UT-BATTELLE

Introduction to Inelastic Neutron Scattering

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With Thanks to:

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HFIR

SNS

SPALLATION NEUTRON SOURCE

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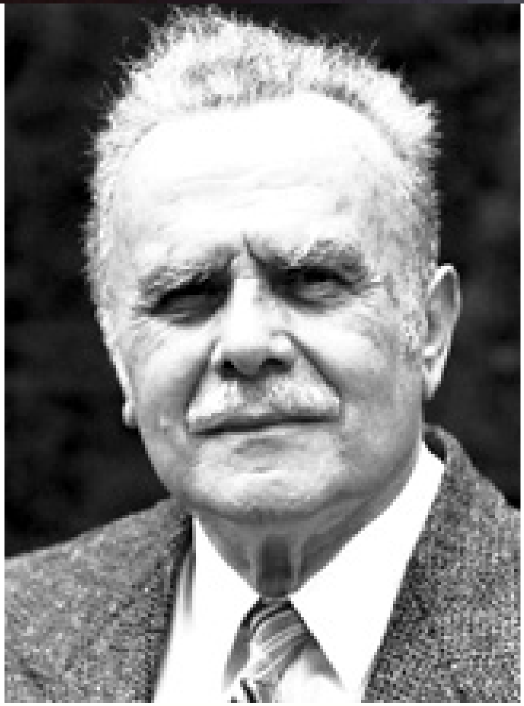
OAK RIDGE NATIONAL LABORATORY
U. S. DEPARTMENT OF ENERGY

The Nobel Prize in Physics 1994

"for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

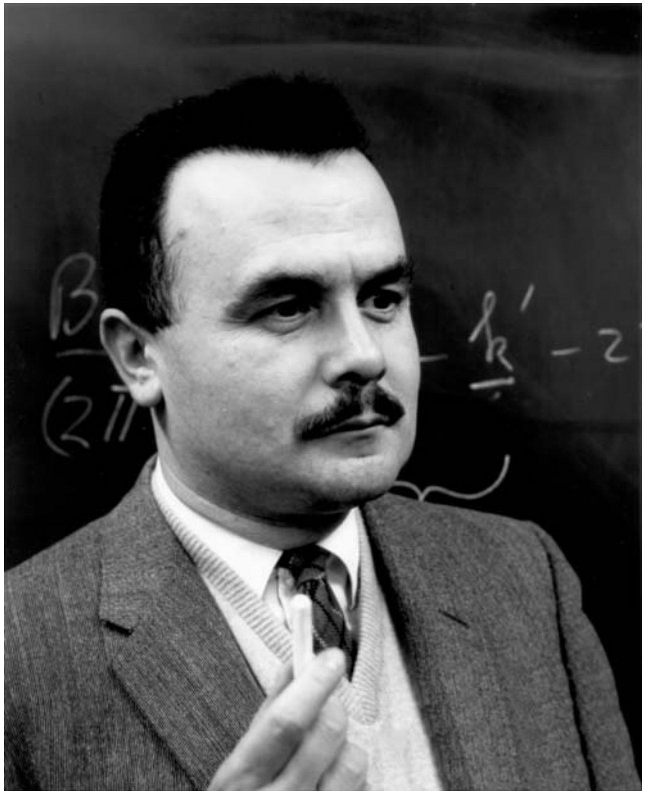
Neutrons show what atoms do



Bertram N. Brockhouse

Neutrons show where atoms are

Clifford G. Shull



"If the neutron did not exist, it would need to be invented."

- B. Brockhouse

Why is the Neutron a Useful Particle?

- $m = 1.675E\text{-}27$ kg, no charge, $S=\frac{1}{2}\hbar$, $\mu_n = -1.913\mu_N$
- Typical de Broglie wavelengths, $\lambda = 2\pi/k$, are similar to lattice spacings.
- Energies of neutrons are tunable to that of excitations in condensed matter.
- Neutrons probe the entire sample, even inside complex sample environments.
- Neutrons interact with nuclei through nuclear force – lattice vibrations.
- Neutrons interact with unpaired electrons – magnetic excitations.

Useful Formulae (non-relativistic neutrons)

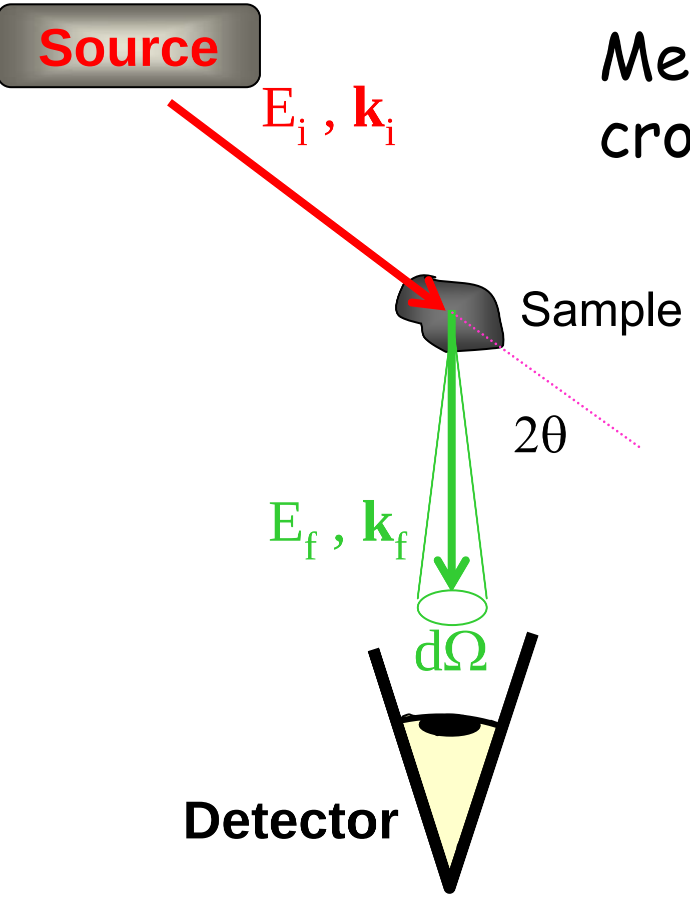
$$p = mv = \hbar k = \frac{h}{\lambda}$$

$$E = \frac{1}{2} m v^2 = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{\lambda^2 m}$$

$$\boxed{E = 2.072 k^2 = \frac{81.81}{\lambda^2}}$$

Units: E (meV) k (Å^{-1}) λ (Å)

Inelastic Scattering: scattering with energy and momentum transfer



Measure the inelastic (double differential) cross section:

$$\frac{d^2\sigma}{d\Omega\, dE_f} = \frac{k_f}{k_i} S(Q,\varepsilon)$$

$S(Q,\varepsilon)$ scattering function - **physics**

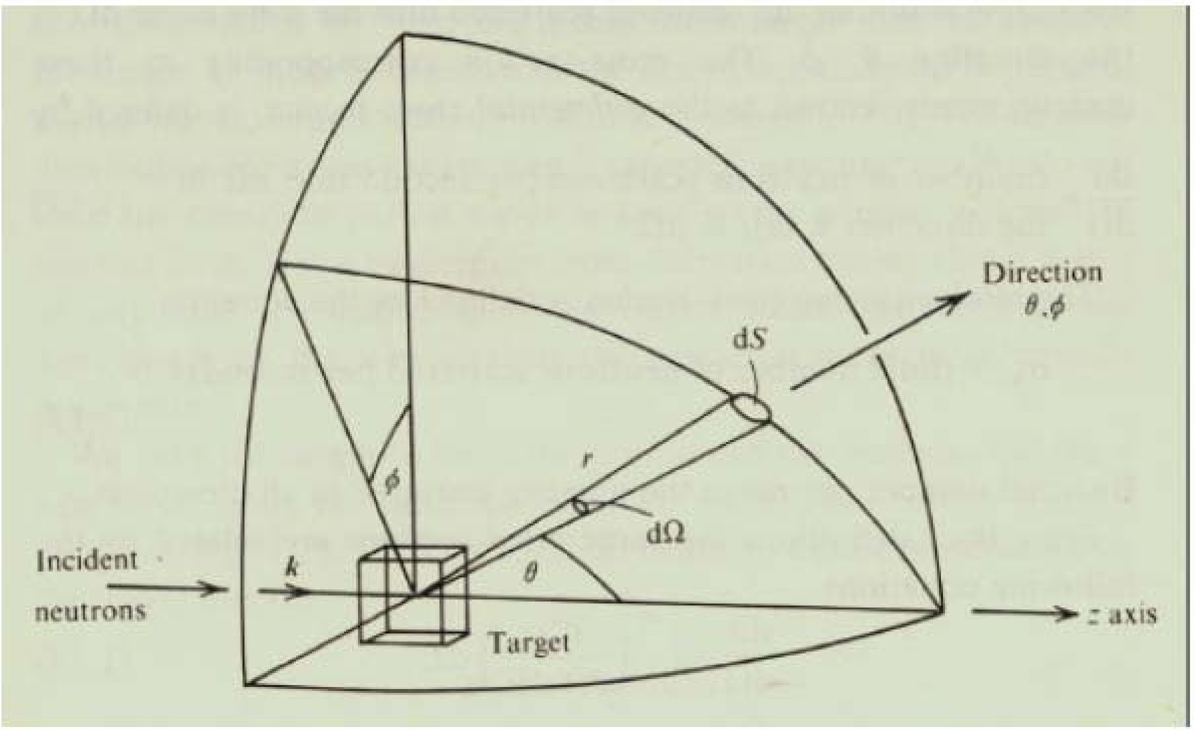
Conservation of energy

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

Conservation of momentum

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

Cross Sections



$$\Phi = \text{number of incident neutrons per cm}^2 \text{ per second}$$

$$\sigma = \text{total number of neutrons scattered per second} / \Phi$$

$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into d}\Omega}{\Phi \; \text{d}\Omega}$$

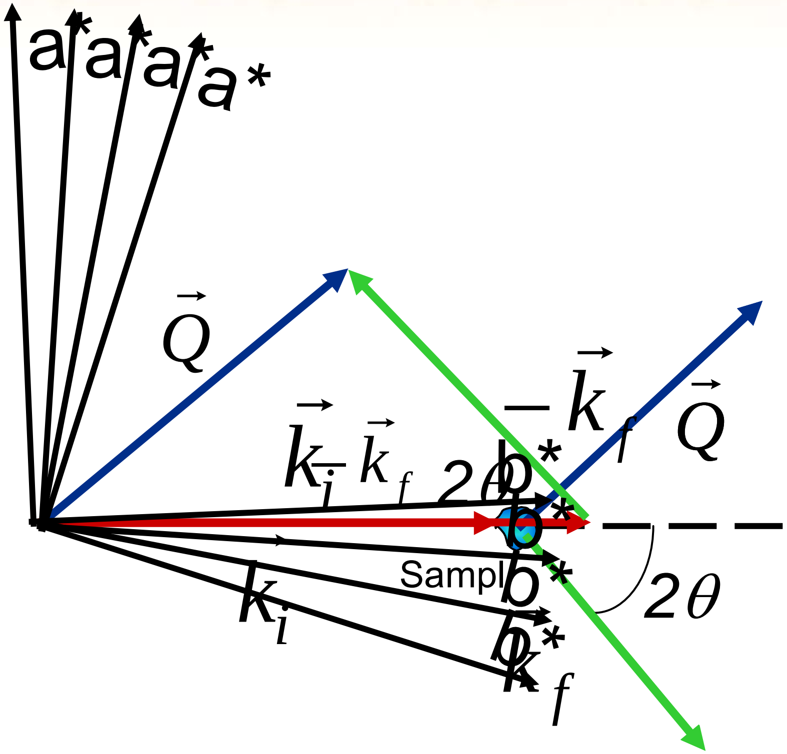
$$\frac{d^2\sigma}{d\Omega dE} = \frac{\text{number of neutrons scattered per second into d}\Omega \; \& \; \text{dE}}{\Phi \; \text{d}\Omega \; \text{dE}}$$

Scattering Functions – $S(Q,\omega)$

Experssions for $S(Q,w)$ can be derived for a number of cases:

- Excitation or absorption of one quantum of lattice vibrational energy (phonon)
- Various models for atomic motions in liquids and glasses
- Various models of atomic & molecular translational & rotational diffusion
- Rotational tunneling of molecules
- Single particle motions at high momentum transfers
- Transitions between crystal field levels
- Magnons and other magnetic excitations such as spinons

Reciprocal Space and the Scattering Triangle

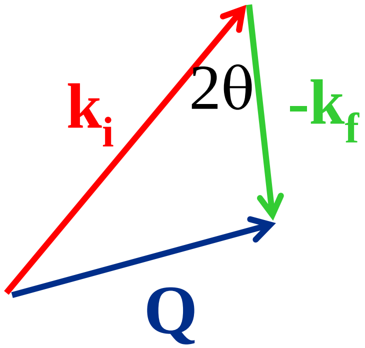


$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

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

Kinematic Constraints for Inelastic Scattering

Guideline I: one can not measure all Q and E



From scattering triangle and law of cosines

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

In terms of E and Q

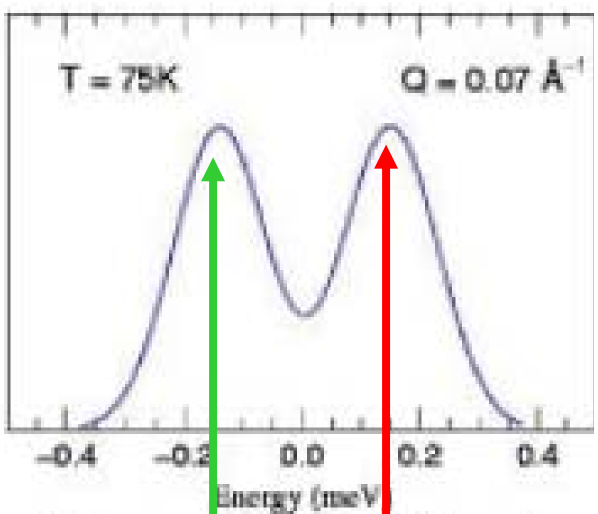
$$\frac{\hbar^2}{2m} Q^2 = E_i + E_f - 2\sqrt{E_i E_f}\,\cos(2\theta)$$

And substituting $E_f = E_i - \varepsilon$

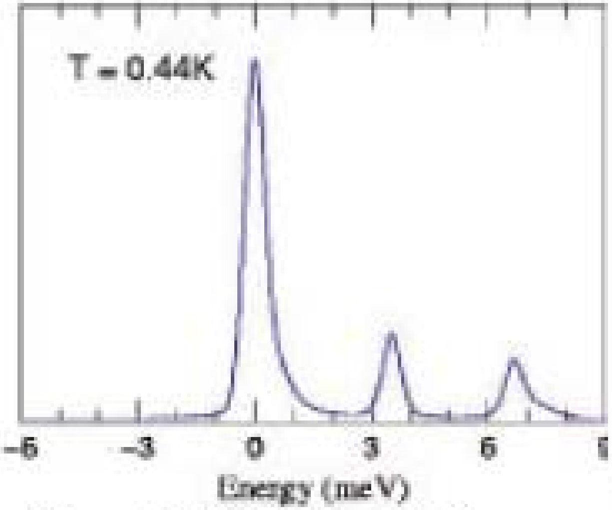
$$\frac{\hbar^2}{2m} Q^2 = 2E_i - \varepsilon - 2\sqrt{E_i(E_i - \varepsilon)}\,\cos(2\theta)$$

- For a given 2θ and E_i, one can only access a locus of Q and ε points. – limits your measurement

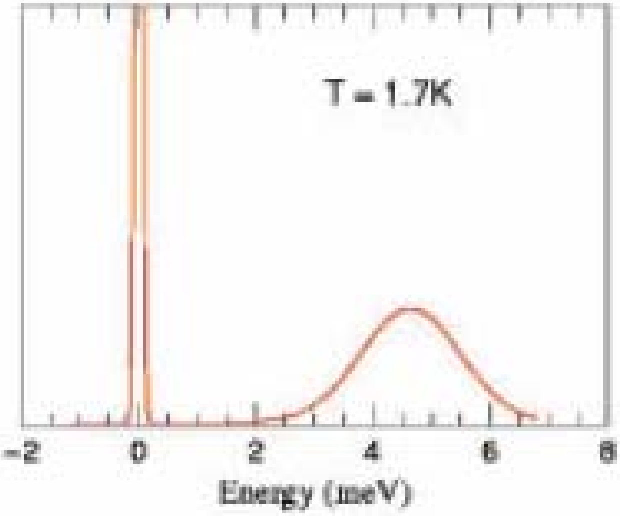
Examples



Spin waves – collective excitations



Crystal Field splittings ($HoPd_2Sn$) – local excitations

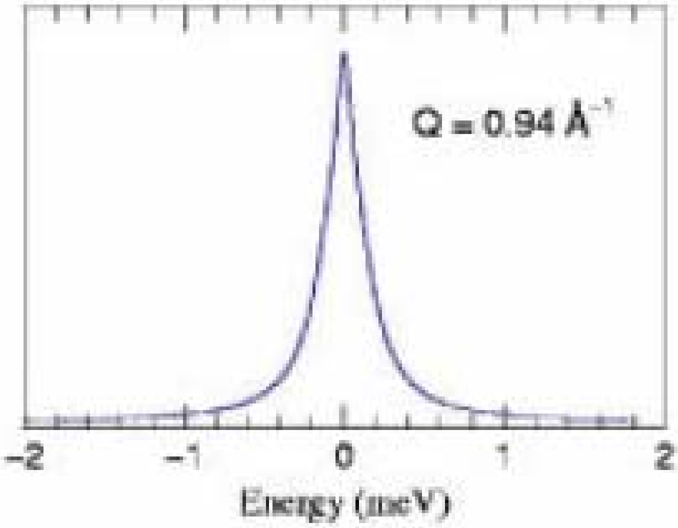


Local spin resonances (e.g. $ZnCr_2O_4$)

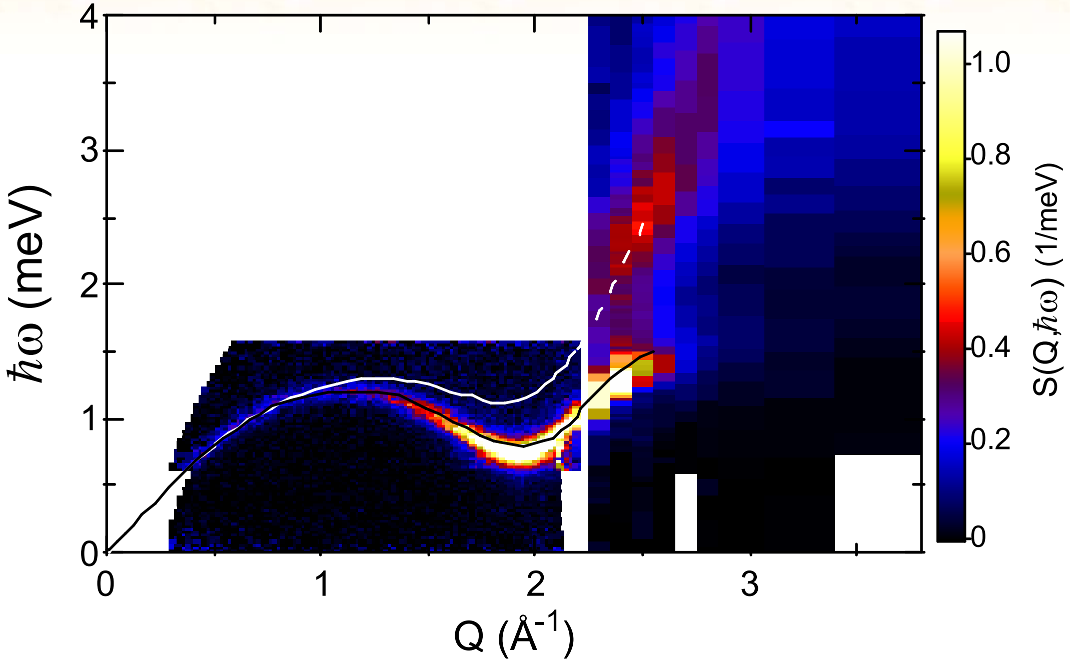
Neutron energy loss

Neutron energy gain

Examples II - Liquids



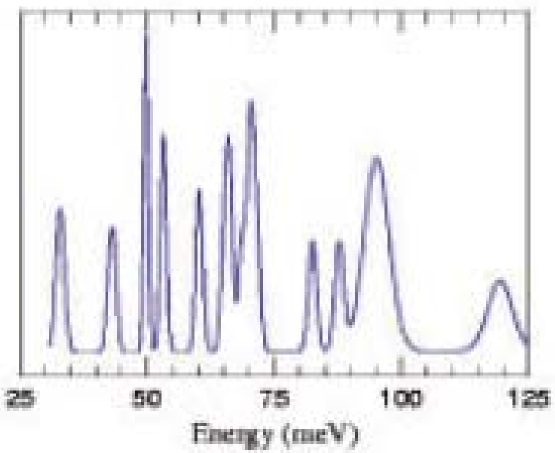
"Simple" liquids (e.g. water)



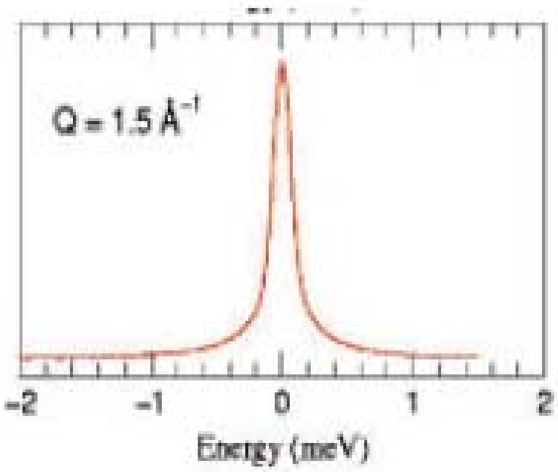
Diffuse scattering

Quantum fluids
Superfluid ^{4}He

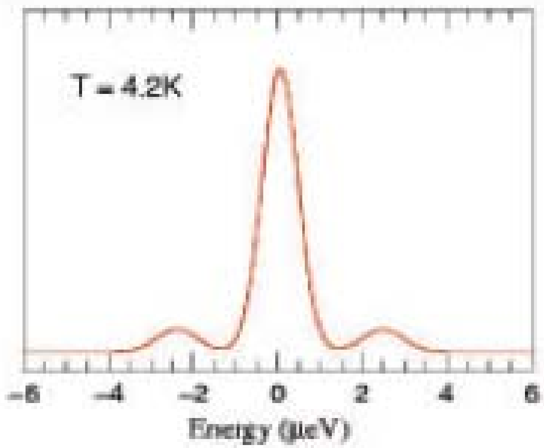
Examples III: molecules (μeV to keV)



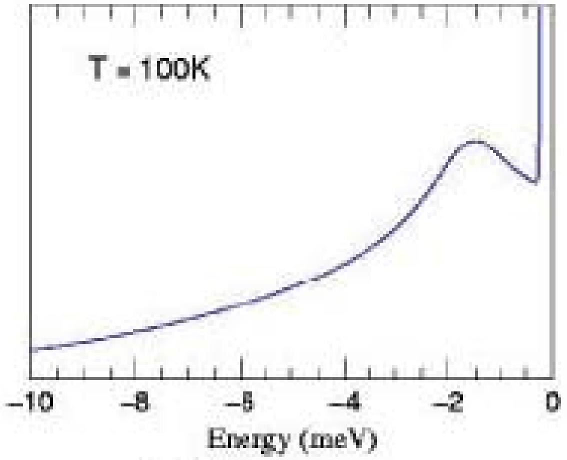
Vibrational spectroscopy
(e.g. C_{60})



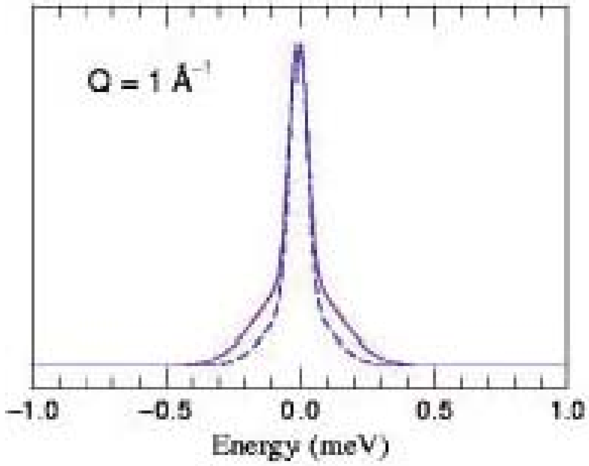
Molecular reorientation
(e.g. pyrazine)



Rotational tunneling
(e.g. CH_3I)



Polymers

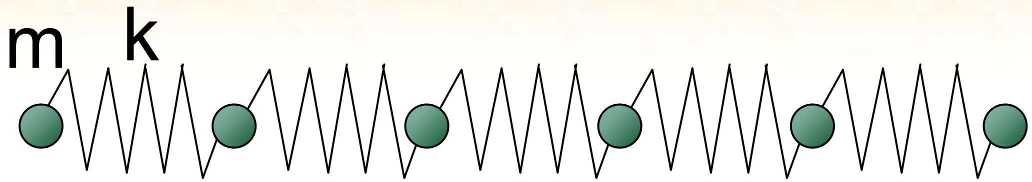


Proteins

Two short case studies

Lattice (phonon) excitations in $Ca_{2-x}Sr_xRuO_4$
and
Magnetic (spin-wave) excitations in $CsMnCl_3\ 2(D_2O)$

Lattice Excitations in Condensed Matter

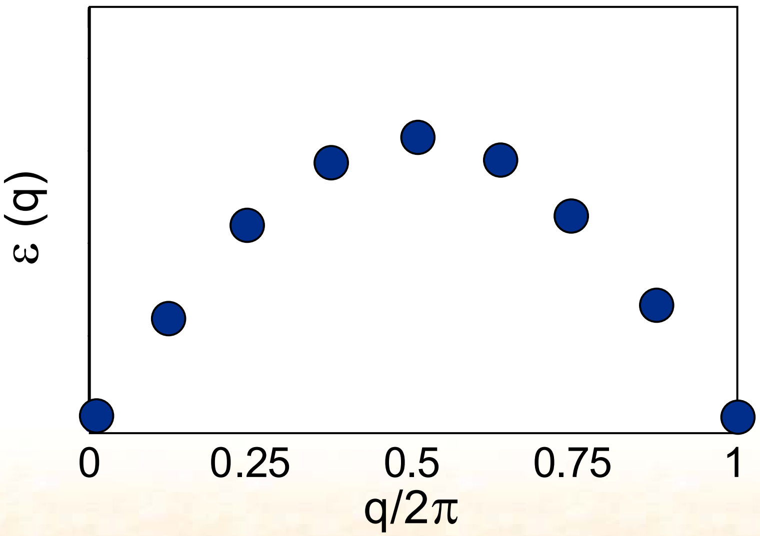


$$F = ma$$

- Well defined excitations out of a long range ordered (LRO) state of atoms in crystal lattice

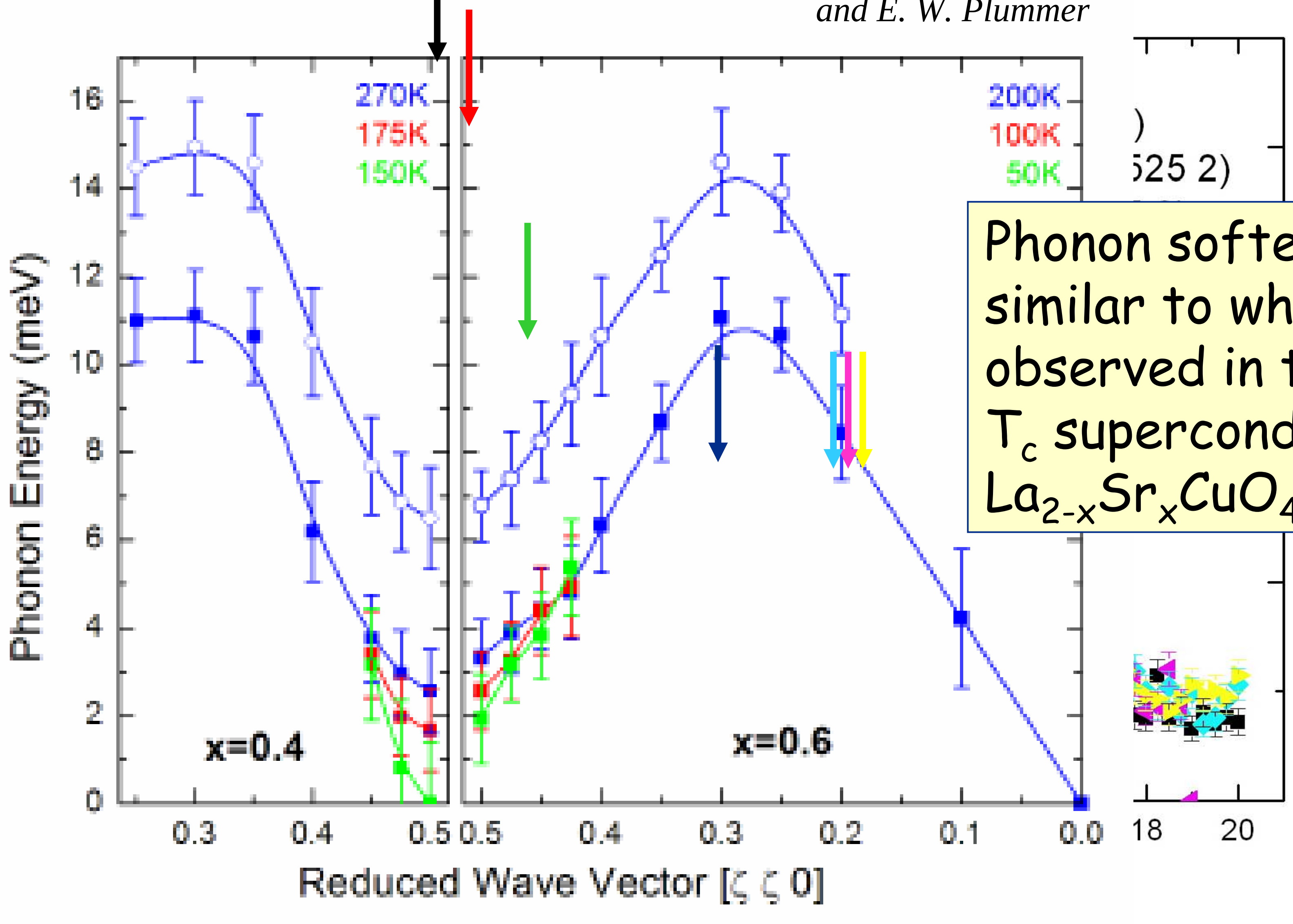
- Transmission of sound – Phonons

- Wave-vector dependent quasiparticles



Phonons in $Ca_{2-x}Sr_xRuO_4$

R. G. Moore, M. D. Lumsden, M. B. Stone, J. Zhang, Y. Chen, J. W. Lynn, R. Jin, D. Mandrus, and E. W. Plummer

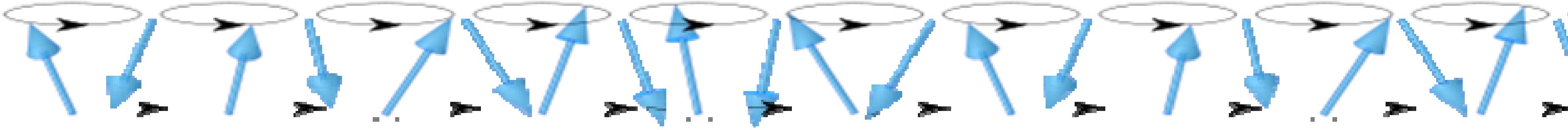


Phonon softening is similar to what is observed in the high T_c superconductor $La_{2-x}Sr_xCuO_4$

Magnetic Excitations in an Ordered Magnet

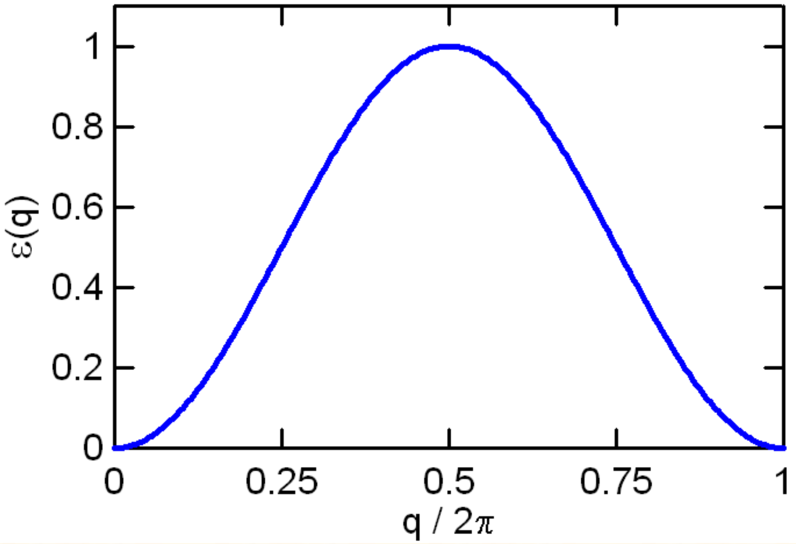
$$H = \sum J(\mathbf{S}\cdot\mathbf{S})$$

- Exchange, J, in Hamiltonian sets energy scale
- ‘Spin-Solid’ – Long range ordered ground state
- Semi-classical spin-wave excitations – a doublet



Antiferromagnetic Spin Waves

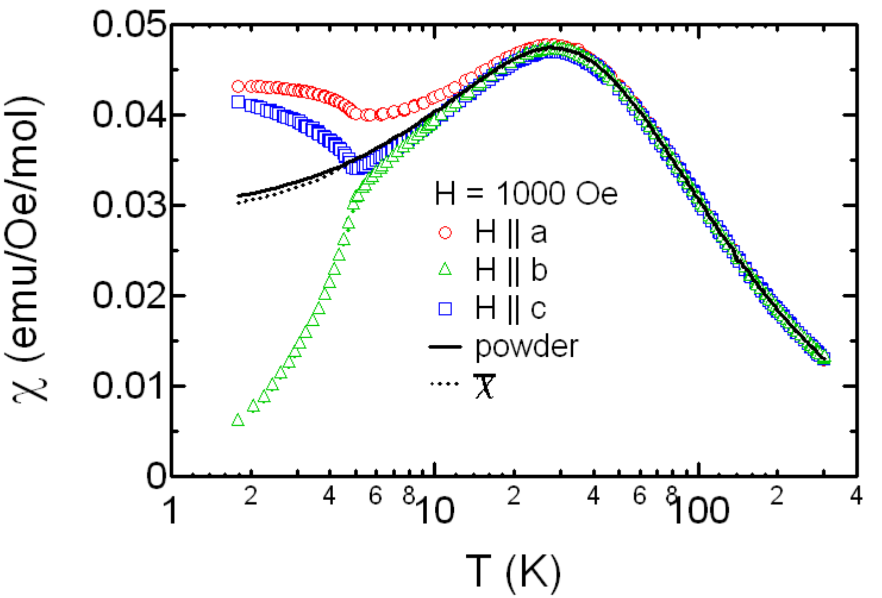
Ferromagnetic Spin Waves



- Wave-vector dependent quasiparticles

A Classic Antiferromagnet

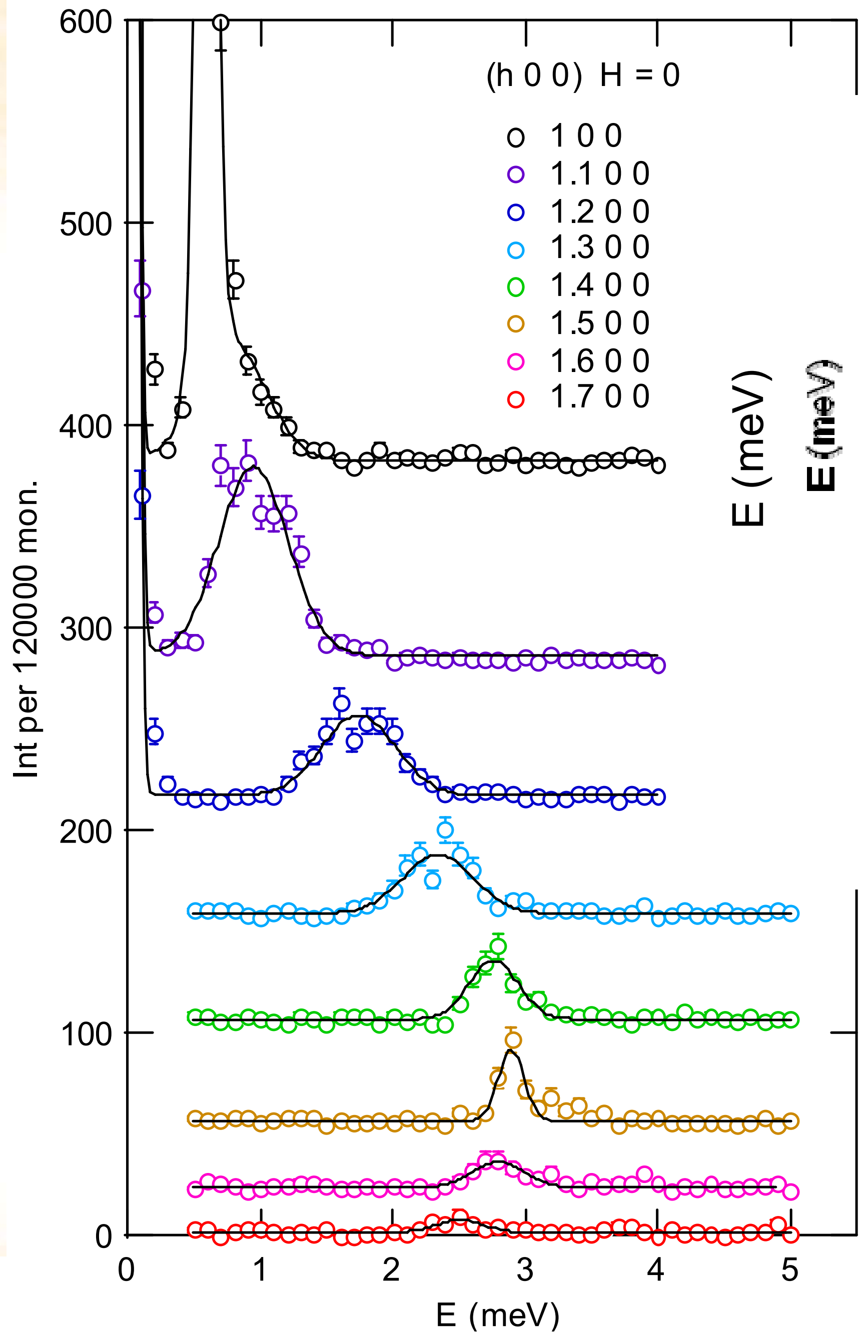
$CsMnCl_3\ 2(D_2O)$

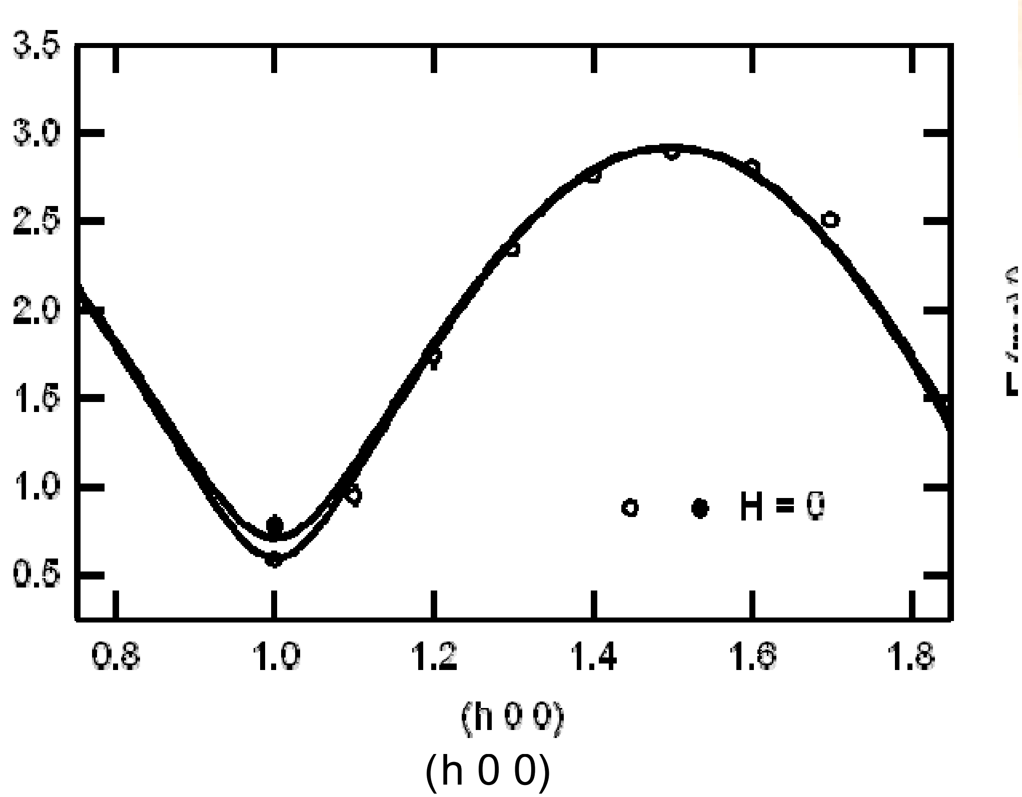


- Mn^{2+}, S=5/2≈∞, semiclassical
- Gas of spins at high T
  Curie-Weiss law, Θ = -48 K
- Long range order "spin solid" $T<T_N = 4.9$ K

With A. Zheludev and I. Zaliznyak

CsMnCl$_3$ 2(D$_2$O)

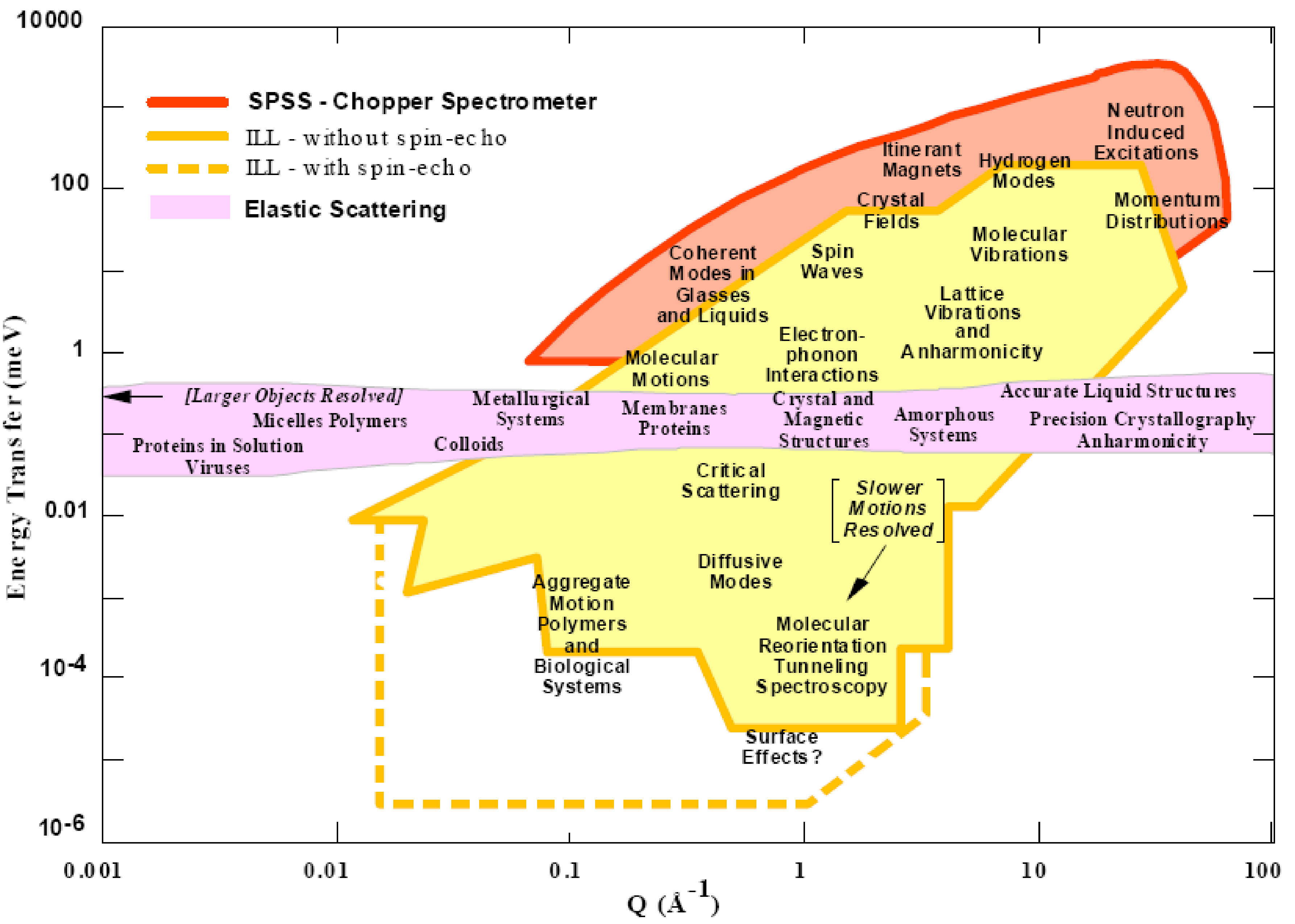




- $J_A = 0.58$ meV
- $J_A/J_B = 0.8\%$
- Semi-classical spin-waves

D ~ -0.007 meV (anisotropy)

Guideline II: There is no Universal Neutron Spectrometer



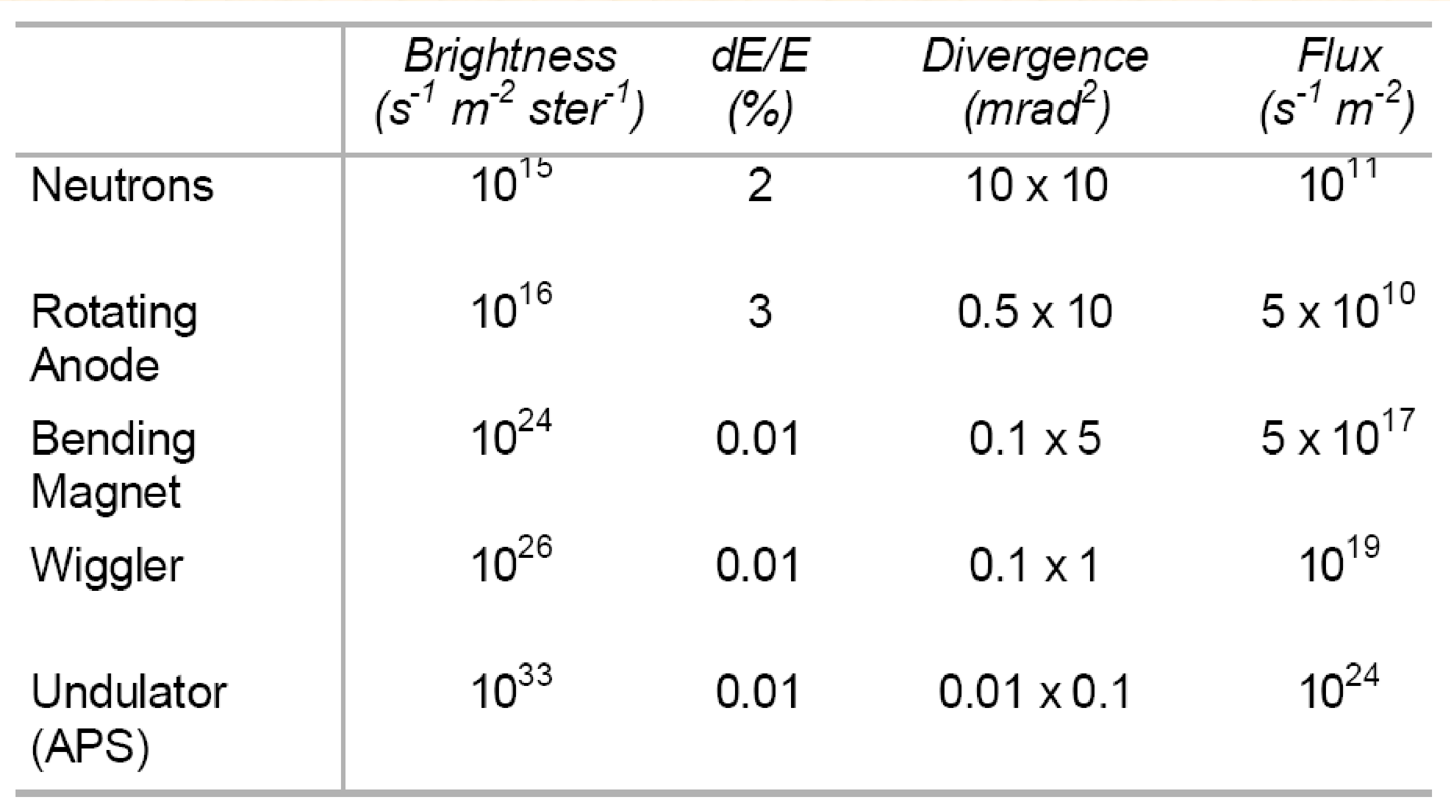
Guideline IIb: Spallation versus Reactor Based Sources

Short Pulse Spallation Source	Reactor
Neutron spectrum is “slowing down” spectrum – preserves short pulses	Neutron spectrum is Maxwellian
Cons e	red ept ator tive
Copio m	y nd slow dynamics
Low background between pulses => good signal to noise	Pulse rate for TOF can be optimized independently for different spectrometers
Polarization possible, but difficult	Neutron polarization easier

- Choose your instrument based upon the physics being probed

- Instrument scientists can discuss possibilities and limitations prior to submission of beam-time proposal

Guideline III: Neutron Flux is comparatively low



	Brightness (s^{-1} m^{-2} $ster^{-1}$)	dE/E (%)	Divergence ($mrad^2$)	Flux (s^{-1} m^{-2})
Neutrons	10^{15}	2	10 x 10	10^{11}
Rotating Anode	10^{16}	3	0.5 x 10	5 x 10^{10}
Bending Magnet	10^{24}	0.01	0.1 x 5	5 x 10^{17}
Wiggler	10^{26}	0.01	0.1 x 1	10^{19}
Undulator (APS)	10^{33}	0.01	0.01 x 0.1	10^{24}

- Implies large single crystals or large quantities of powder.
- Calculate or Compare to prior measurements to determine appropriate sample size.
- Can use broad and tunable resolution to advantage!

Closing thoughts

- **Inelastic neutron scattering allows for the measure of excitations over a range of energy and length scales.**
- **Need to choose the right instrument.**
- **Need appropriate samples (mass, powder, single crystal, isotopic purity, etc.).**
- **Often need to know what you are looking for.**
- **Don’t hesitate to discuss experiments with instrument scientists prior to submission of proposal (feasibility, length of time, instrument considerations, etc.).**
- **Submit proposals to** http://www.ornl.gov/sci/iums/ipts/

Or Google: ORNL neutron proposal