optical phonons in  $\text{Nd}_{0.85}\text{Ce}_{0.15}\text{CuO}_4$   
 Braden, et al, PRB, 72 184517 (2005).

# Configurations

- **$E_f$ -fixed mode**
  - Mono moves during  $\omega$ -scan
  - Beam monitor accounts for variations in incident flux
- **$E_i$ -fixed mode**
  - Analyzer moves during  $\omega$ -scan
  - Useful for expts requiring low background
  - Analysis more complicated
- **Magic numbers**
  - $\lambda/2$  contamination
  - $E_i$  or  $E_f = 13.7, 14.7, 30.5, 41$  meV



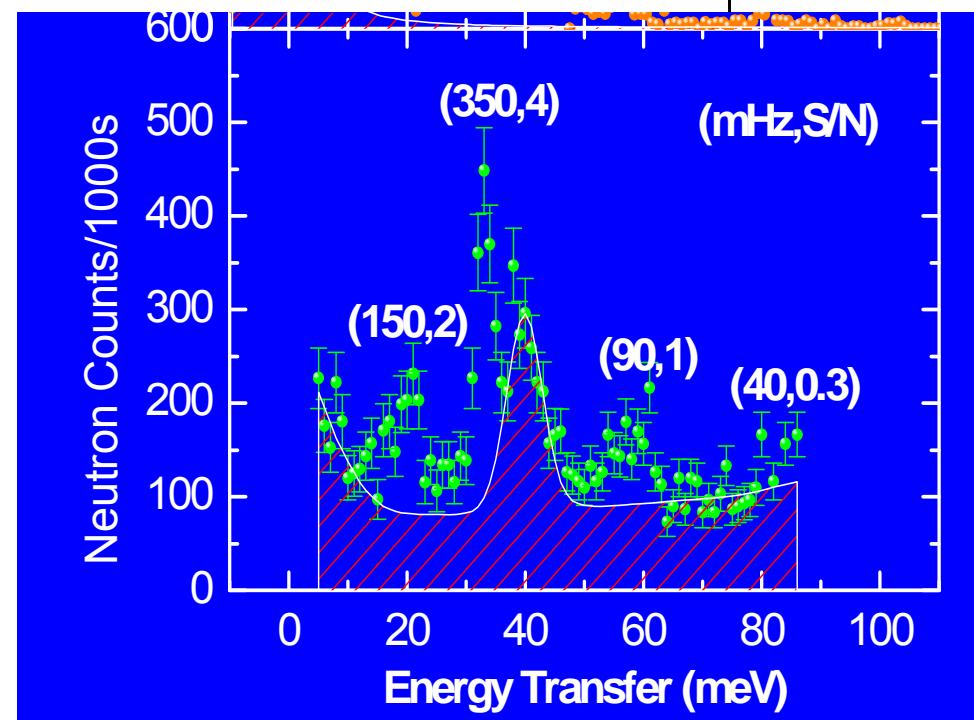
**Fixed- $E_f$  mode**



# Spurions

- Bragg – incoherent – Bragg

- Eg.  $k_i - 2k_f$ 
  - $\hbar\omega = 41.1 \text{ meV}$
  - $E_f = 13.7 \text{ meV}$   
 $E_i = 54.8 \text{ meV}$   
 $4E_f = 54.8 \text{ meV}$
  - Incoherent elastic scattering visible from analyzer  $\lambda/2$



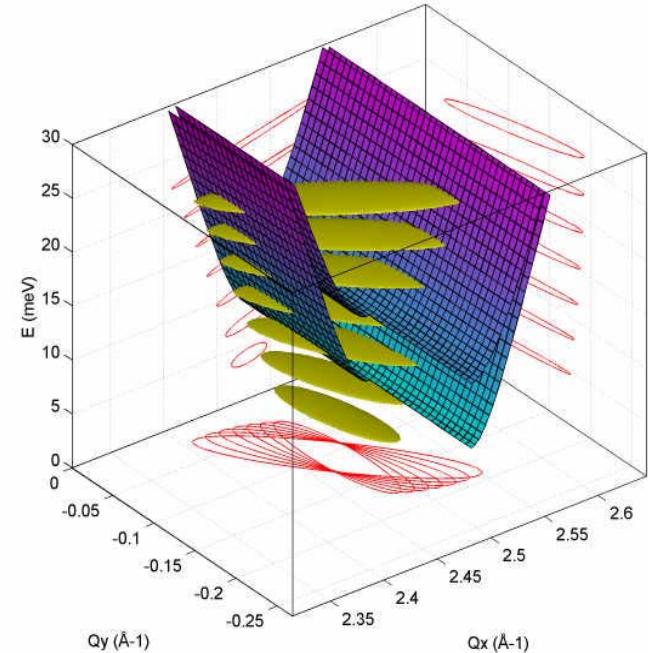
- incoherent – Bragg – Bragg

- Sample  $2\theta$  in Bragg condition for  $k_f - k_f$
- Even for inelastic config, weak incoherent from mono

# Resolution

- **Resolution ellipsoid**

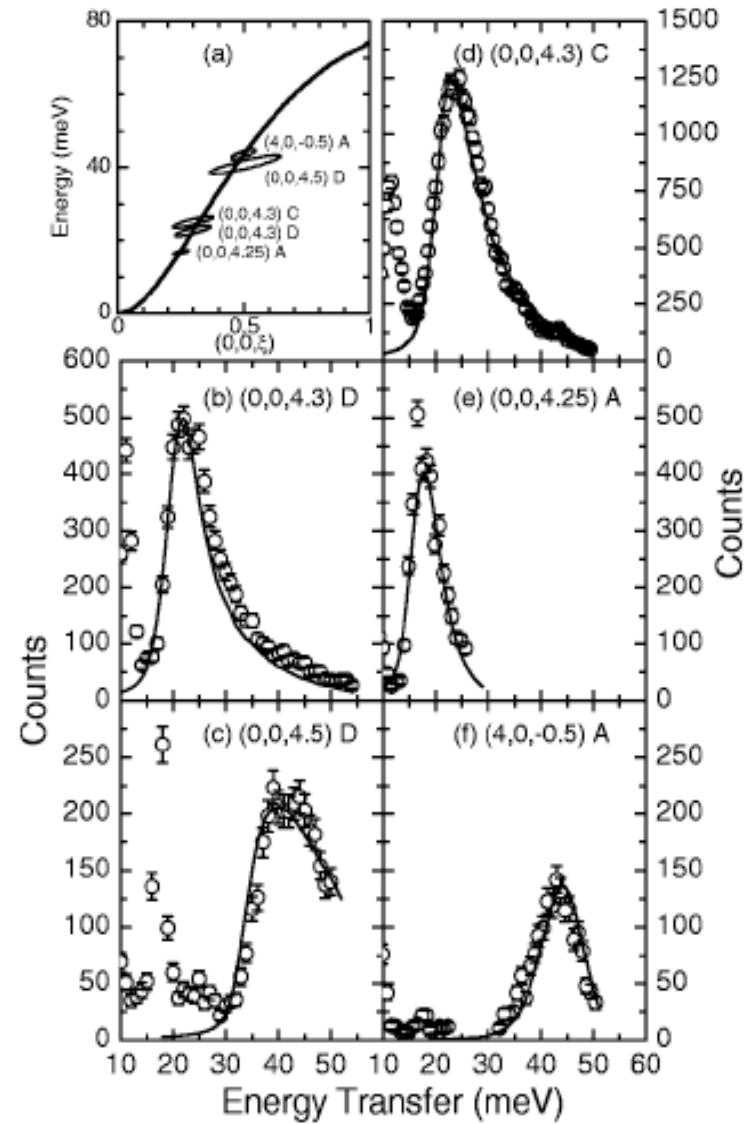
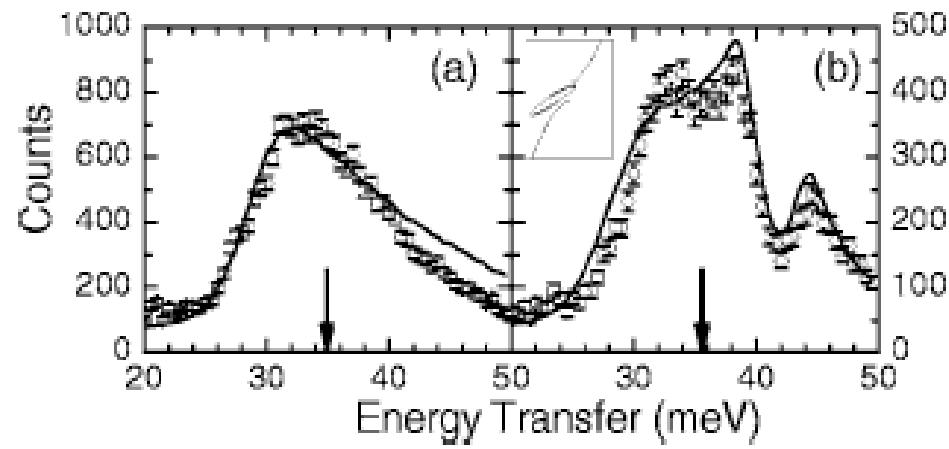
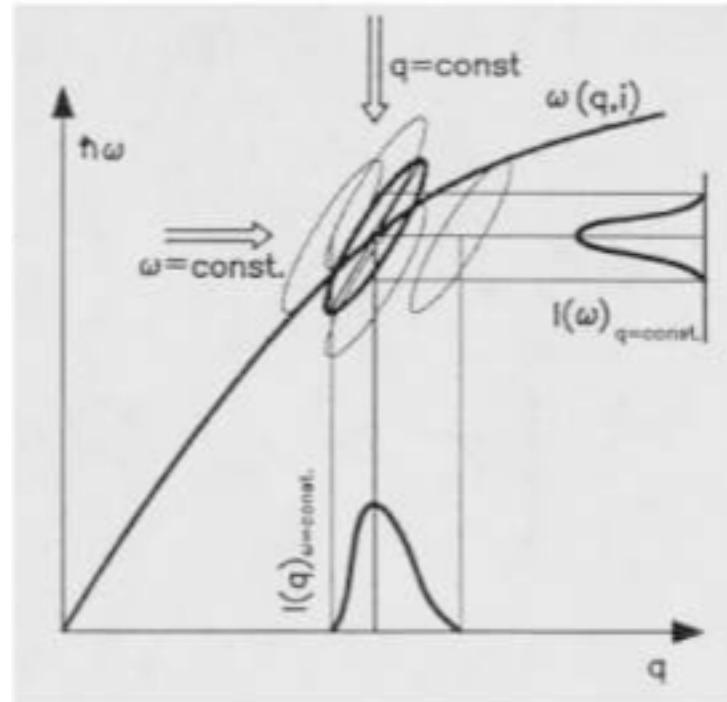
- Beam divergences
- Collimations/distances
- Crystal mosaics/sizes/angles



- **Resolution convolutions**

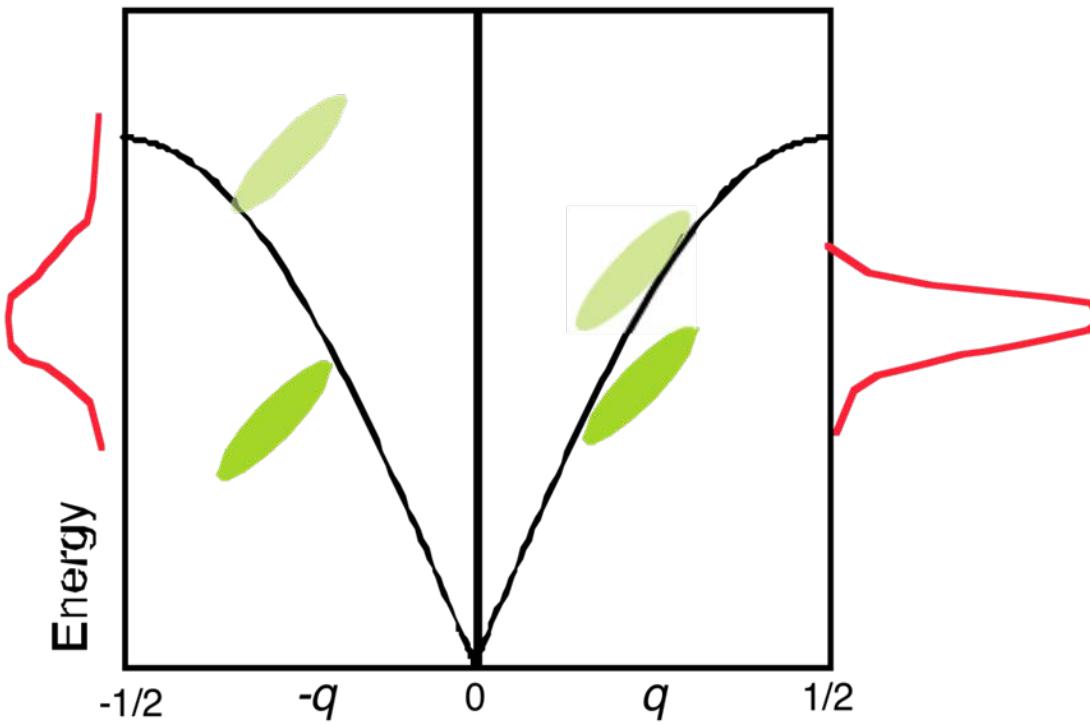
$$I(Q_0, \omega_0) = \int S(Q_0, \omega_0) R(Q - Q_0, \omega - \omega_0) dQ d\omega$$

# Resolution effects

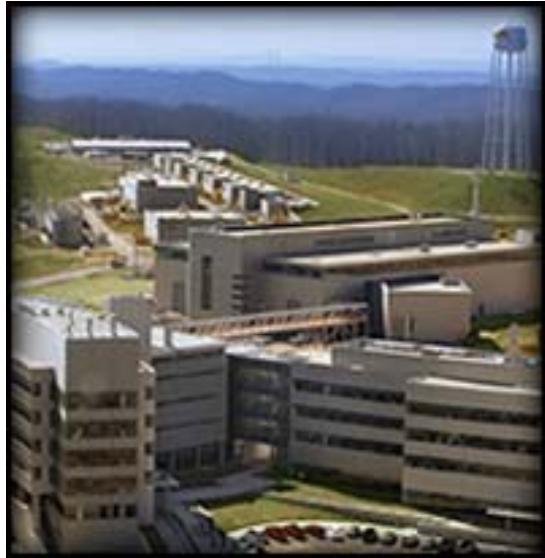


# Resolution focusing

- Optimizing peak intensity
- Match slope of resolution to dispersion



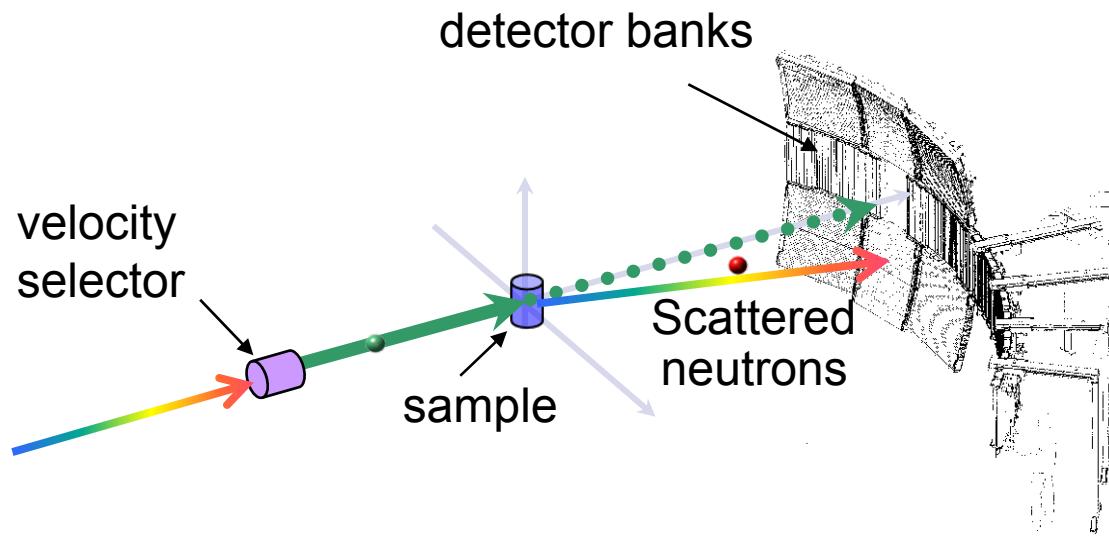
# Time-of-flight methods



Spallation neutron source



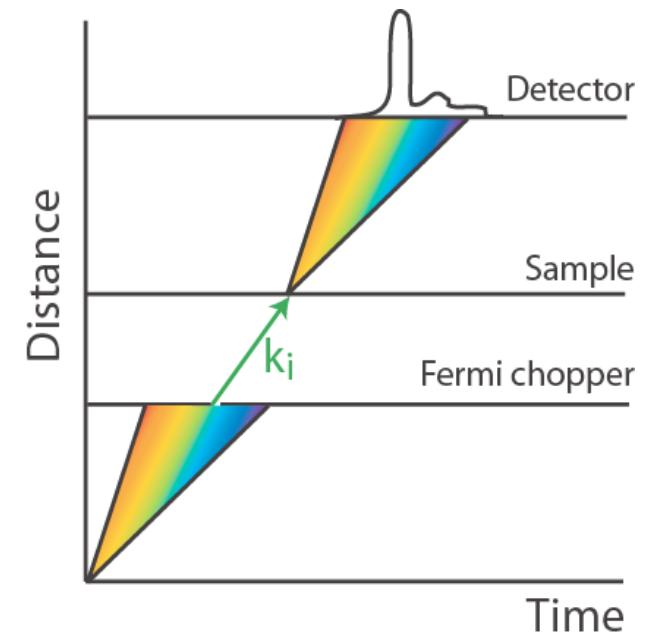
Pharos – Lujan Center



May 31, 2009

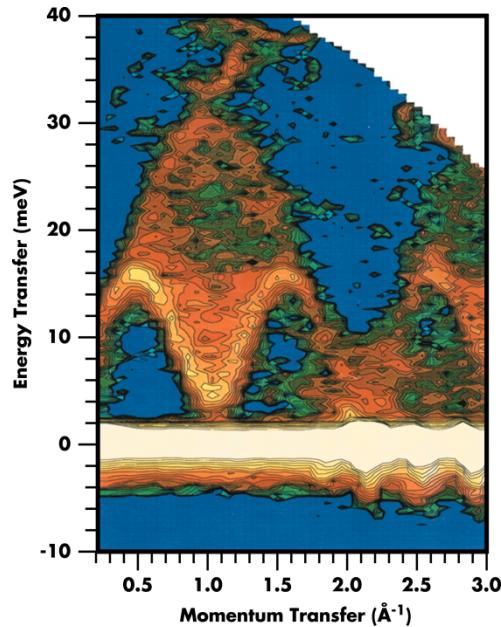
- Effectively utilizes time structure of pulsed neutron groups

$$t = \frac{d}{v} = \left( \frac{m}{h} d \right) \lambda$$

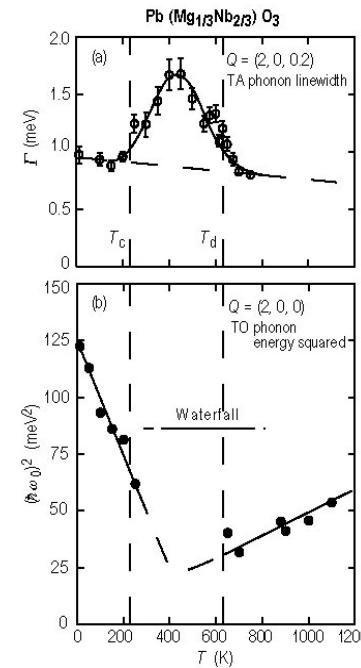


# TOF vs. 3-axis

- epithermal (up to 2 eV)
- Total spectra (esp. powder samples)
- Absolute normalization
- Low-dimensional systems
- Hardware inflexible
- Software intensive



- High flux of thermal neutrons
- Focused studies in  $Q, \omega$  (soft modes, gaps, etc.)
- Three-dimensional systems
- Hardware intensive
- Software inflexible



# Fermi Choppers

- Body radius ~ 5 cm
- Curved absorbing slats
  - B or Gd coated
  - ~mm slit size
- $f = 600$  Hz (max)
- Acts like shutter,  $\Delta t \sim \mu\text{s}$

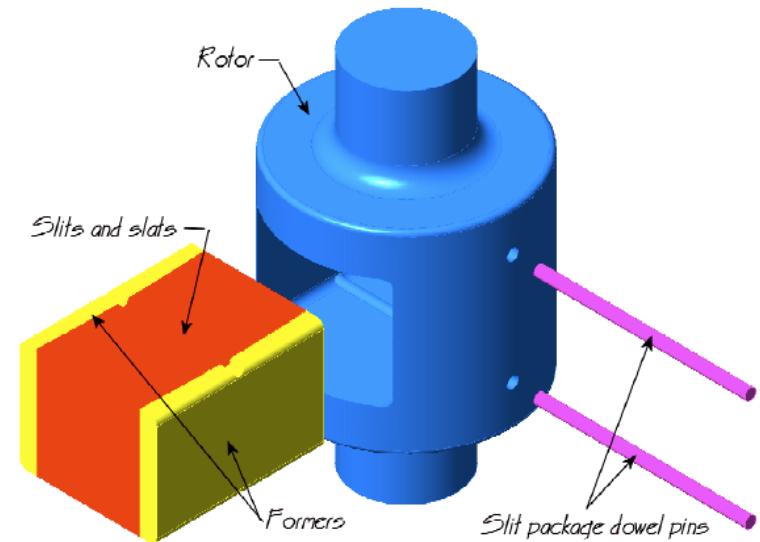
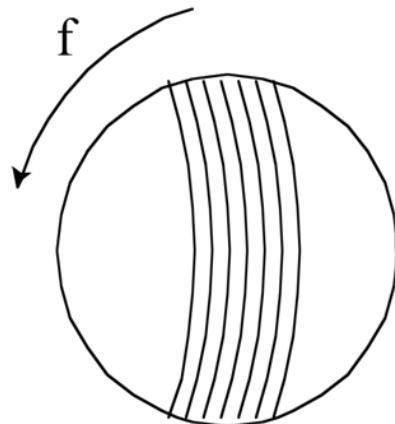
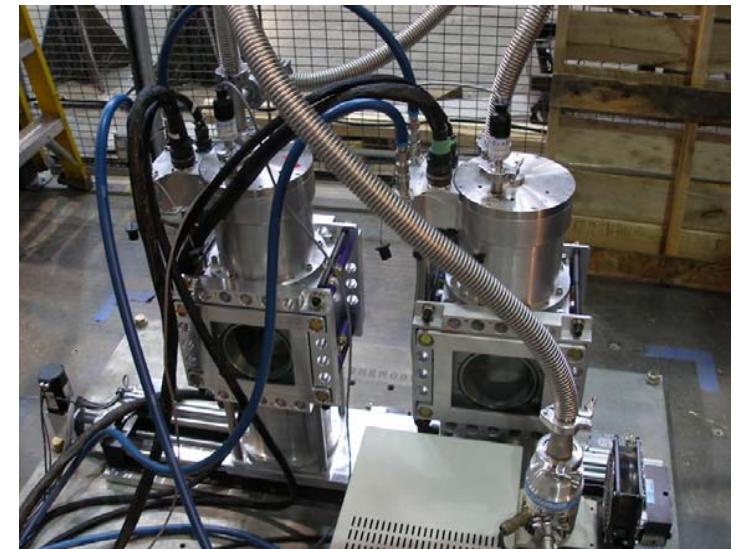


Figure 1. ISIS MAPS chopper and slit package assembly – exploded view

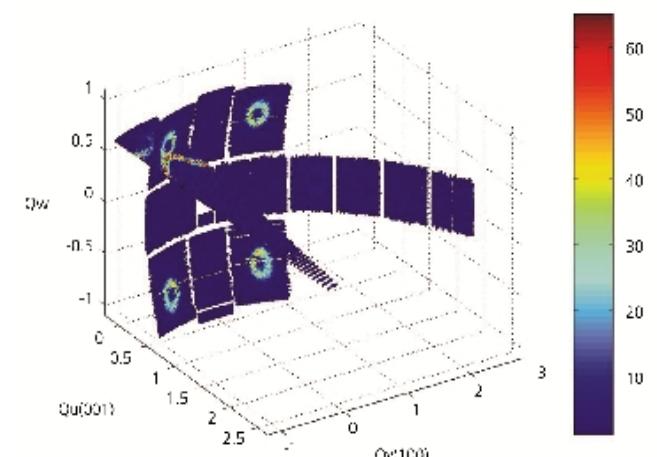


# Position sensitive detectors

- $^3\text{He}$  tubes (usu. 1 meter)
- Charge division
- Position resolution  $\sim \text{cm}$
- Time resolution  $\sim 10 \text{ ns}$

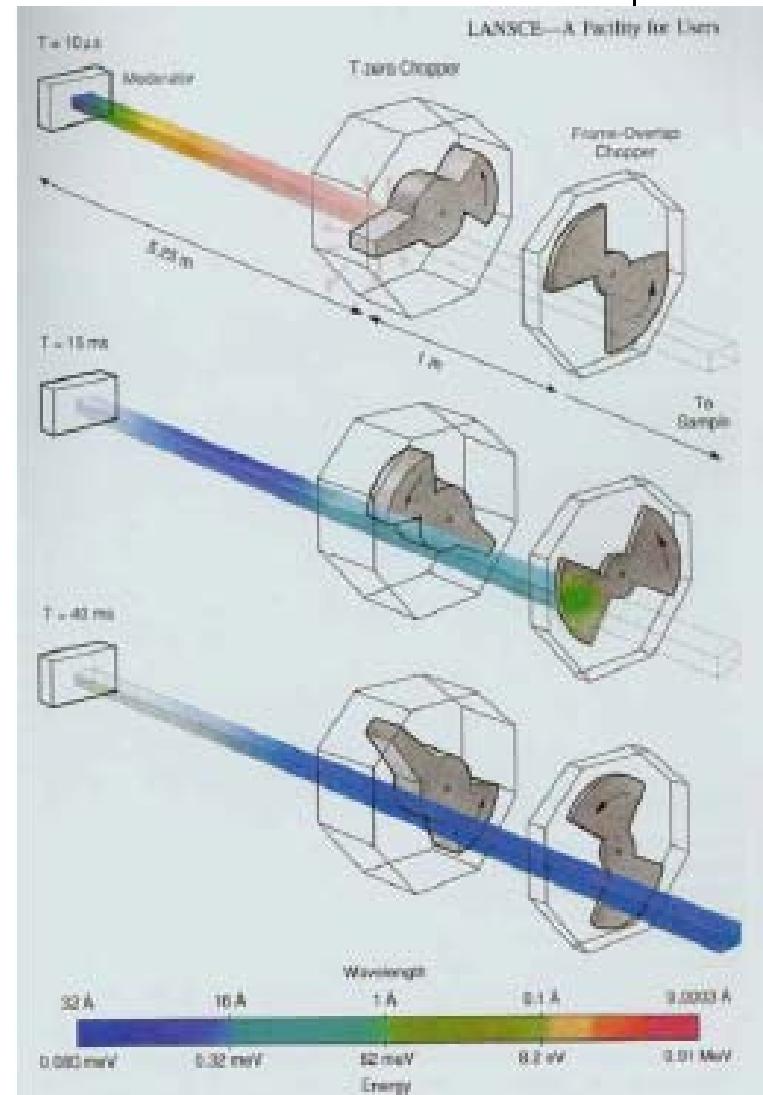
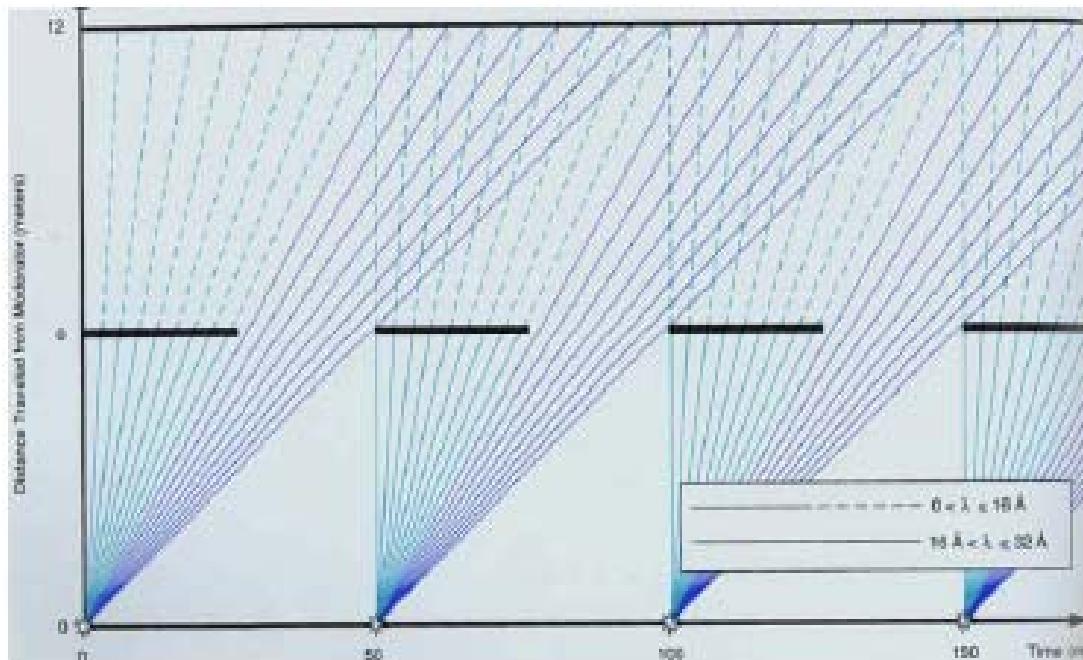


MAPS detector bank



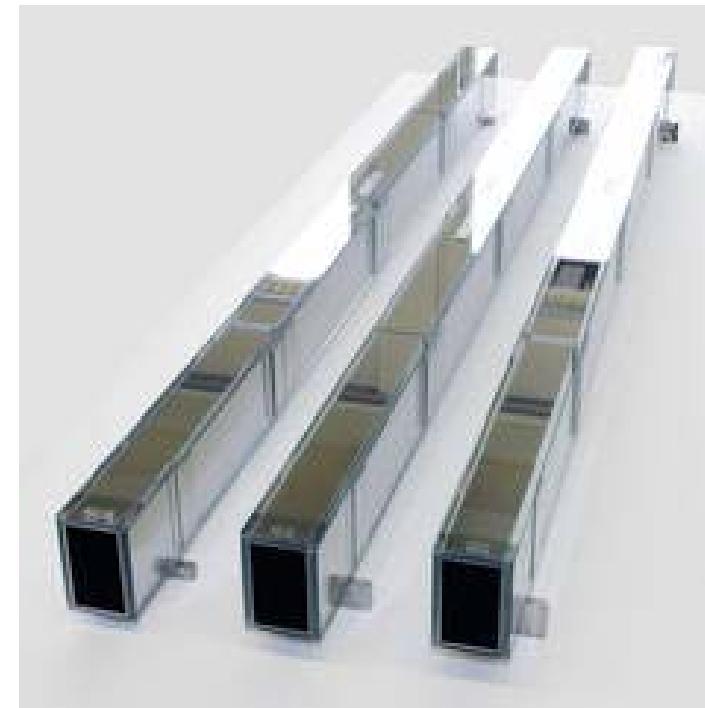
# T-zero chopper

- Background suppression
- Blocks fast neutron flash



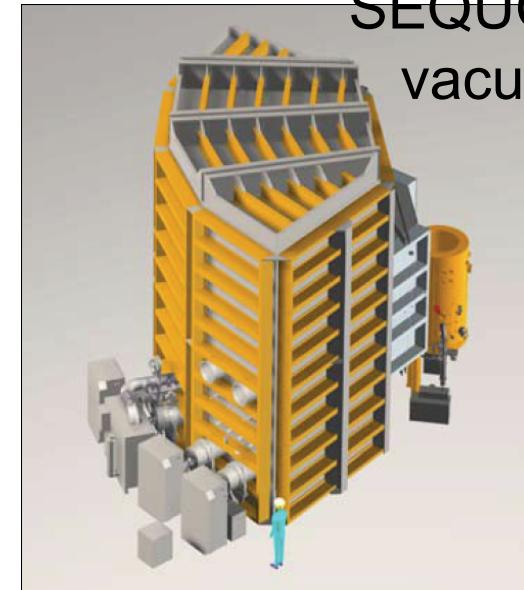
# Guides

- Transport beam over long distances
- Background reduction
- Total external reflection
  - Ni coated glass
  - Ni/Ti multilayers (supermirror)



# Size matters

- **Length = resolution**
  - Instruments ~ 20 – 40 m long
  - E-resolution ~ 2-4%  $E_i$
- **More detectors**
  - SEQUOIA – 1600 tubes, 144000 pixels
  - Solid angle coverage 1.6 steradians
- **Huge data sets**
- 0.1 – 1 GB

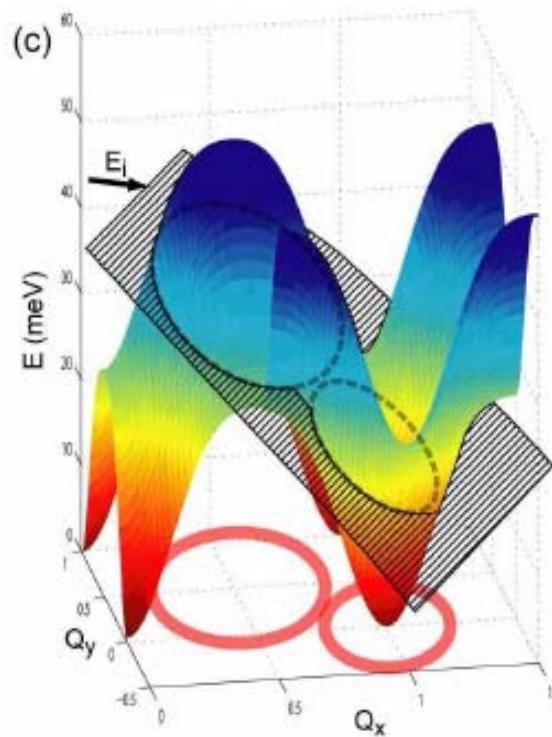


SEQUOIA detector  
vacuum vessel

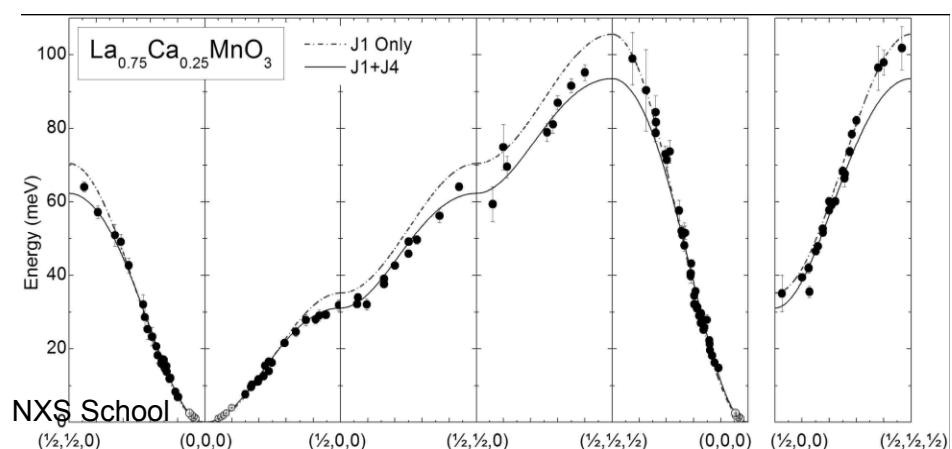
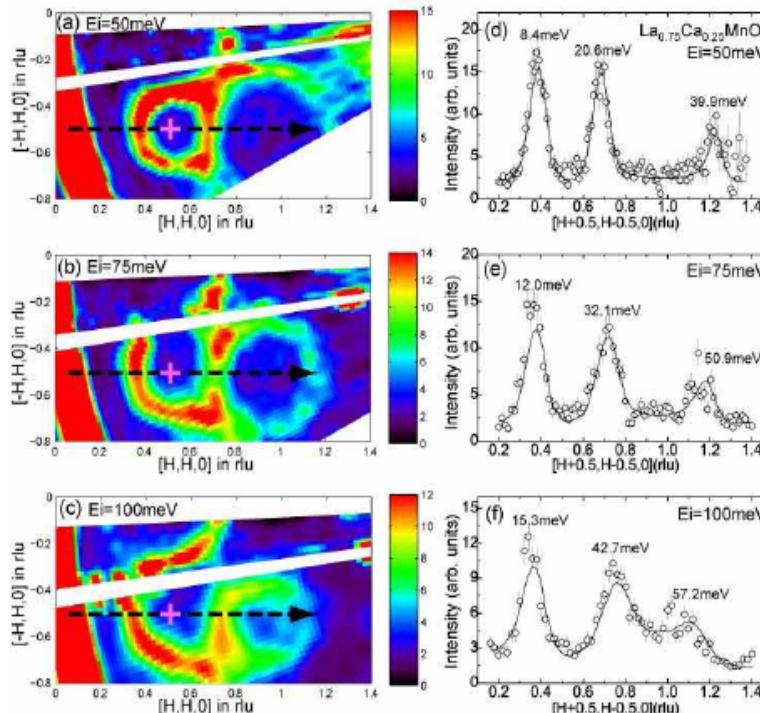


# Data visualization

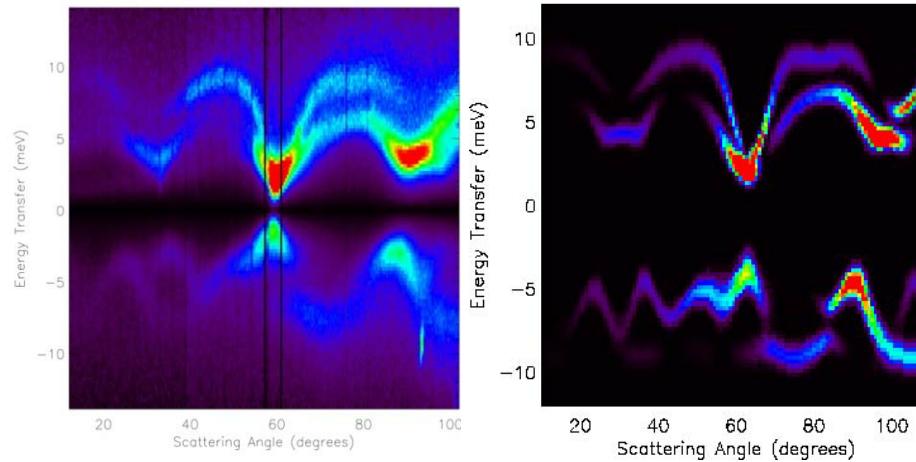
- Large, complex data from spallation sources
- Measure  $S(\mathbf{Q}, \omega)$  – 4D function



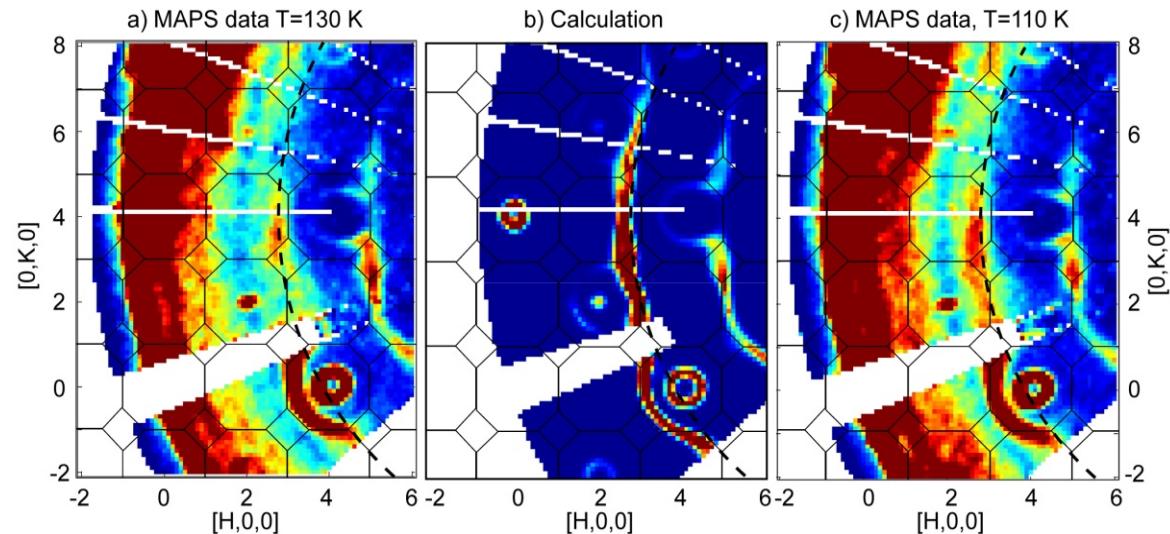
Ye et al., Phys. Rev. B, 75 144408 (2007).



# Computation



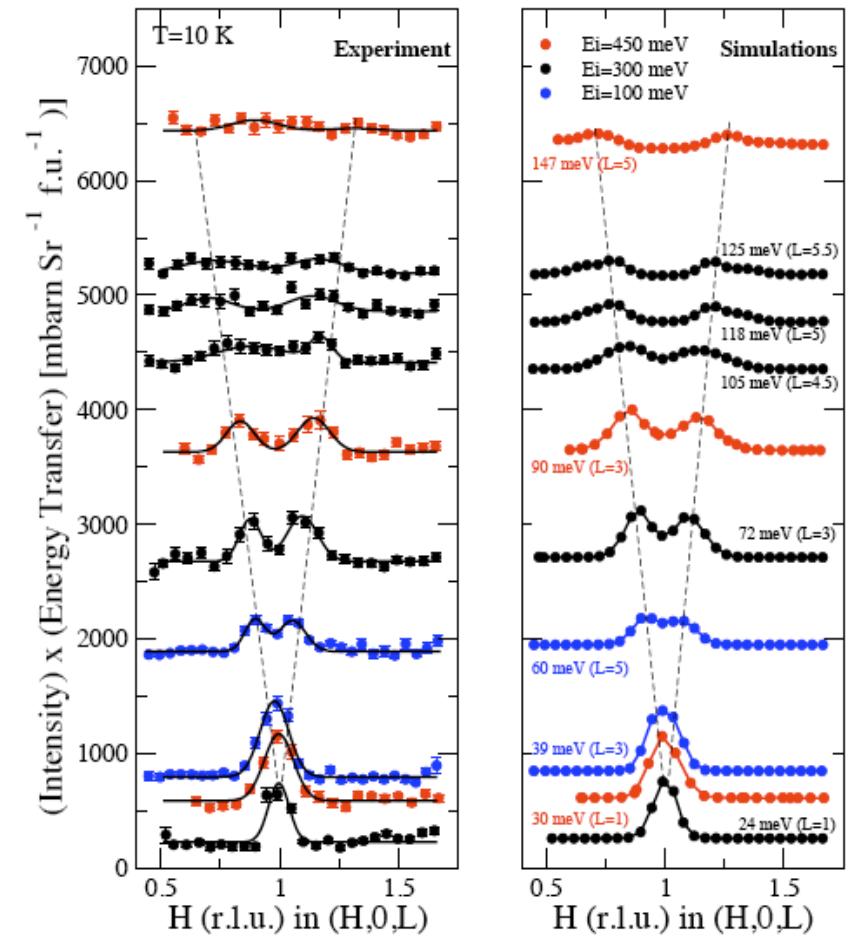
**Pb phonons**



**Fe<sub>3</sub>O<sub>4</sub> spin waves**

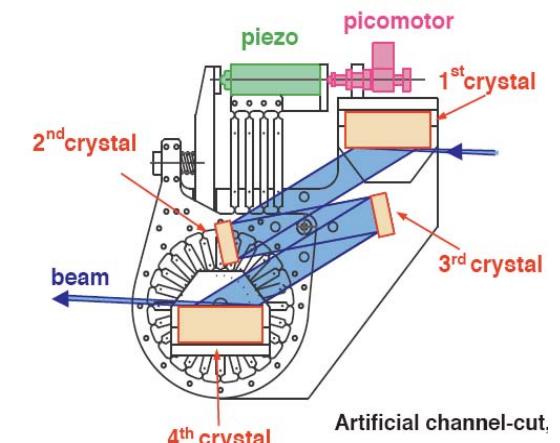
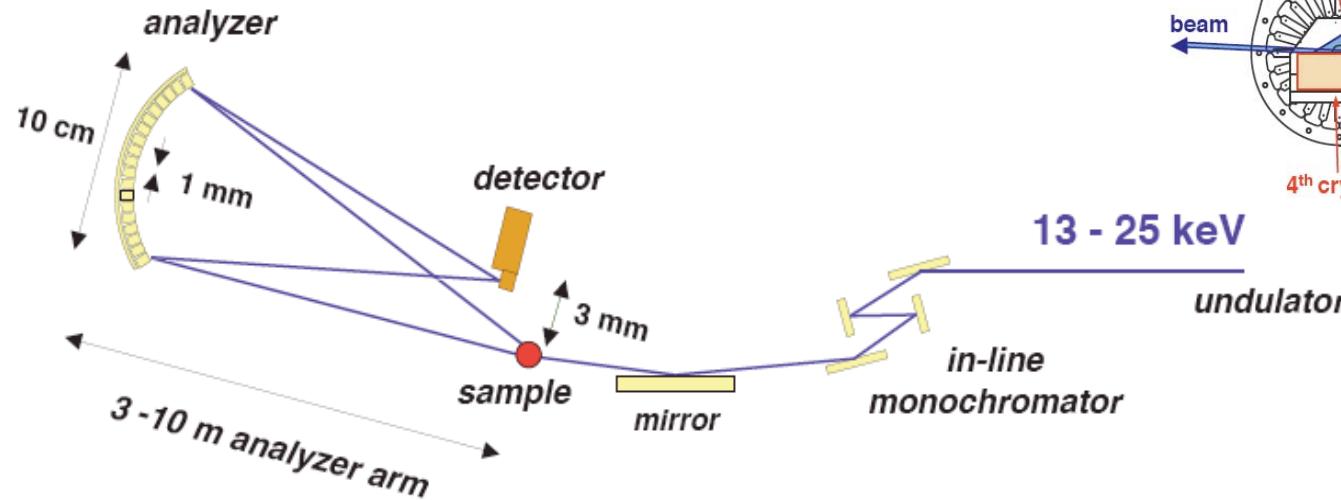
# Absolute normalization

- **Absolute normalization**
  - Using incoherent scattering from vanadium
  - $\sigma/4\pi = 404 \text{ mbarns/Sr}$

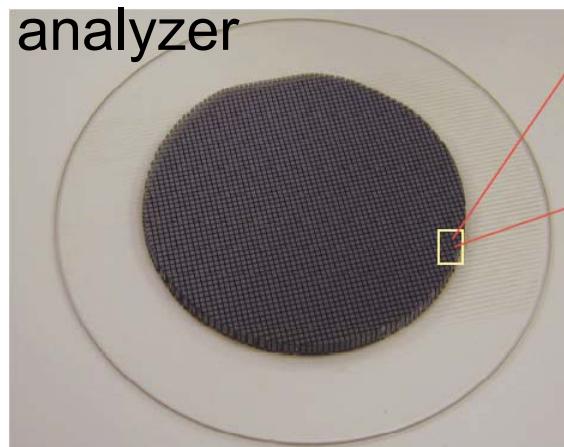


# Inelastic x-ray scattering

- $E_i=20 \text{ keV}$ , need 1 meV resolution
- $\Delta E/E_i \sim 10^{-7}$  !!!



Sector-3, APS



$\phi$ -scan of monochromator  
1 meV  $\Rightarrow$   $\mu\text{rad}$

T-scan of monochromator  
1 meV  $\Rightarrow$  0.02 K  
NXS School

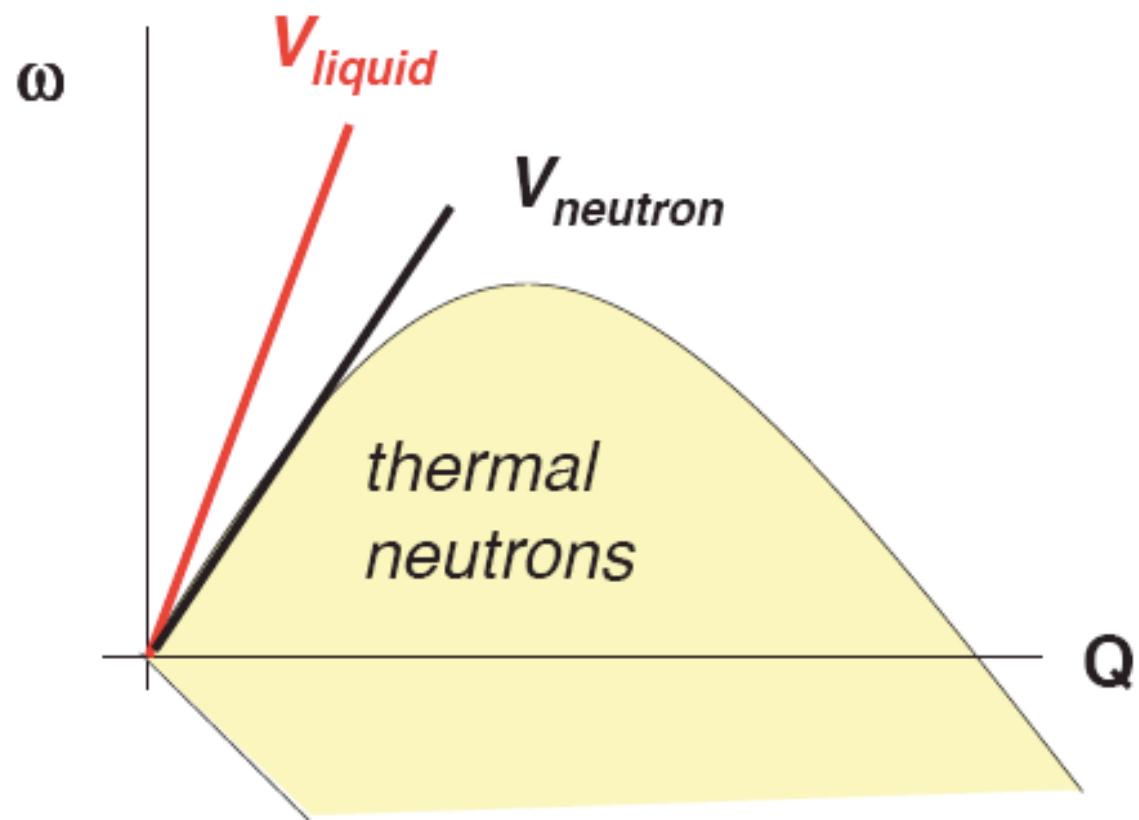


# Kinematics

- Essentially elastic scattering
- No kinematic limits

$$Q \approx 2k_i \sin \theta$$

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



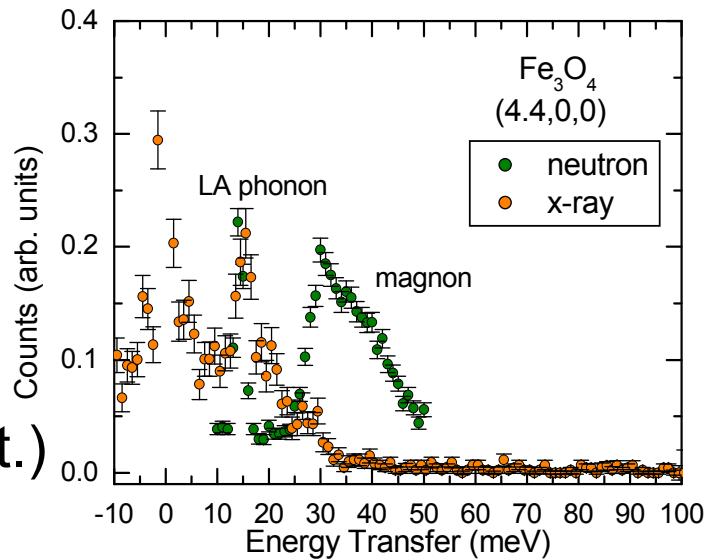
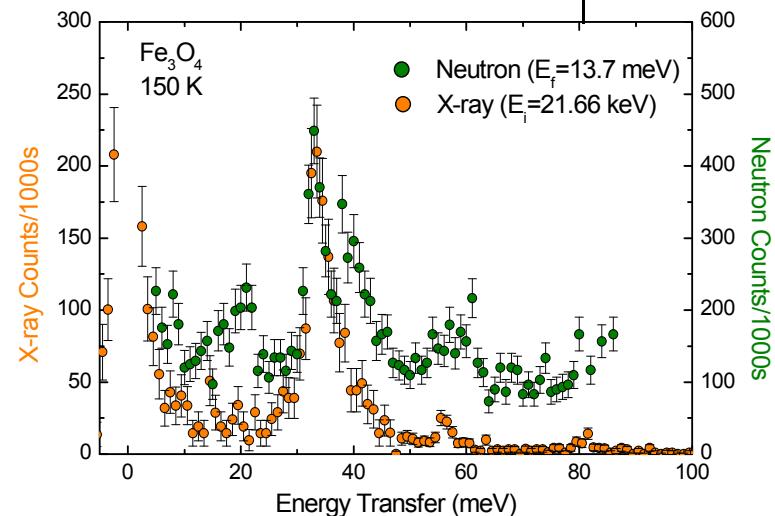
# IXS vs. INS

- SAMPLE SIZE



- IXS

- Simple scattering geometry ( $k_i \approx k_f$ )
- Resolution function simpler  
(most angles fixed, E-scans only)
- No spurious  
(high-order refs. keV, no incoherent scat.)
- Can only do lattice excitations*



# References

## General neutron scattering

- G. Squires, "Intro to theory of thermal neutron scattering", Dover, 1978.  
S. Lovesey, "Theory of neutron scattering from condensed matter", Oxford, 1984.  
R. Pynn, <http://www.mrl.ucsb.edu/~pynn/>.

## Polarized neutron scattering

Moon, Koehler, Riste, Phys. Rev **181**, 920 (1969).

## Triple-axis techniques

Shirane, Shapiro, Tranquada, "Neutron scattering with a triple-axis spectrometer", Cambridge, 2002.

## Time-of-flight techniques

B. Fultz, [http://www.cacr.caltech.edu/projects/danse/ARCS\\_Book\\_16x.pdf](http://www.cacr.caltech.edu/projects/danse/ARCS_Book_16x.pdf)