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Magnetic phase transition and spin fluctuations in the geometrically frustrated antiferromagnetic spinel $CdCr_2O_4$: An experiment using the SPINS cold-neutron triple axis spectrometer

Group A

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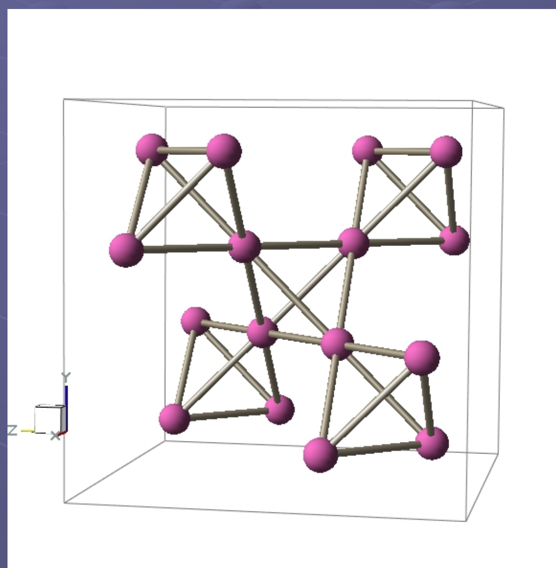
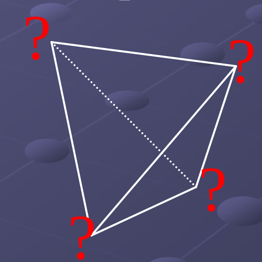
NIST Center for Neutron Research

$CdCr_2O_4$: Cr^{3+} ($3d^3$, S =3/2)

Magnetic Cr^{3+} ions form a lattice of corner-shared tetrahedra
Similar lattices are found in spinel (AB_2O_4) B-sites or pyrochlores ($A_2B_2O_7$)

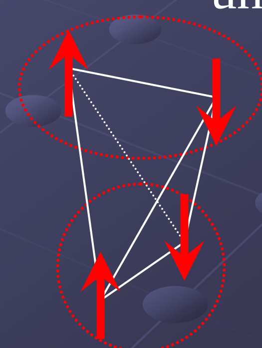


But $CdCr_2O_4$ eventually orders at very low temperatures. How?

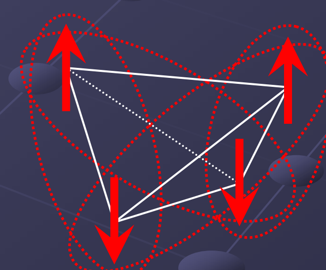


frustrated

unfrustrated



$CdCr_2O_4$



$ZnCr_2O_4$

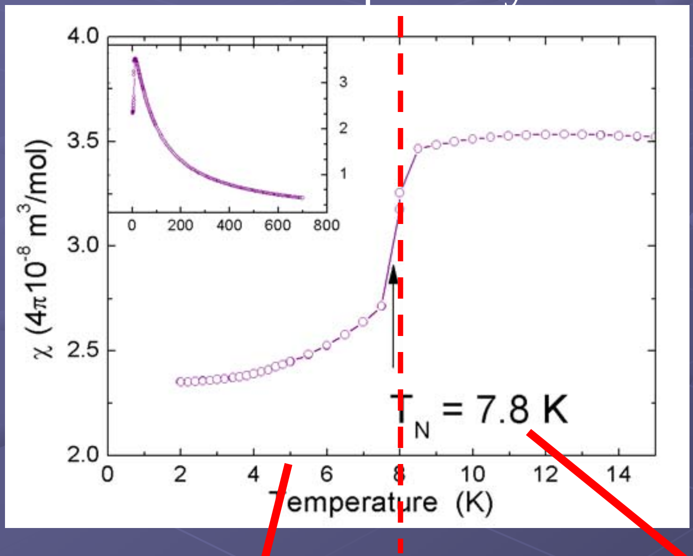
Magnetic exchange energy between a pair of spins is $H = J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j$. If $J_{ij} > 0$, then $\mathbf{S}_i$ and $\mathbf{S}_j$ will become antiparallel to each other.

Magnetic phase transition in $CdCr_2O_4$

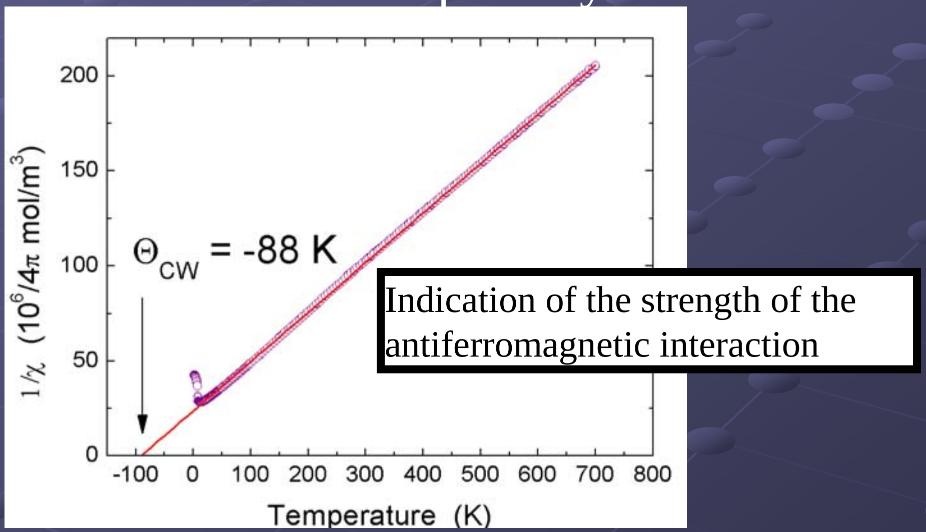
Magnetic susceptibility
$\chi = dM/dH$

M: magnetization of the material
H: applied magnetic field

susceptibility

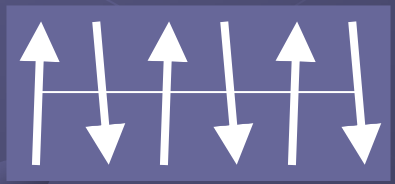


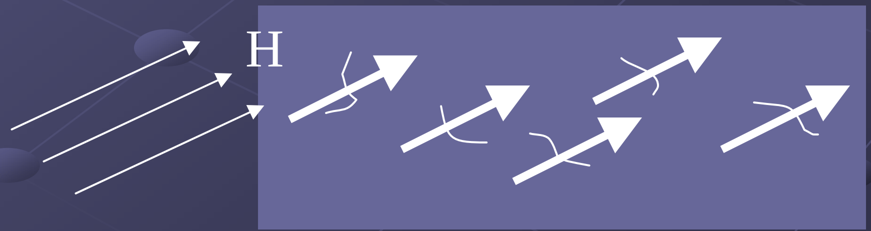
inverse susceptibility



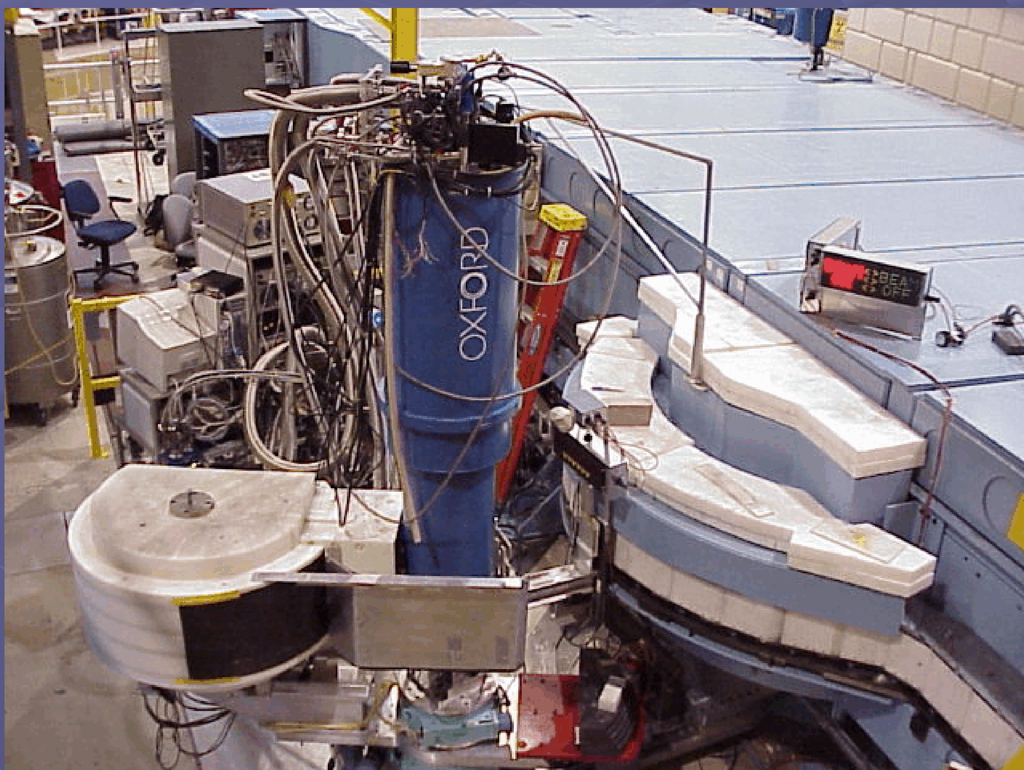
$|\Theta_{CW}| \cong T_N$: normal antiferromagnet

$|\Theta_{CW}| >> T_N$: strong frustration





SPINS cold neutron triple axis spectrometer

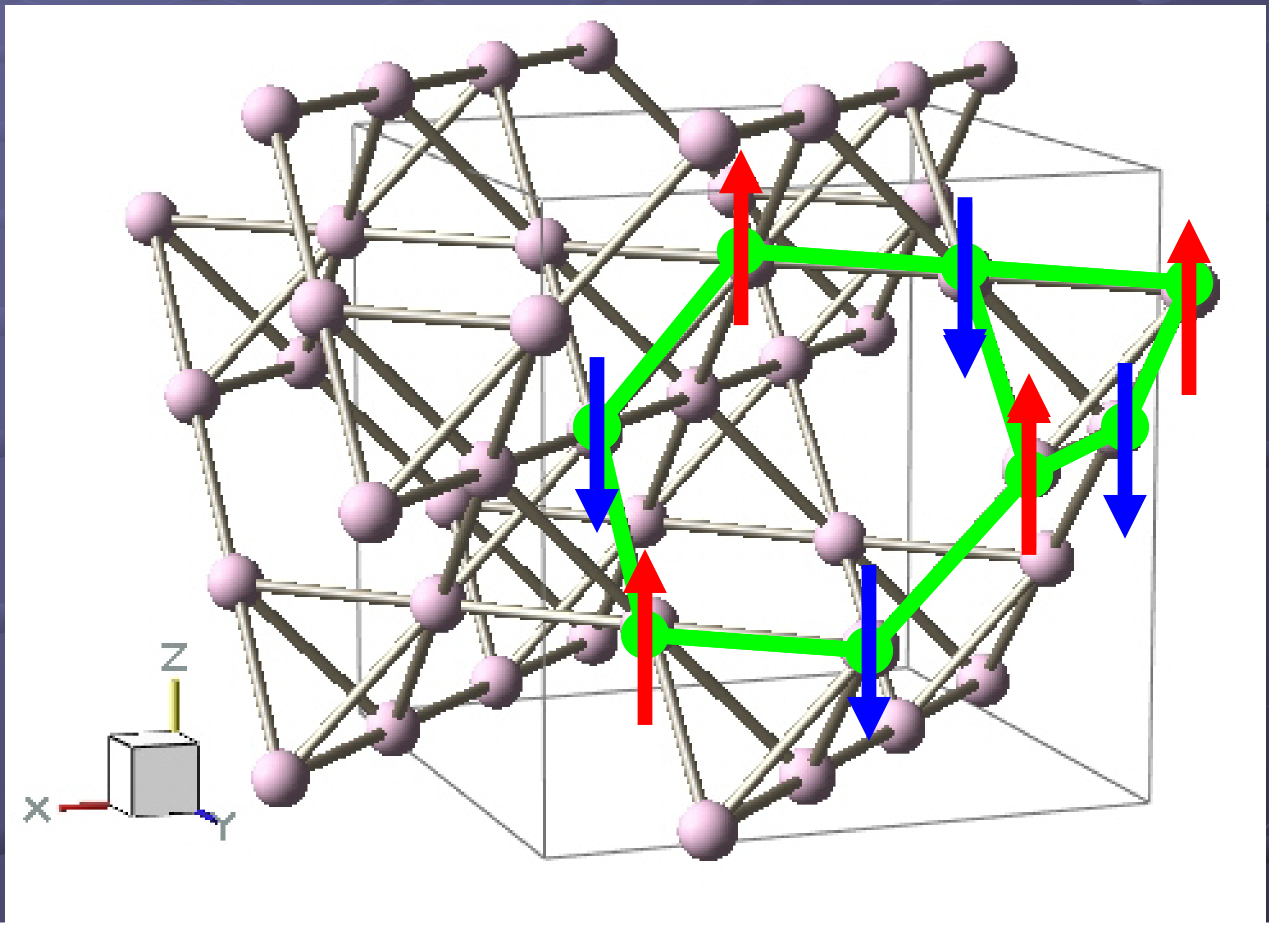


Why SPINS for this study?
Because SPINS

- Precisely access desired Q and $\hbar\omega$
- Covers $\hbar\omega$ in the range between 0.1 to 10 meV
- Perform diffraction measurement
- Provides a flexible choice of high resolution or high intensity

Looking for the degenerate ground states in the geometrically frustrate phase

Using simulations, we can try to determine the magnetic structure by comparing to the collected data.



Simple calculation of magnetic neutron scattering intensity

- Magnetic neutron scattering cross section

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}\omega} = r_o^2 \frac{k_f}{k_i} S(\mathbf{Q},\omega)$$

$$\text{where,}\quad S(\mathbf{Q},\omega) = \sum_{\alpha,\beta} (\delta_{\alpha\beta} - \tilde{Q}_\alpha \tilde{Q}_\beta) \sum_{\lambda,\lambda'} p_\lambda \sum_{l,d} \sum_{l',d'} f_d^*(\mathbf{Q}) f_{d'}(\mathbf{Q}) \exp\{ i\mathbf{Q}\cdot(\mathbf{R}_{l'd'} - \mathbf{R}_{ld})\}$$
$$\times \left\langle \lambda \middle| \hat{S}_{ld}^{\alpha} \middle| \lambda' \right\rangle \left\langle \lambda' \middle| \hat{S}_{l'd'}^{\beta} \middle| \lambda \right\rangle \delta(\hbar\omega + \hbar\omega_\lambda - \hbar\omega_{\lambda'})$$

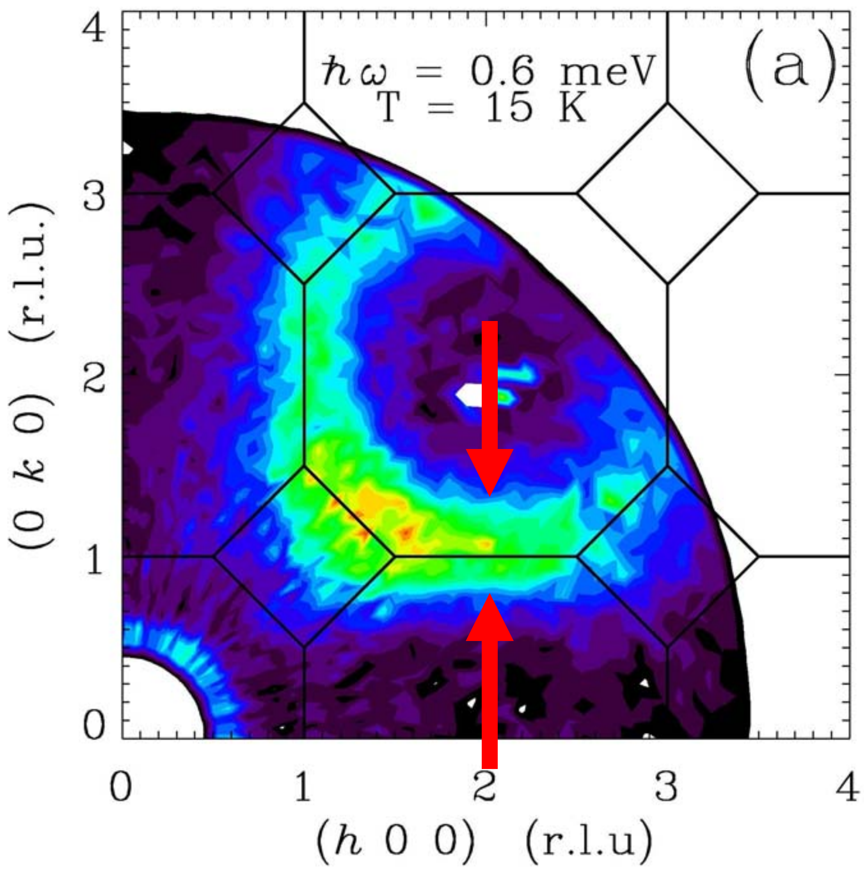
- But if we consider only up and down spins for diffuse quasi-elastic scattering, all we need is the following simple equation:

$$I(\mathbf{Q}) \propto \left| \sum_{\mathbf{R}} f_{\mathbf{R}}(\mathbf{Q}) \sigma_{\mathbf{R}} e^{i\mathbf{Q}\cdot\mathbf{R}} \right|^2 \qquad f: \text{magnetic form factor}$$

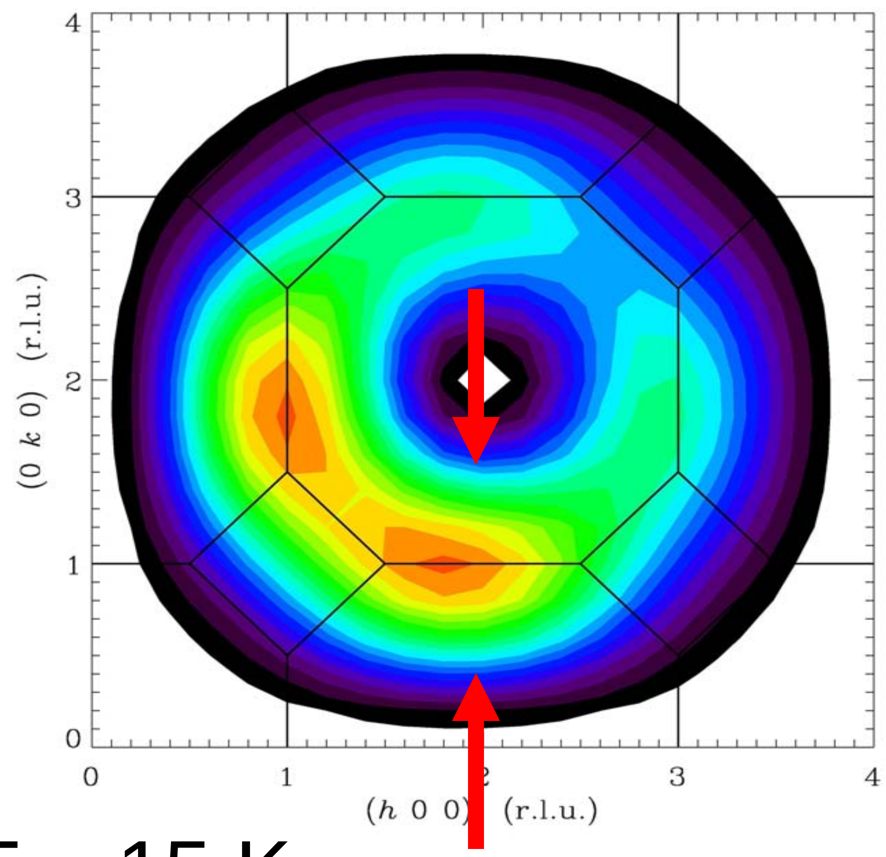
$$\sigma = -1, \text{ or } 1$$

Q-dependence along the (h,0,0) and (0,k,0) crystal configurations

Experimental Data



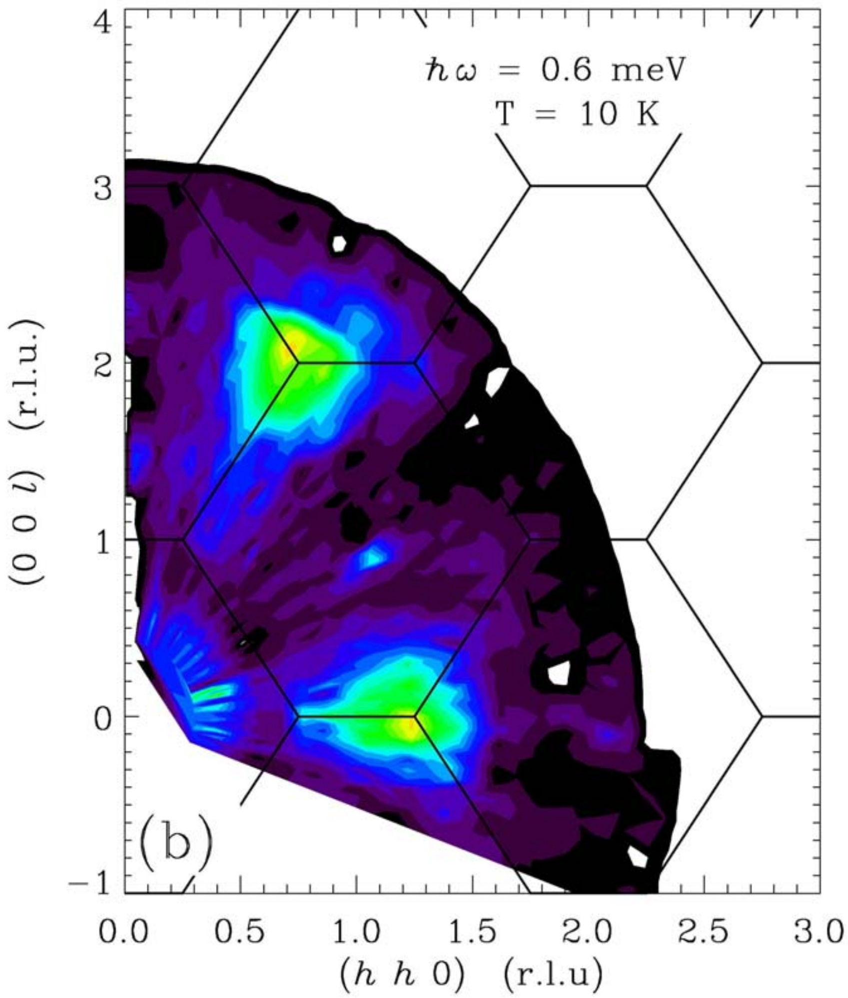
Theoretical Simulation



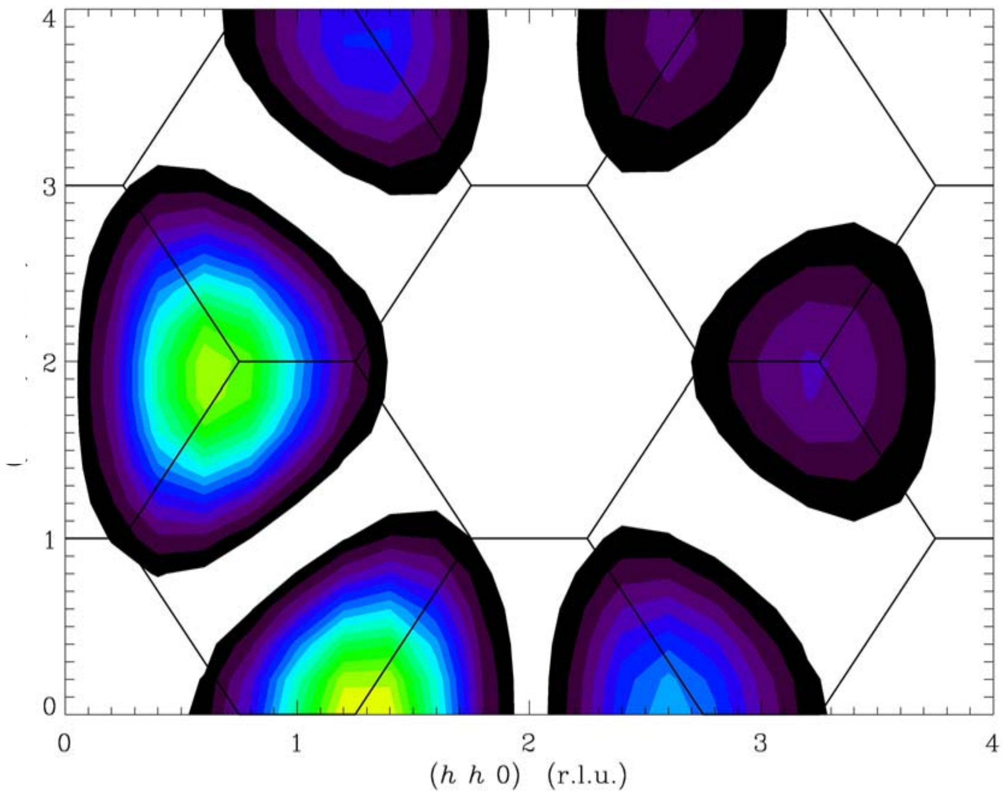
T = 15 K

Q-dependence along the (h,h,0) and (0,0,l) crystal configurations

Experimental Data

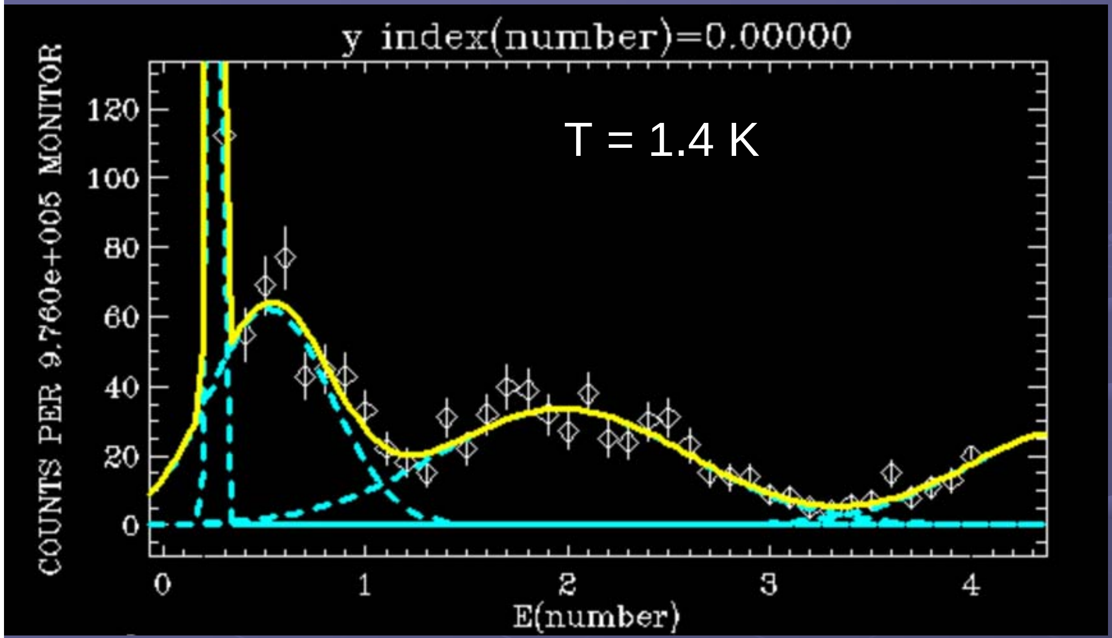


Theoretical Simulation



T = 10 K

Temperature Dependence

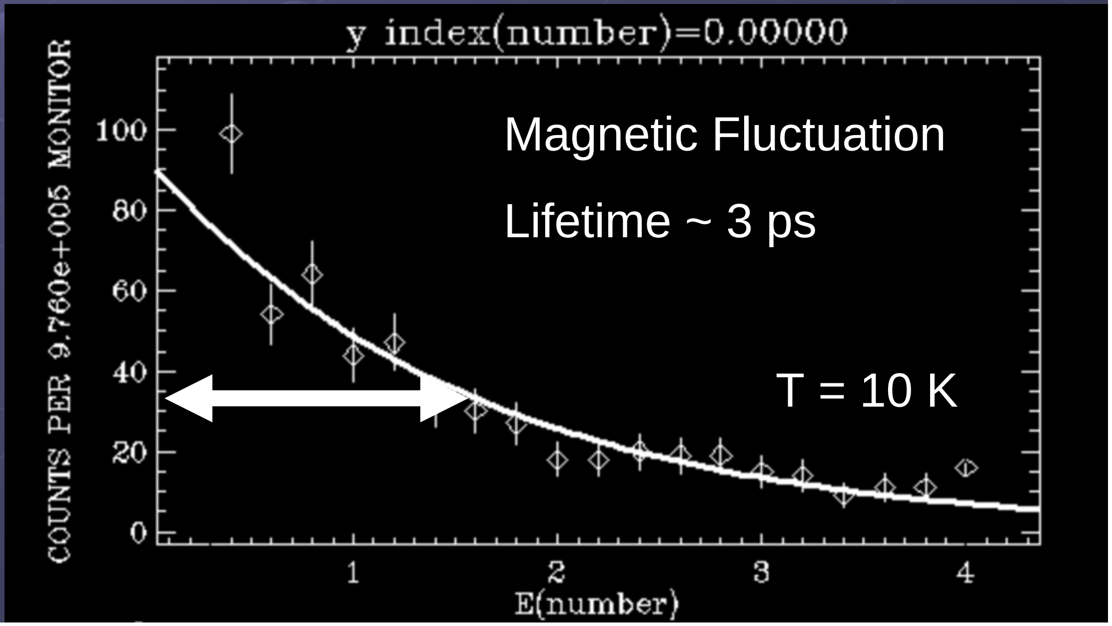


Low Temperature

Magnon Excitations

High Temperature

Short Range Quasi-elastic
Spin Fluctuation



Summary

- Using the Triple-Axis Spectrometer, we studied the magnetic phase transitions in $CdCr_2O_4$, which is a spinel with antiferromagnetic interactions between Cr^{3+} ions on B sites.
- We examined the Q-dependence on different crystal planes.
- Using a theoretical simulations, we were able to determine the basic magnetic structure.
- Through the use of temperature dependence, we were able to find that the discovered peaks are consistent with magnetic excitations.
- The examination of the line width for the quasi-elastic fluctuation shows the lifetime to be on the pico-second scale.

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