The Magnetic phase transition in the frustrated antiferromagnet $ZnCr_2O_4$ using SPINS

Group B

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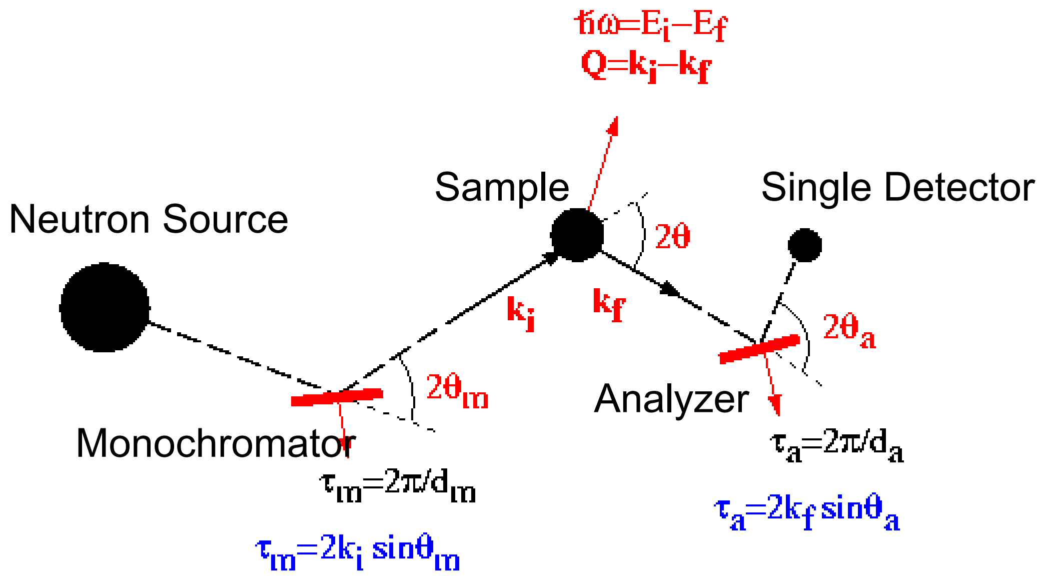
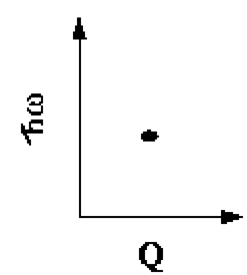
Outline

- Principle of triple axis neutron spectrometry
- Sample properties: crystal and magnetic structure
- Sample behavior: macroscopic (magnetic) properties
- Neutron results: structural and dynamic information

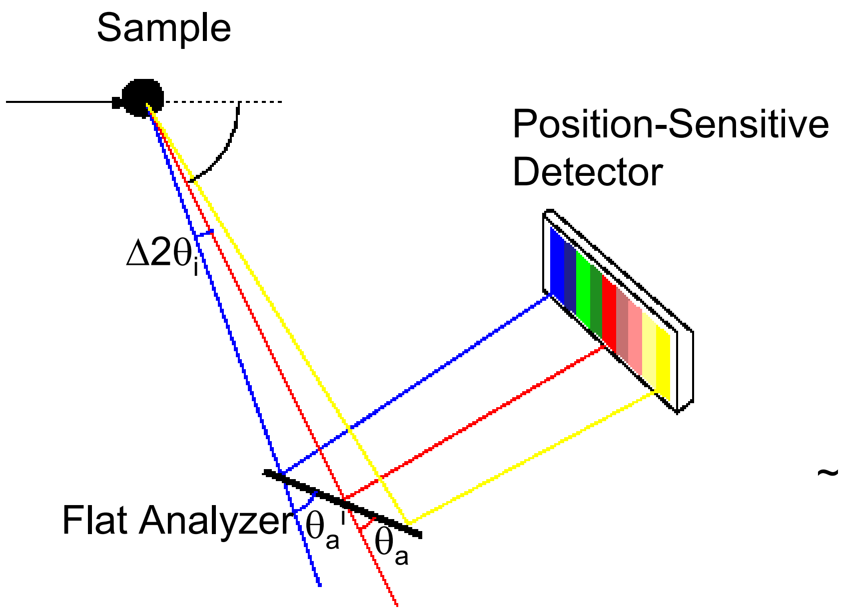
Conventional Triple-Axis Spectroscopy (TAS)



A single point at a time



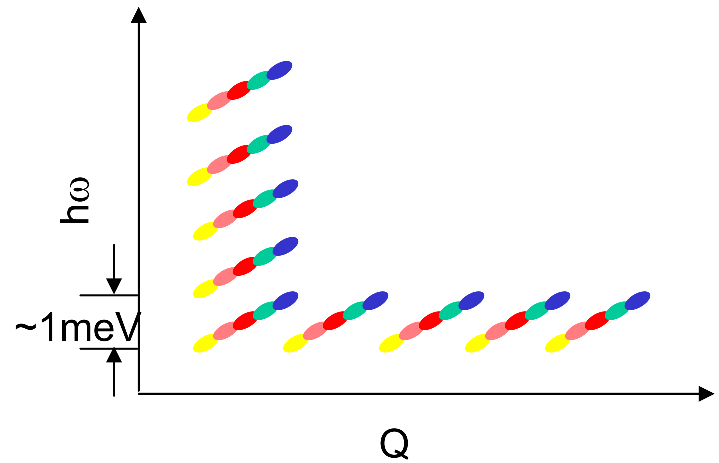
Multiplexing Detection System for TAS

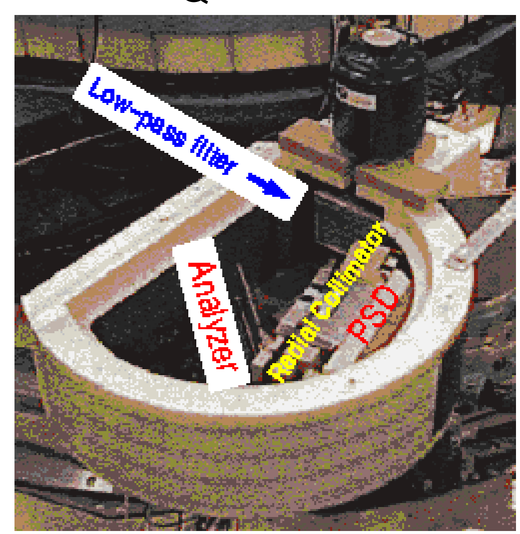


$\theta_a^i = \theta_a + \Delta 2\theta_i = \theta_a - \mathrm{atan}(x \sin\theta_a/(L+x\cos\theta_a))$

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

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



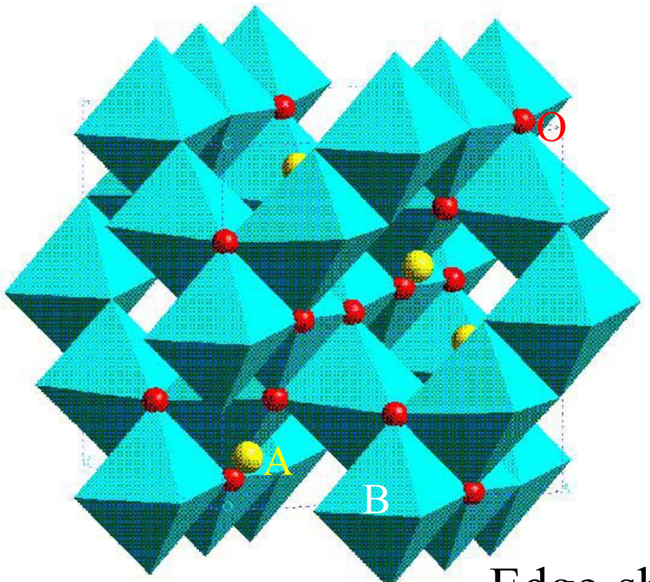


Probes scattering events at different energy and momentum transfers simultaneously

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

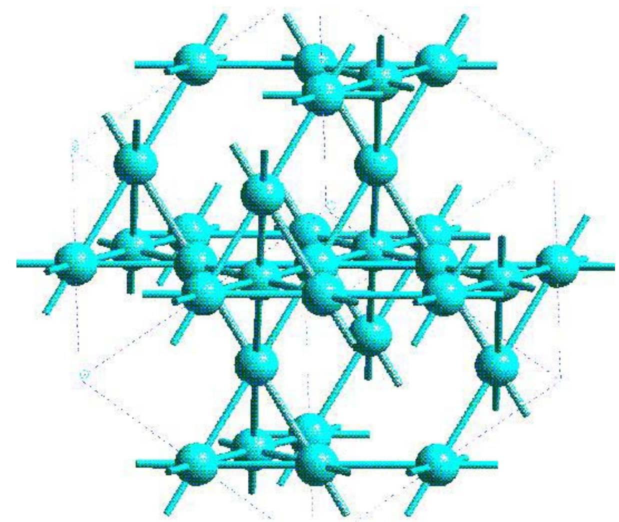
Sample structure ($ZnCr_2O_4$)

Space group Fd3m

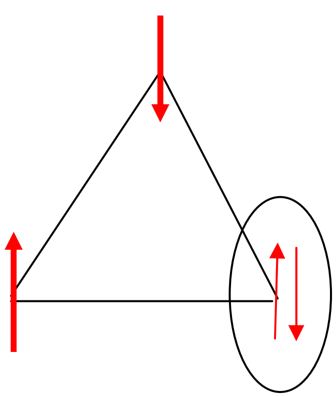


Edge-sharing
octahedra

Lattice of B sites
: Corner-sharing tetrahedra

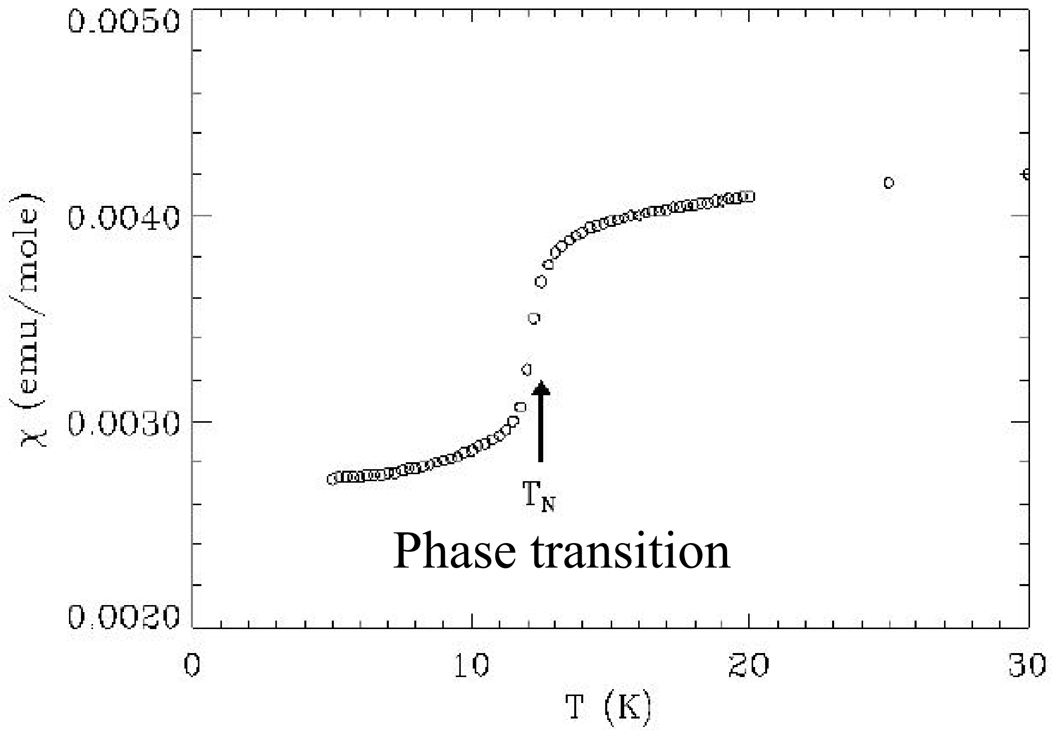


$$H = -J \sum_{nn} \mathbf{S_i} \cdot \mathbf{S_j}$$



? Multiple energetically equivalent configurations:
Geometric frustration

Magnetic Phase Transition in $ZnCr_2O_4$



$\Theta_{CW} = 390$ K

$T_N = 12.5$ K

What information do we expect to get from neutron scattering?

- Static information: crystal structure and magnetic ordering, thus perform elastic scattering.

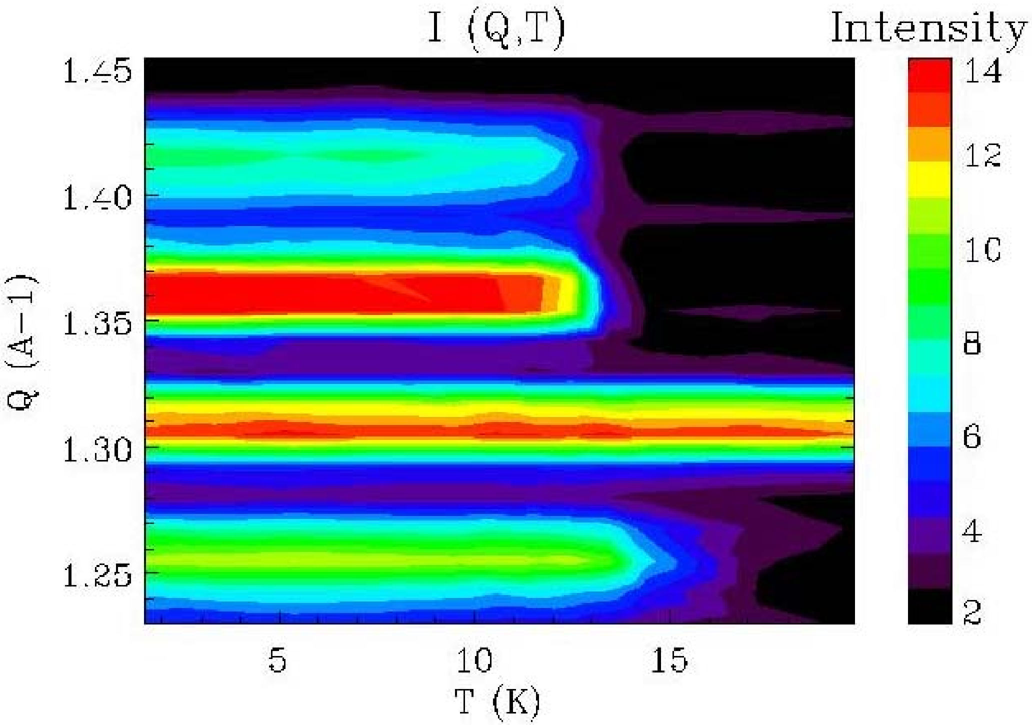
- Dynamic information: what “excitations” do we observe and how they evolve with temperature, thus look for inelastic peaks

- Dynamic and static correlations, thus look at peak linewidths.

- How are the fluctuating spins in the spin liquid phase correlated with each other?

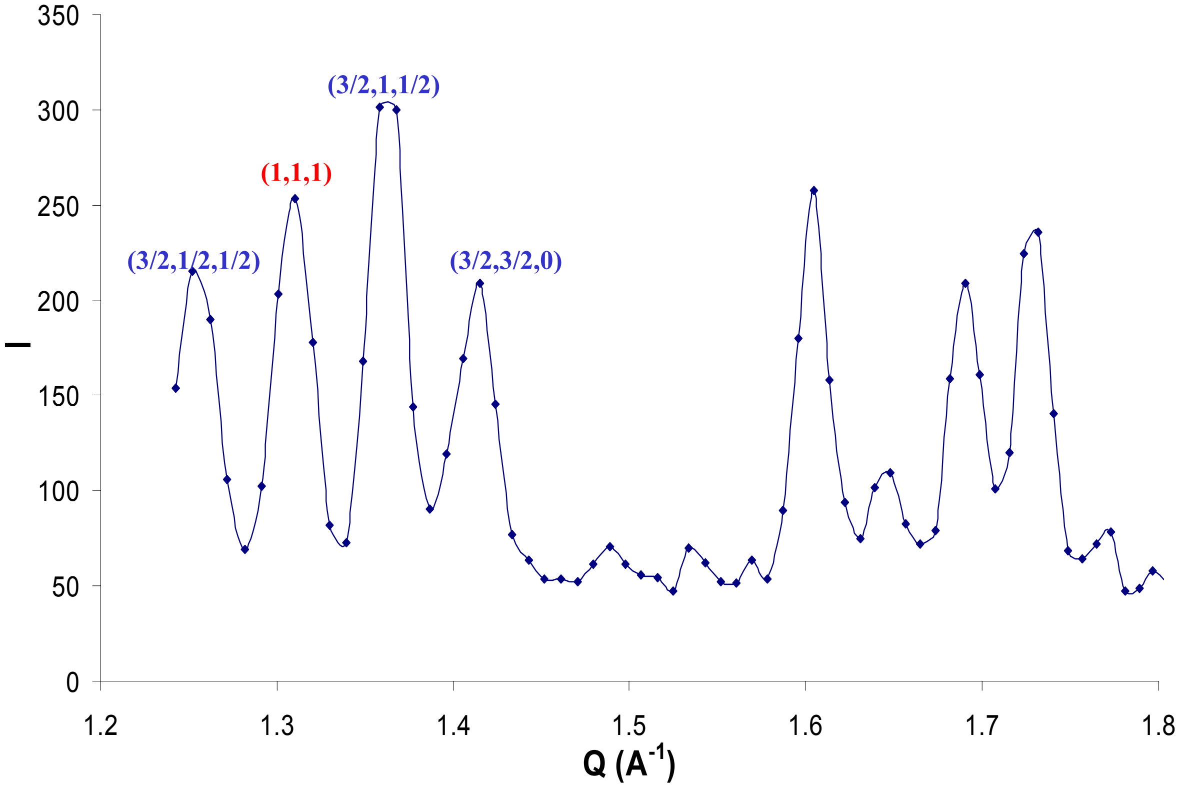
- How do the spin correlations change with the phase transition?

I. Structural data



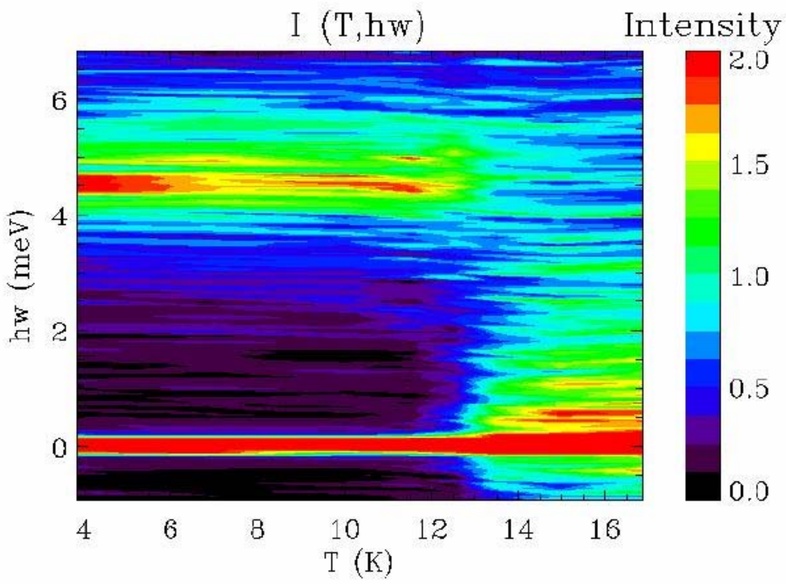
- Perform Q scan at zero energy transfer at several temperatures
- Estimate Q resolution: $\Delta Q_{FWHM} \approx 0.2 Å^{-1}$
- Estimate energy resolution: $\Delta(\hbar\omega)_{FWHM} \approx 0.2 meV$
- Appearance of several magnetic peaks below the AF T_N

Structural insight gained



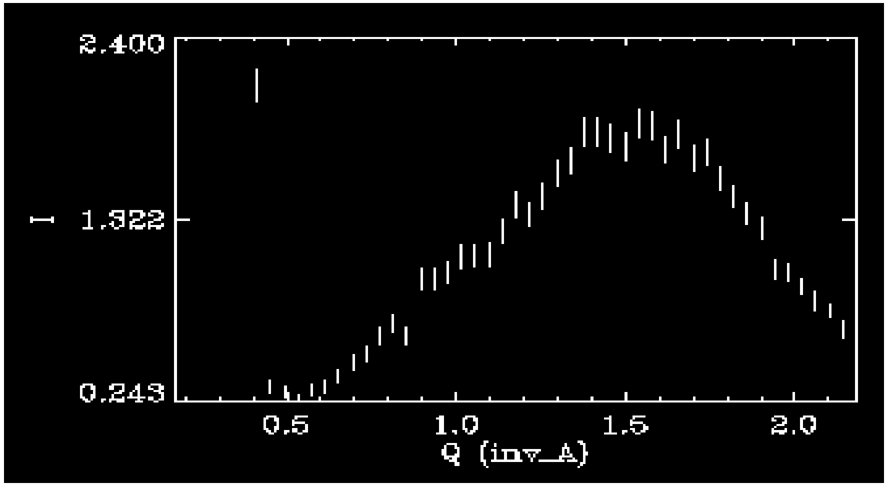
- Position of (1,1,1) nuclear peak doesn't shift
- Several half integer indexed peaks appear
- Comparable peak linewidths: Long range structural order

II. Dynamical data

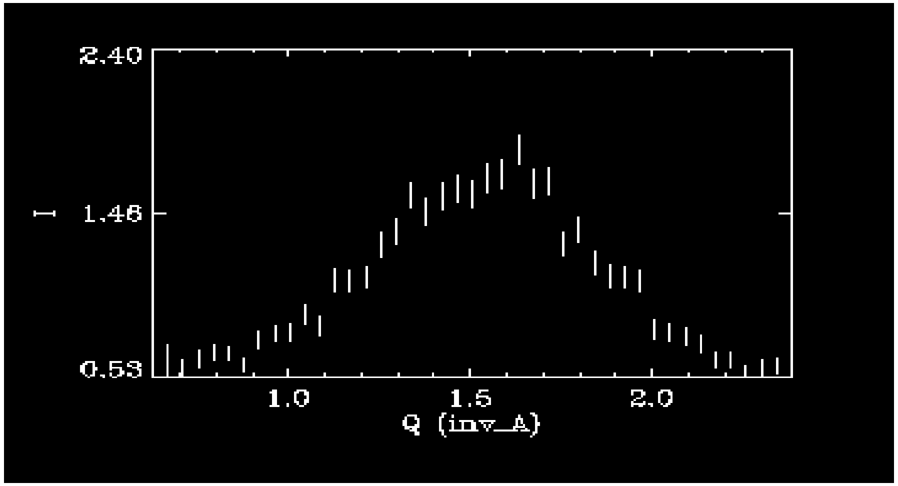


- Scan for energy spectral weight at $Q=1.5Å^{-1}$
- Shift in spectral weight from low (quasielastic)to high (inelastic) energy at T_N.
- $T>T_N$: Thermal energy broadening.
- $T<T_N$: 4.5meV peak FWHM≈0.5meV (lifetime≈8ps).
- What excitation is it?
- Why the jump in energy?

II. More dynamical data



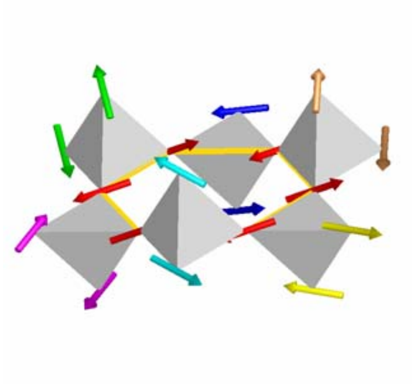
ħω=1.5meV, T=15K



ħω=4.5meV, T=1.5K

- Q scans at low and high T
- Correlation length at ħω =1.5meV and T=15K is ~2.5 Å
- Correlation length at ħω =4.5meV and T=1.5K is ~3.2 Å
- Approximately same range of dynamic spin correlations; comparable to nearest neighbor distance

Resolution: The nature of the AF state.



- Antiferromagnetic spin hexagons form under T_{CW}.

•These can move independently (new degrees of freedom)

- Still only spin liquid state can be formed (frustration)

- Dynamical correlations of the formed hexagon span its size only

- Frustration disappears due to crystal distortion at T_N (lifting of degeneracy). New AF ordered state appears.

- Why the jump in energy? What is the **Q** dependence? *To be continued…*

Acknowledgements

Seung-Hun Lee

Peter Gehring

Sungil Park