Triple-Axis Spectroscopy

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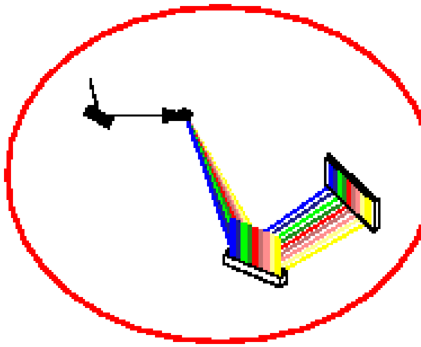
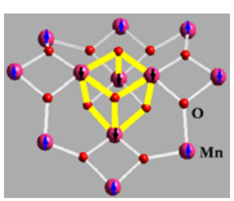
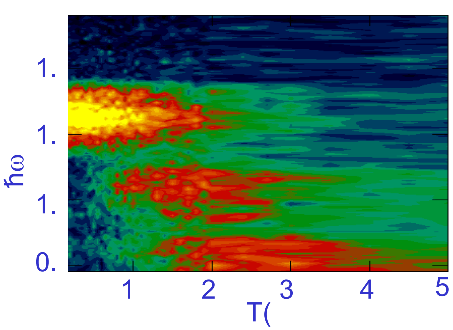
Outline

- Basic principles of TAS
- Multiplexing detection modes for TAS
    1. Horizontally focusing mode
    2. Position-sensitive-detector (PSD) mode
- Examples of science utilizing the PSD mode

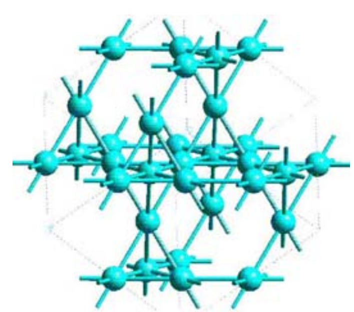


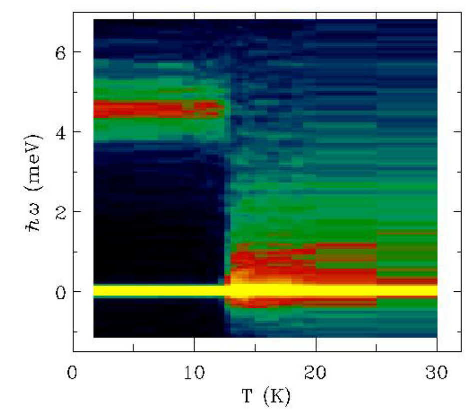
Mn_{12} : Magnetic Molecule



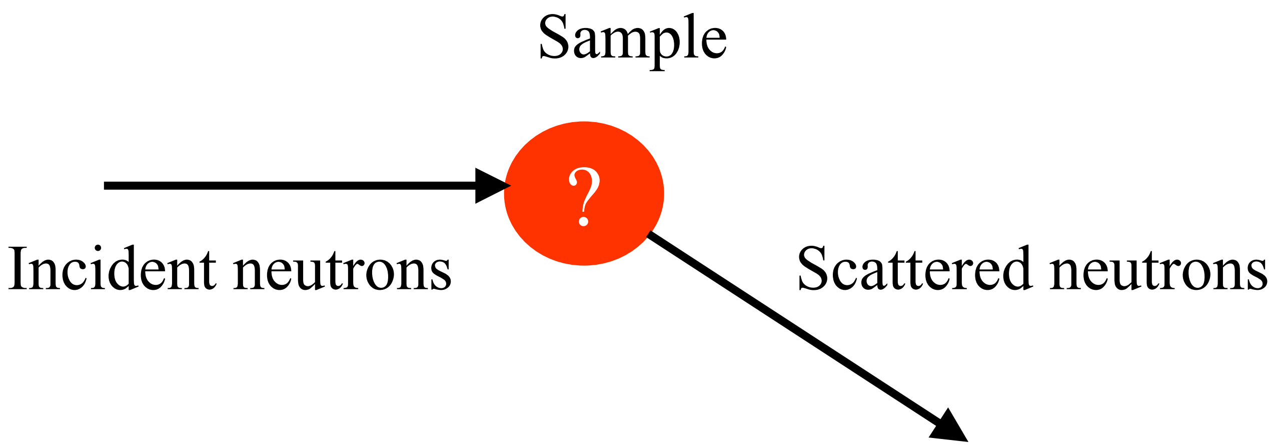


$ZnCr_2O_4$: Geometrically Frustrated Magnet





Neutron Scattering



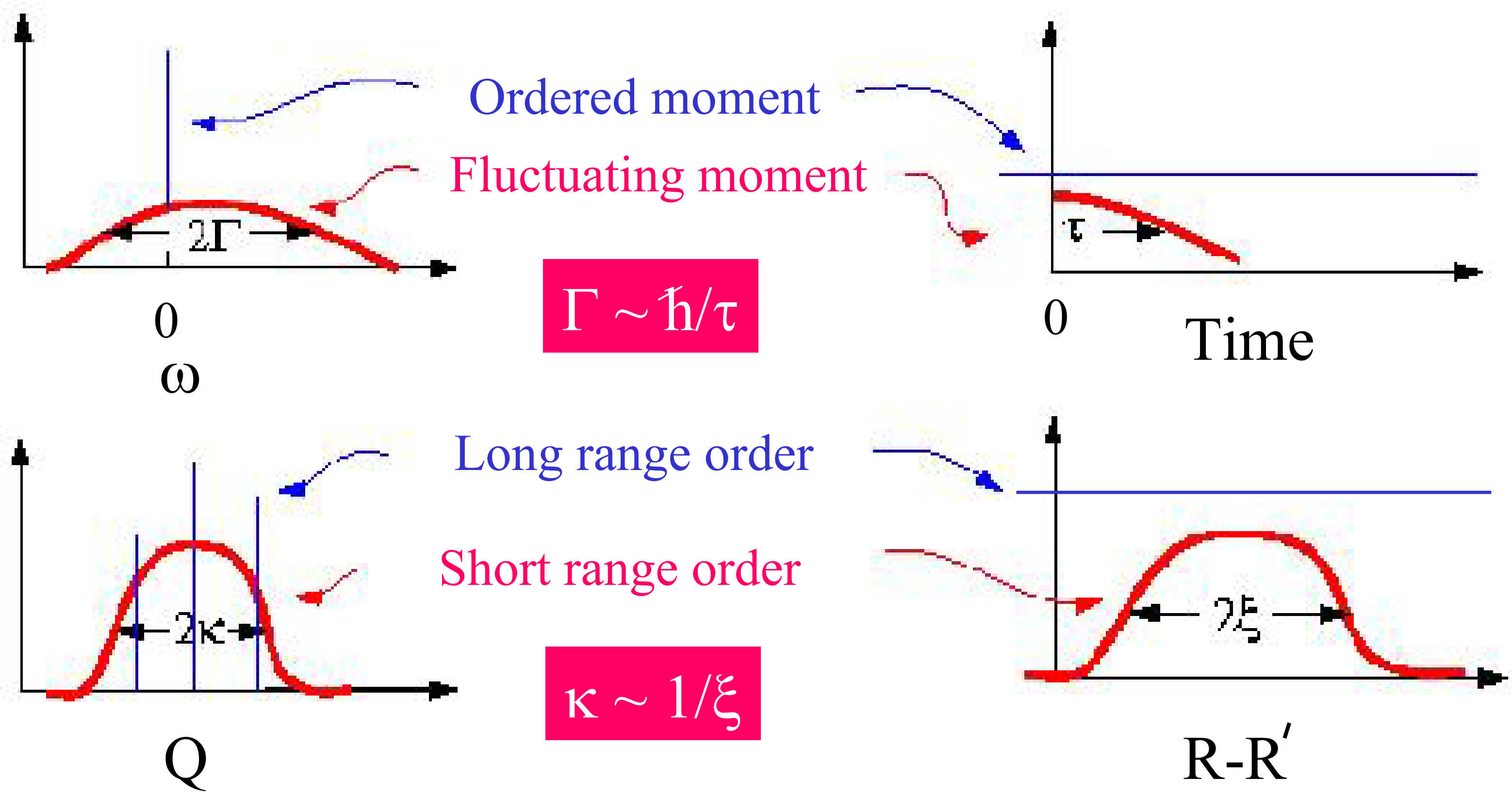
measures scattering cross section as a function of Q and ω

$$\frac{d^2\sigma}{d\Omega d\omega}(\mathbf{Q},\omega)$$

Neutron Scattering Cross Section

Correlation Function

$$\frac{d^2\sigma}{d\Omega d\omega} \quad \xleftrightarrow{\text{Fourier Transform}} \quad \langle S_R(t)\, S_{R'}(0) \rangle$$



Γ : relaxation time

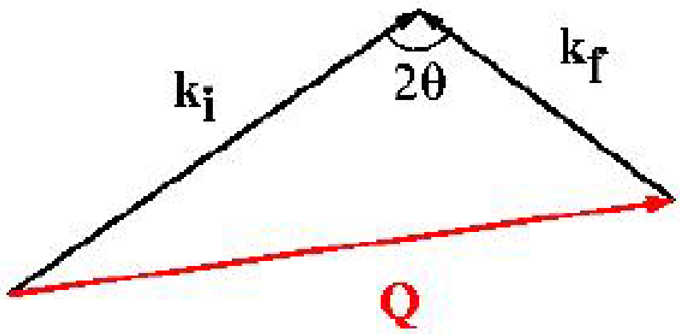
κ : intrinsic linewidth

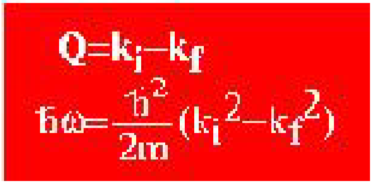
τ : lifetime

ξ : correlation length

How can we determine Q and ω ?

Scattering triangle : Energy and momentum are conserved in the scattering process

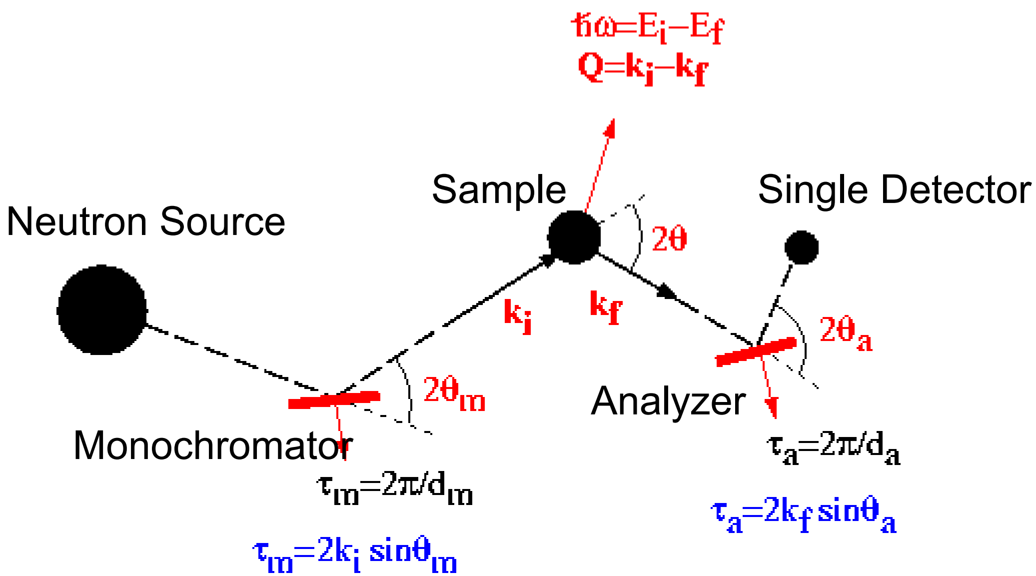




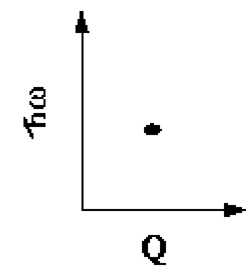
Now, how to determine k_i, k_f, and 2θ ?

- Triple-axis spectroscopy (TAS)
- Time-of-flight spectroscopy (TOF)

Conventional Triple-Axis Spectroscopy (TAS)



A single point at a time



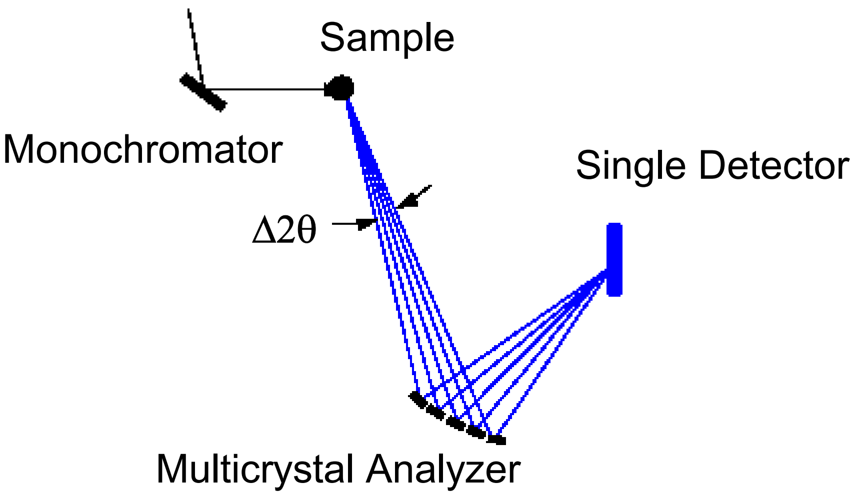
TAS is ideally suited for probing small regions of phase space

Shortcoming: Low data collection rate

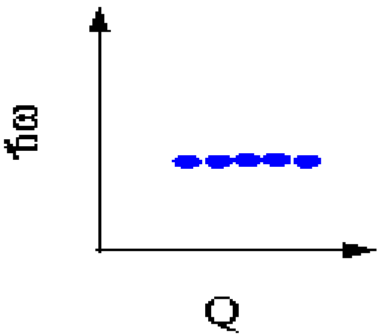
Improvement

Multicrystal analyzer and position-sensitive detector

Horizontally Focusing (HF) Analyzer Mode



Relaxed Q-resolution

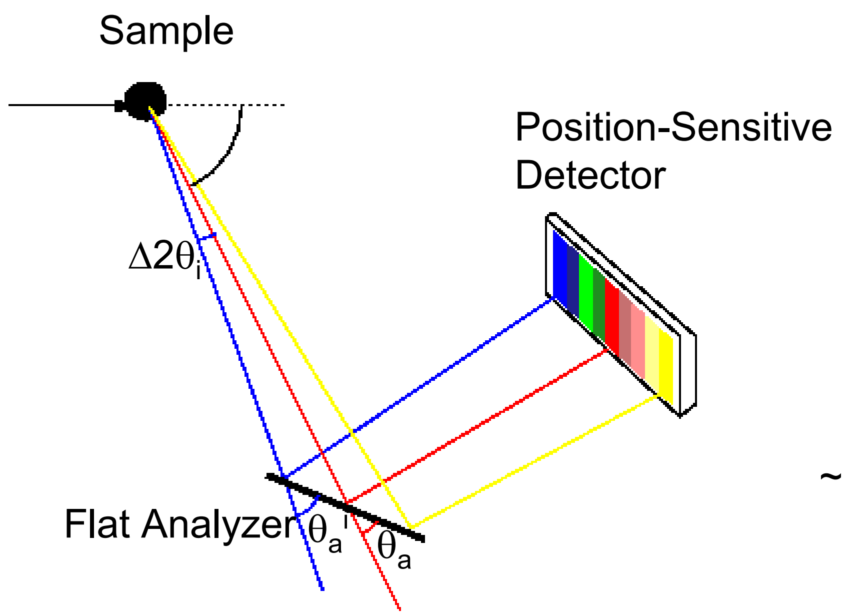


L = distance from sample to HF analyzer
w_a = total width of HF analyzer

$\Delta 2\theta = w_a \sin\theta_a / L \sim 9$ degree for E_f=5 meV at SPINS

Useful for studying systems with short-range correlations

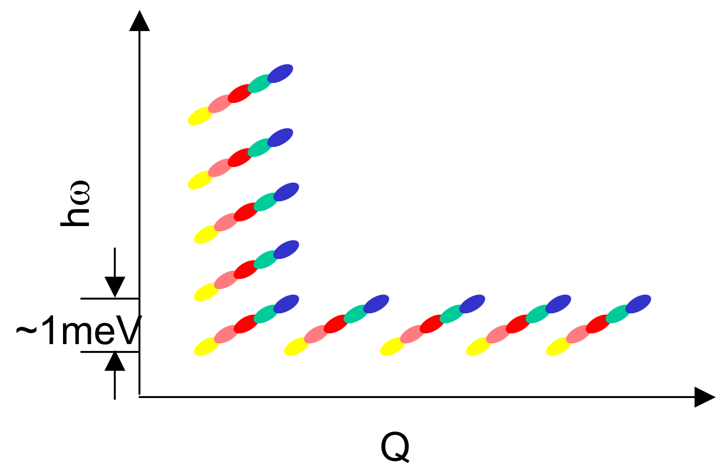
Multiplexing Detection System for TAS



$\theta_a^i = \theta_a + \Delta 2\theta_i = \theta_a - \mathrm{atan}(x \sin\theta_a/(L+x\cos\theta_a))$

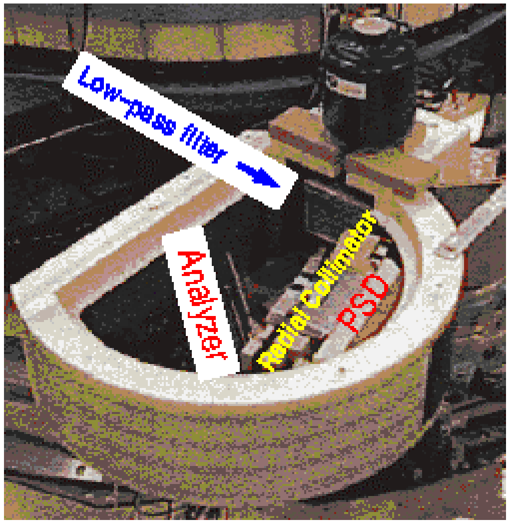
$k_f^i = \tau_a/2\sin\theta_a^i$

$\mathbf{Q_i = k_i - k_f^i}$

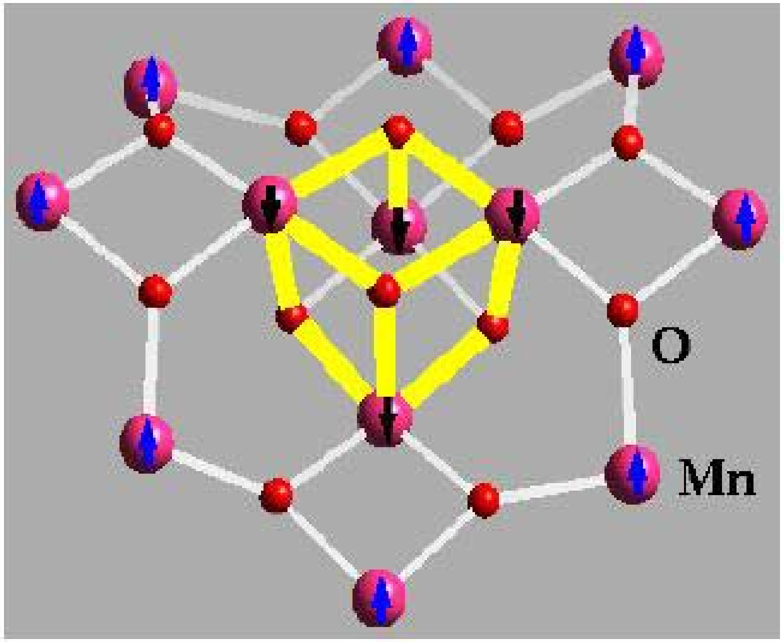


Probes scattering events at different energy and momentum transfers simultaneously

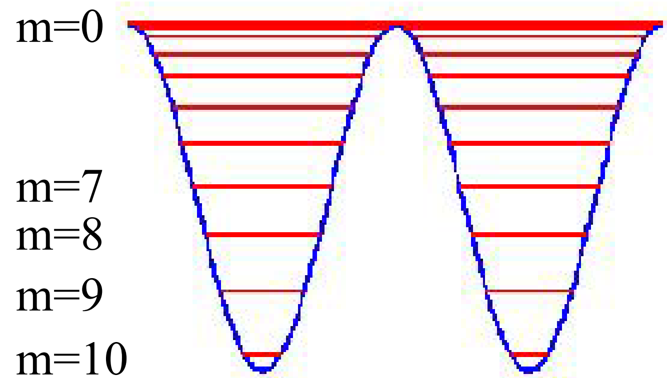
Survey (hω-Q) space by changing the incident energy and scattering angle



Mn_{12}: Magnetic Molecule



Energy levels : $H = -D\, S_z^2$

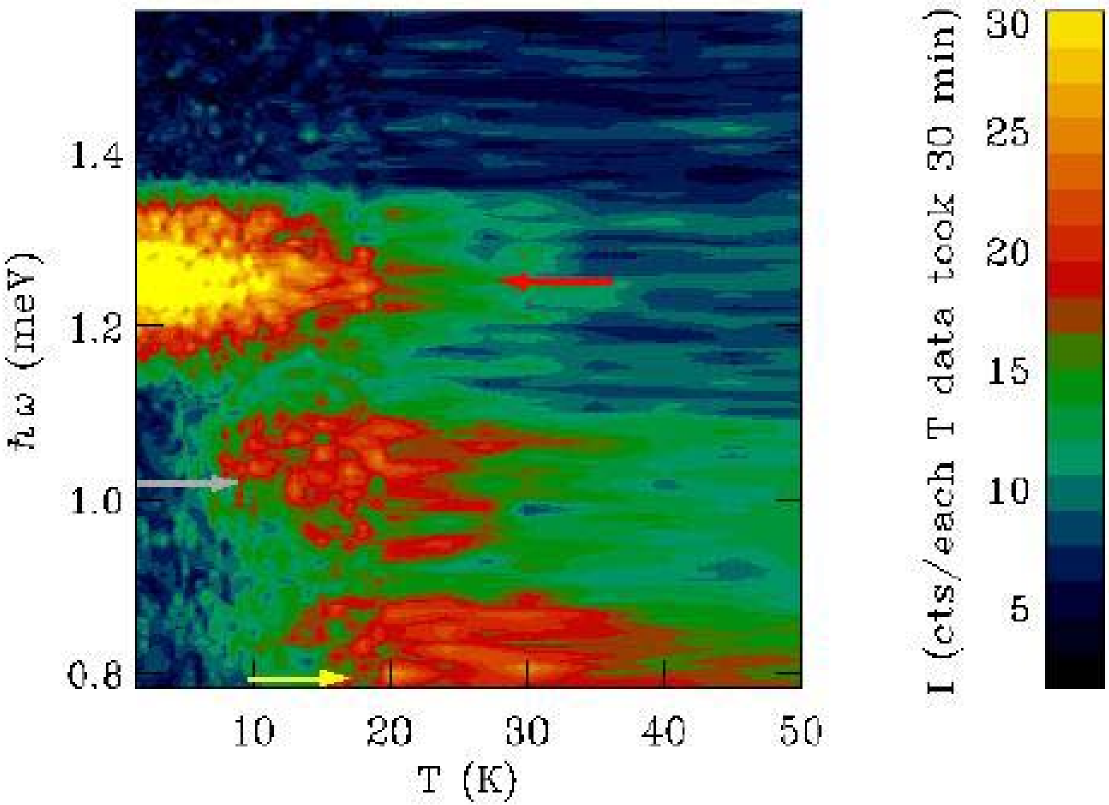


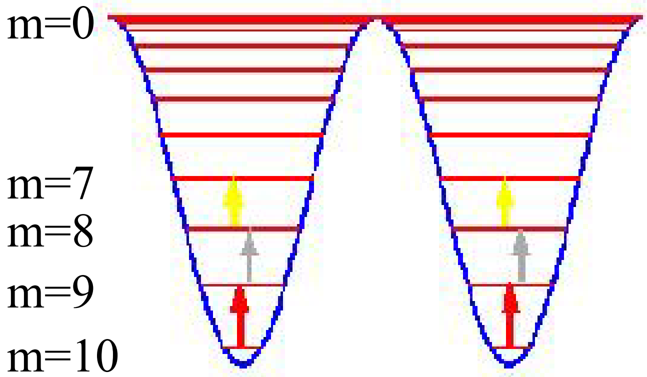
Mn^{3+} (S=2)

Mn^{4+} (S=3/2)

$S_{tot} = 10$

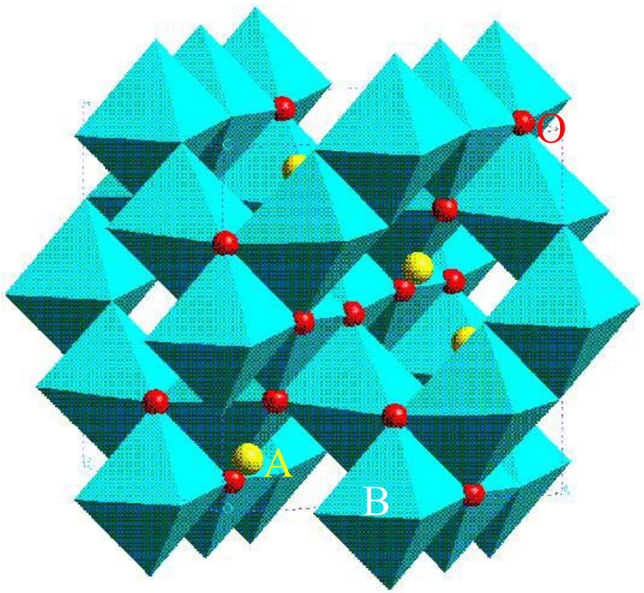
Mn_{12} Magnetic Molecule : I (T,w) at Q = 1 A^{-1}





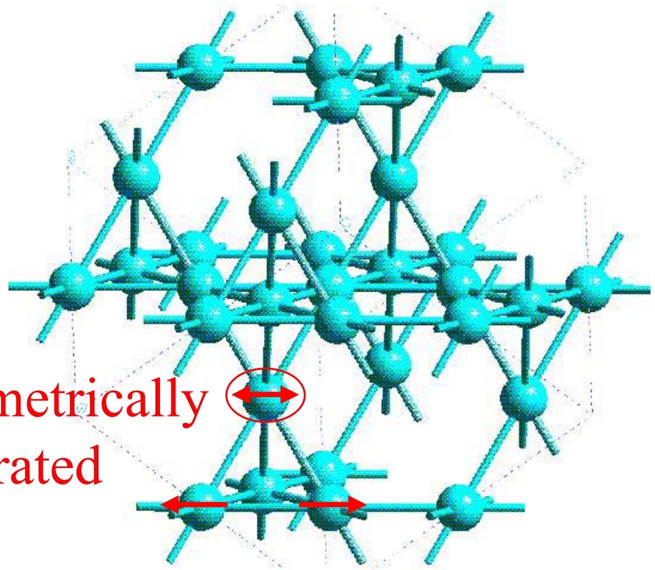
The peaks correspond to transitions between different energy states

Crystal Structure of Spinel $ZnCr_2O_4$



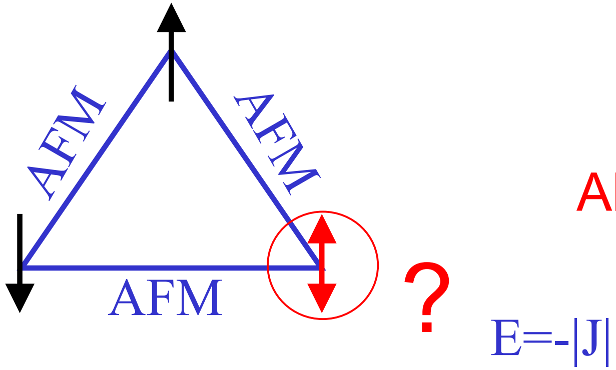
Space group Fd3m
B site: the center of O octahedron with a slight trigonal distortion

B sites form a network of corner-sharing tetrahedra -> Frustrating lattice for antiferromagnetic spins



Geometrical Frustration

A simplest example: a Triangle of three antiferromagnetic Ising spins

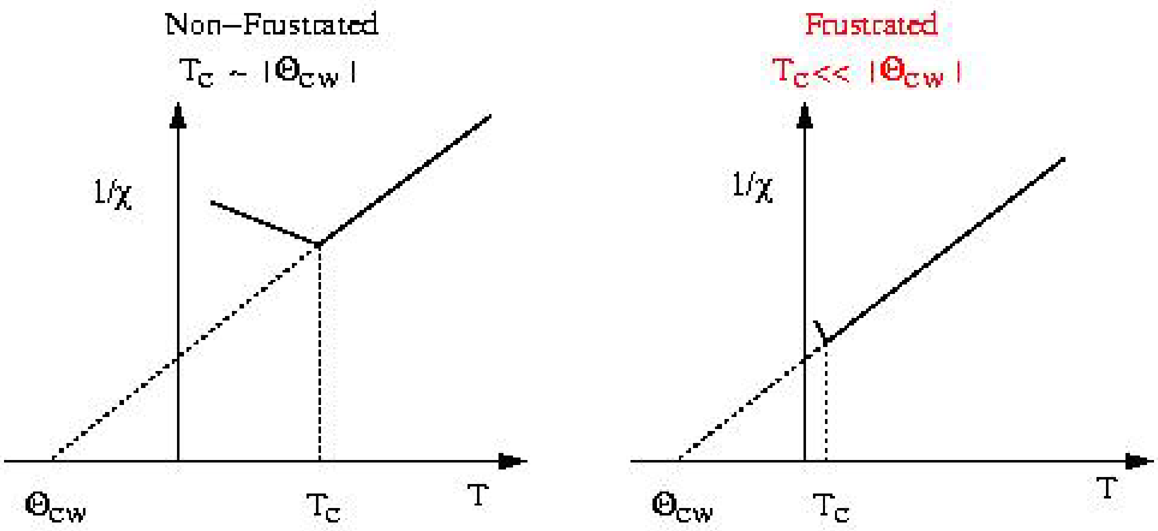


$$H = -J \sum \mathbf{S}_i \cdot \mathbf{S}_j$$

All exchange interactions can not be satisfied.

Geometrical frustration leads to a large degeneracy in the ground state

Effect of Geometrical Frustration

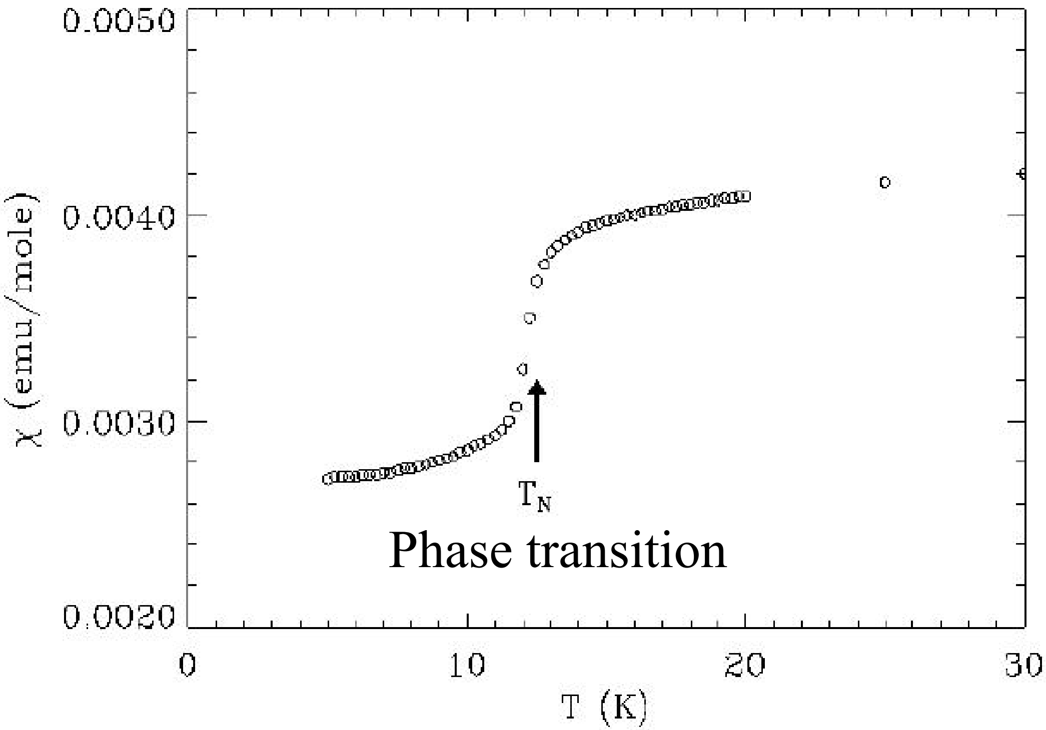


Frustration suppresses the magnetic ordering

A new state of matter ?

Initial Experimental Planning :

Bulk susceptibility from $ZnCr_2O_4$

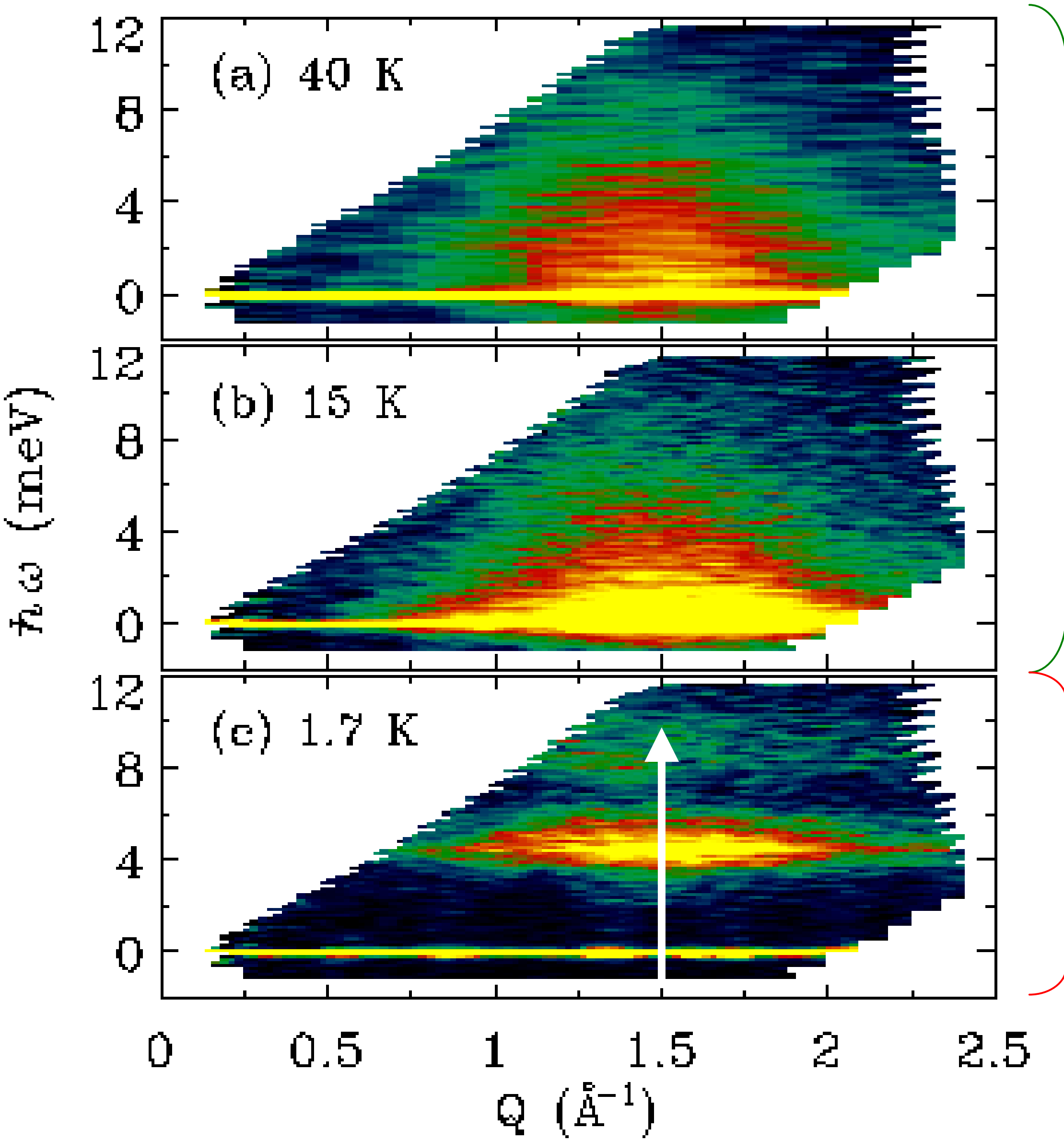


Θ_{CW} = -390 K

T_N = 12.5 K

How do the spin correlations change through the phase transition ?

Neutron Scattering from $ZnCr_2O_4$



Paramagnetic fluctuations in frustrated AFM

Local spin resonance in magneto-elastic LRO phase

Keywords for SPINS Hand-on Experiments

- Triple-axis spectroscopy

  Multiplexing detection system for a TAS
- Spin correlations
- Magnetic phase transition

- Long range vs Short range order

- Static spin correlations — Elastic neutron scattering
- Dynamic spin correlations — Inelastic neutron scattering