Title: Quasiparticle breakdown in the quantum pyrochlore Yb2Ti2O7 in magnetic field

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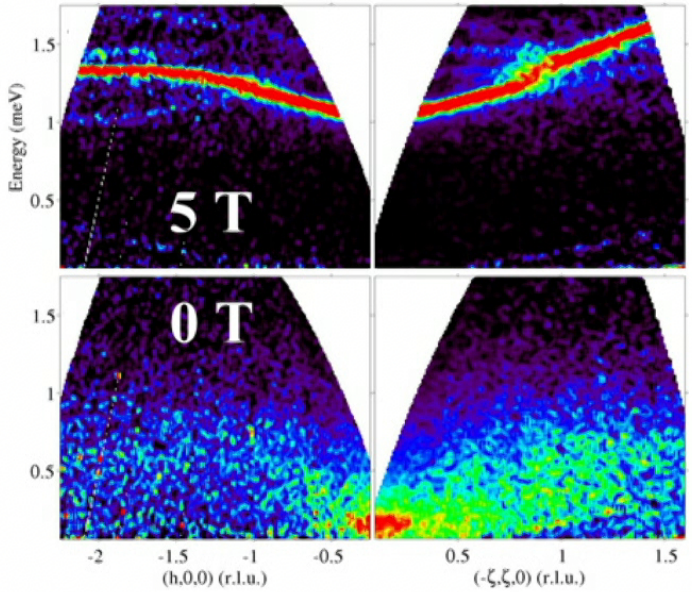
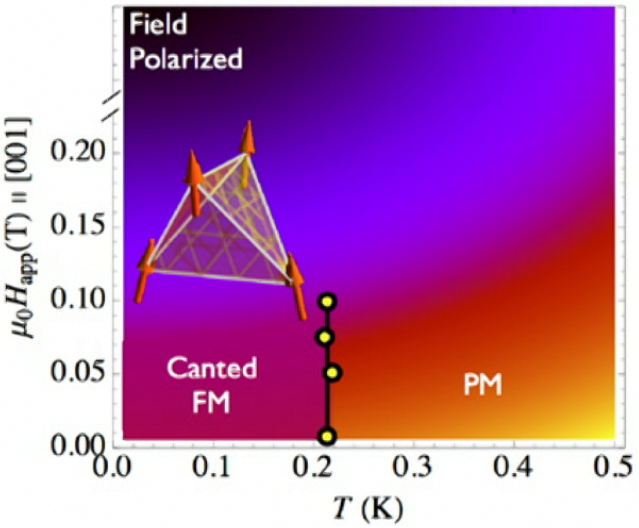
Abstract: The pyrochlore magnet Yb2Ti2O7 has the remarkable property that it orders magnetically, but has no propagating magnons over wide regions of reciprocal space. Using inelastic neutron scattering we observe that at high magnetic fields, in addition to dispersive magnons there is also a two-magnon continuum, which grows in intensity upon reducing field, overlaps with one-magnon states at intermediate fields leading to strong dispersion renormalizations and magnon decays. We re-evaluate the Hamiltonian finding dominant quantum exchange terms, which we propose are responsible for the anomalously strong quantum fluctuation effects observed at low fields.

Quasiparticle breakdown in the quantum pyrochlore $Yb_2Ti_2O_7$ in magnetic field

Radu Coldea (Oxford)





Collaborators

Jordan Thompson

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Paul McClarty

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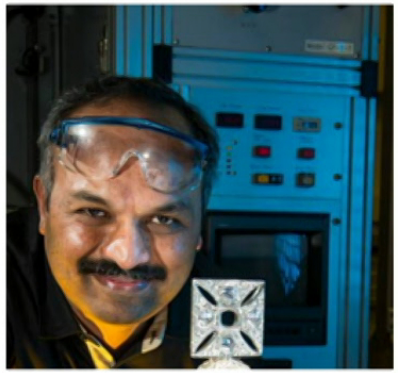

D. Prabhakaran

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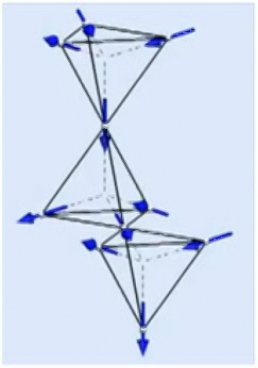
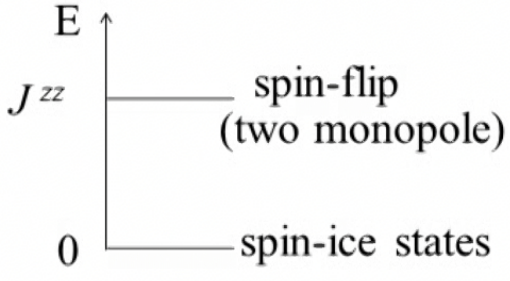
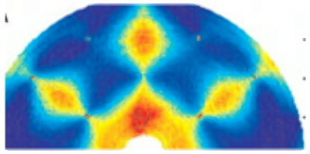
Inelastic Neutron Scatering on LET spectrometer @ ISIS Facility

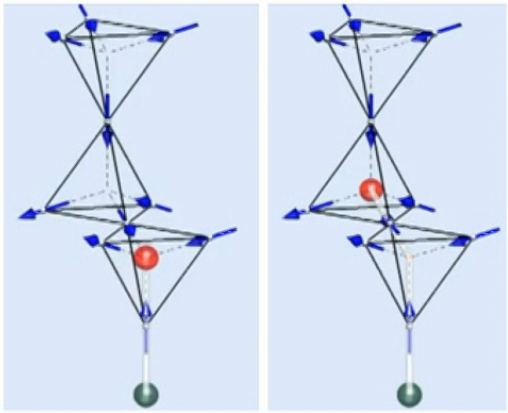
Spin ice physics on the pyrochlore lattice



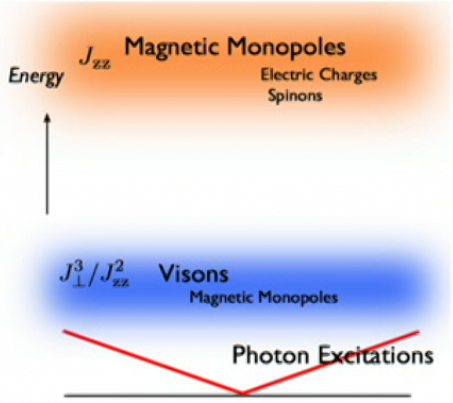
- corner-shared tetrahedra, Ising spins (local 111 axis) coupled FM many degenerate states => Spin Ice, 2 in 2 out, $Ho_2Ti_2O_7$



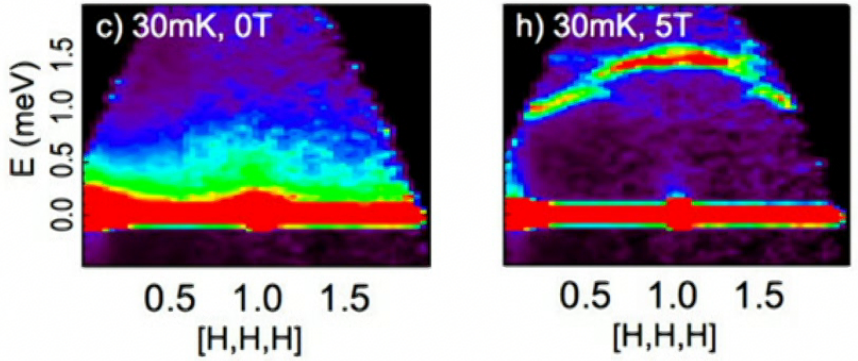




- additional "transverse exchange" terms -> "**quantum spin ice**" (photon + propagating monopoles)



$Yb_2Ti_2O_7$ spin dynamics : open questions



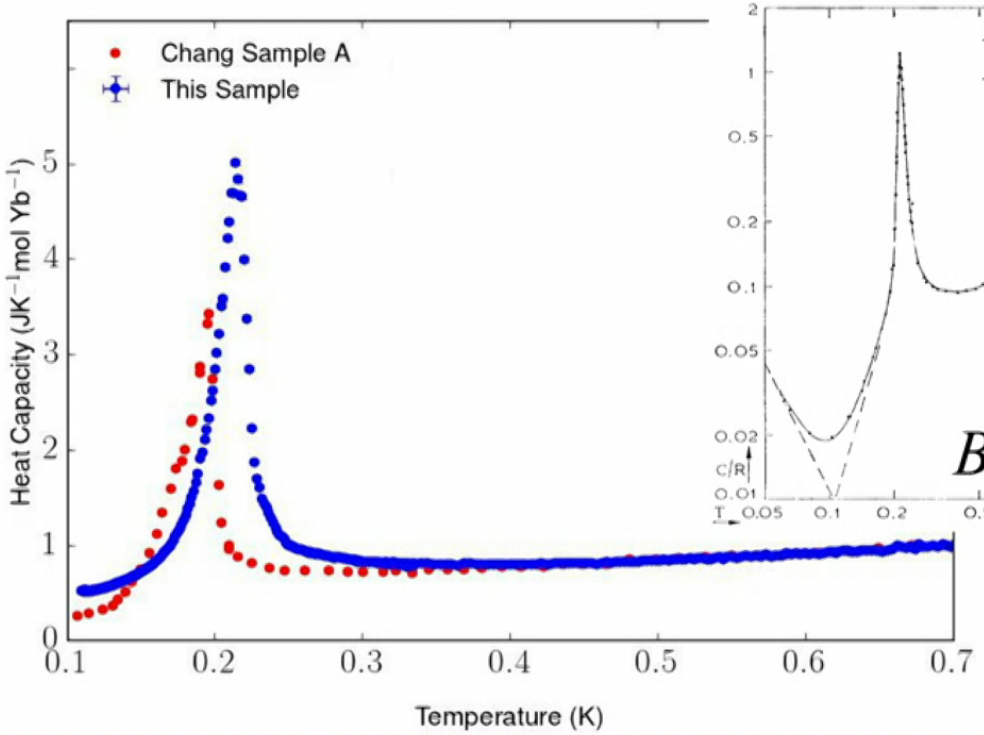
B=0 broad scattering reported

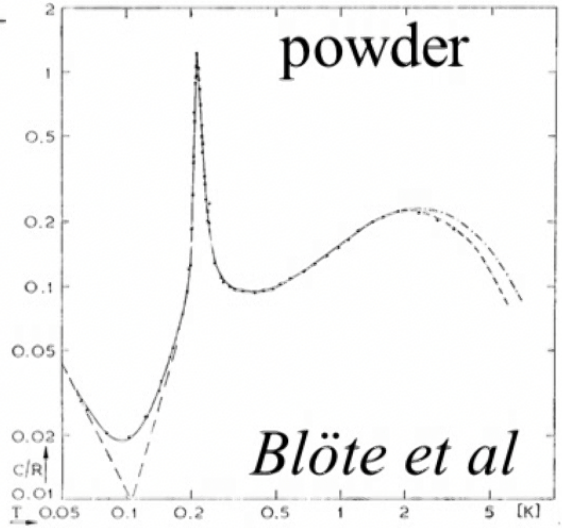
Field-polarized state sharp magnon modes

Ross et al. (2009,2011)

- **how magnons disappear upon lowering field**?
- if broad scattering at B=0 is due to quantum fluctuations, are fluctuations still present at high field, what is their manifestation, **how do fluctuations evolve upon lowering field** (gradually or with a sharp onset below a critical field) ?

$Yb_2Ti_2O_7$ single crystal specific heat

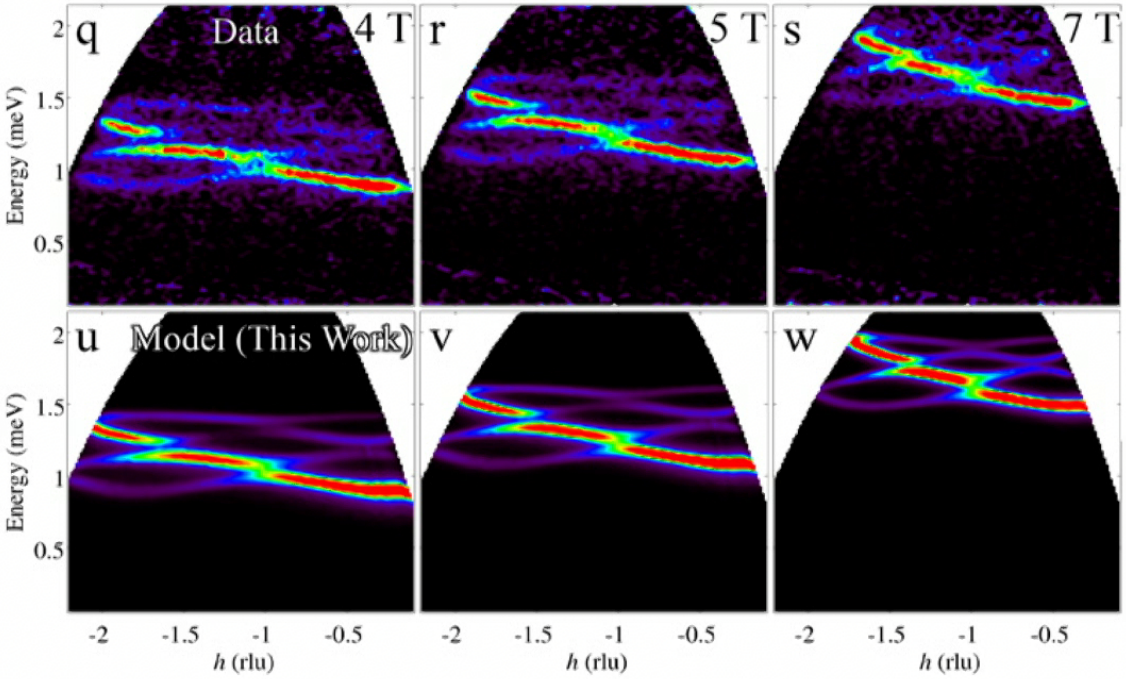


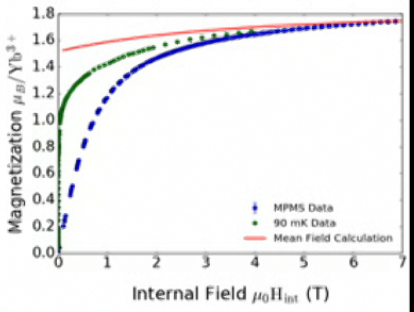


- our image furnace "slow"-grown & annealed single crystal shows a single, sharp specific heat peak at 0.214 K -> similar in behaviour to high purity limit (stoichiometric powders have 1st order transition 0.24-0.26 K)

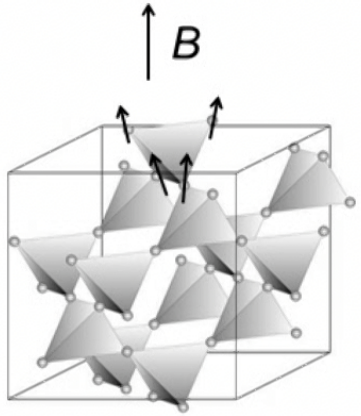
Chang et al (2012) *Arpino ...McQueen (2017)*

Spin dynamics at high magnetic field // [001] 0.15 K





- observe sharp modes with gap increasing in field, as seen by *Ross et al*. in B//[-1,1,0]
- coherently-propagating spin-flips on 4 sublattices

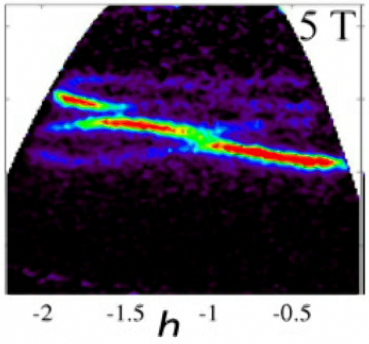


Parameterization by spin waves of a nn Hamiltonian

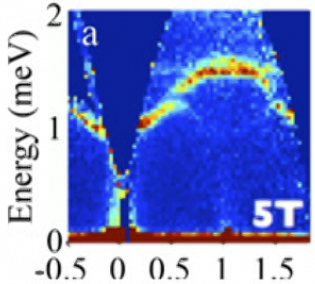
$$\mathcal{H}_{\text{Exchange}} = \sum_{\langle ij \rangle} \{ J_{zz} S_i^z S_j^z - J_{\pm} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + J_{\pm\pm} \left(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^- \right) + J_{z\pm} \left[S_i^z \left(\zeta_{ij} S_j^+ + \zeta_{ij}^* S_i^- \right) + (i \leftrightarrow j) \right] \}$$

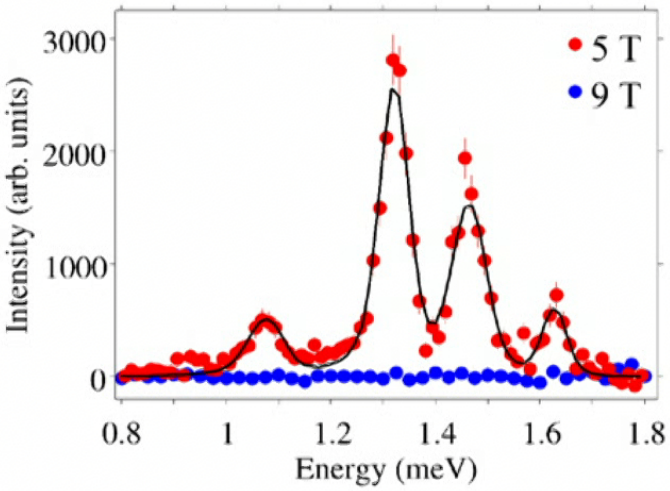
$$\mathbf{g} = \begin{pmatrix} g_\perp & 0 & 0 \\ 0 & g_\perp & 0 \\ 0 & 0 & -g_\parallel \end{pmatrix}$$

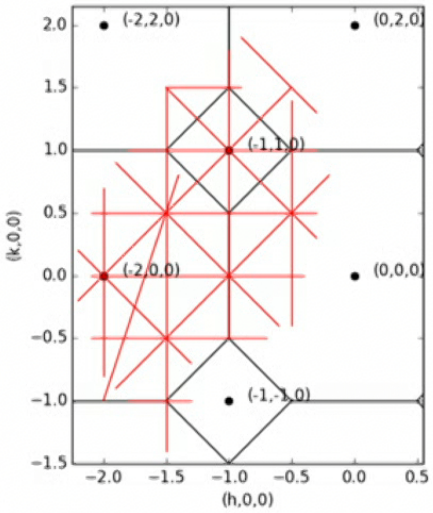
Ross, Savary, Gaulin, Balents (2011)



Ross et al. Data

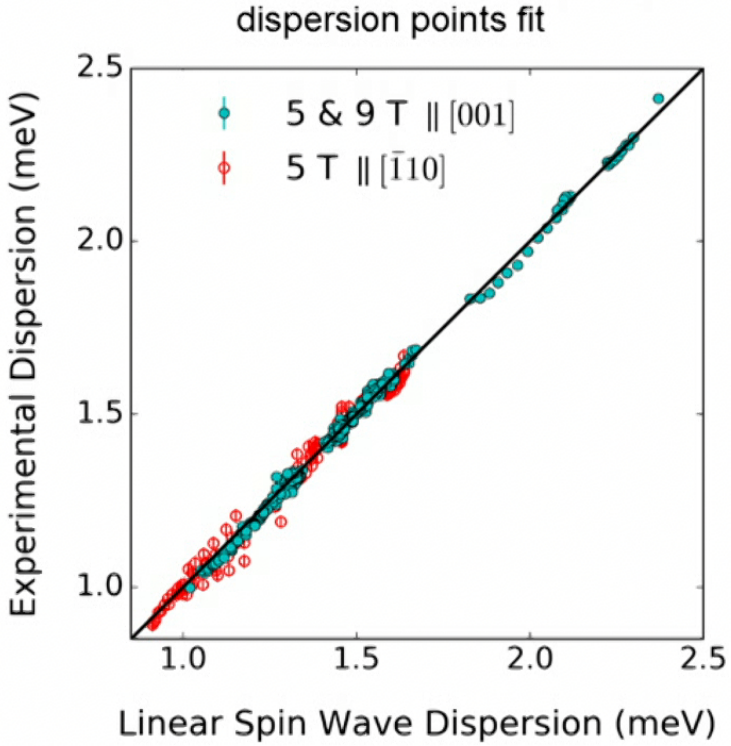


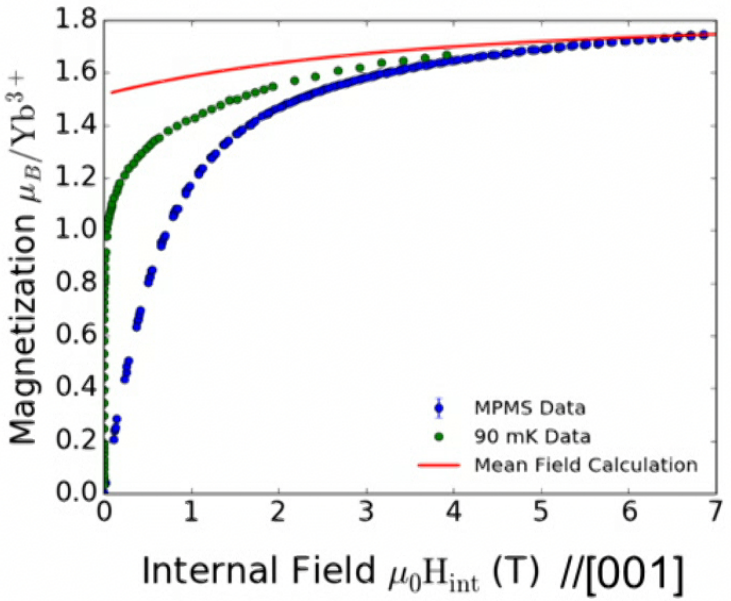




- pick dispersion points throughout the full volume of data (17 directions total) get (h,k,l,E) and mode index 1-4
- **fit 6 parameters** (4 symmetry-allowed nn exchange terms) + g tensor (2 terms) to data from **both** neutron experiments B//[001] and published B//[-1,1,0]

Parameterization by spin waves of a nn Hamiltonian

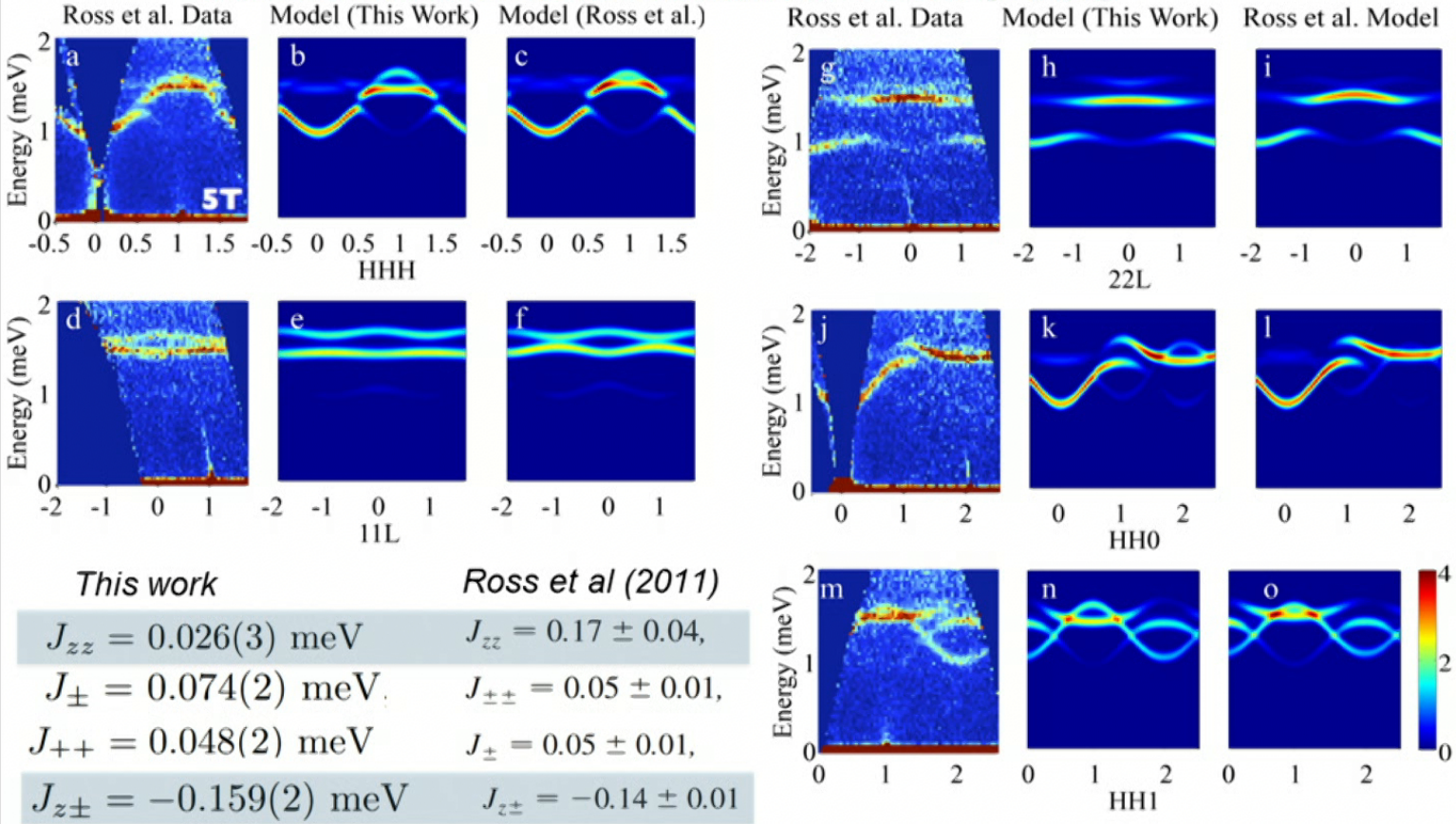




- to fit all Hamiltonian parameters without any constraints use neutron data for the **two field orientations** (over 550 dispersion points) and **magnetization near saturation** (7 T)

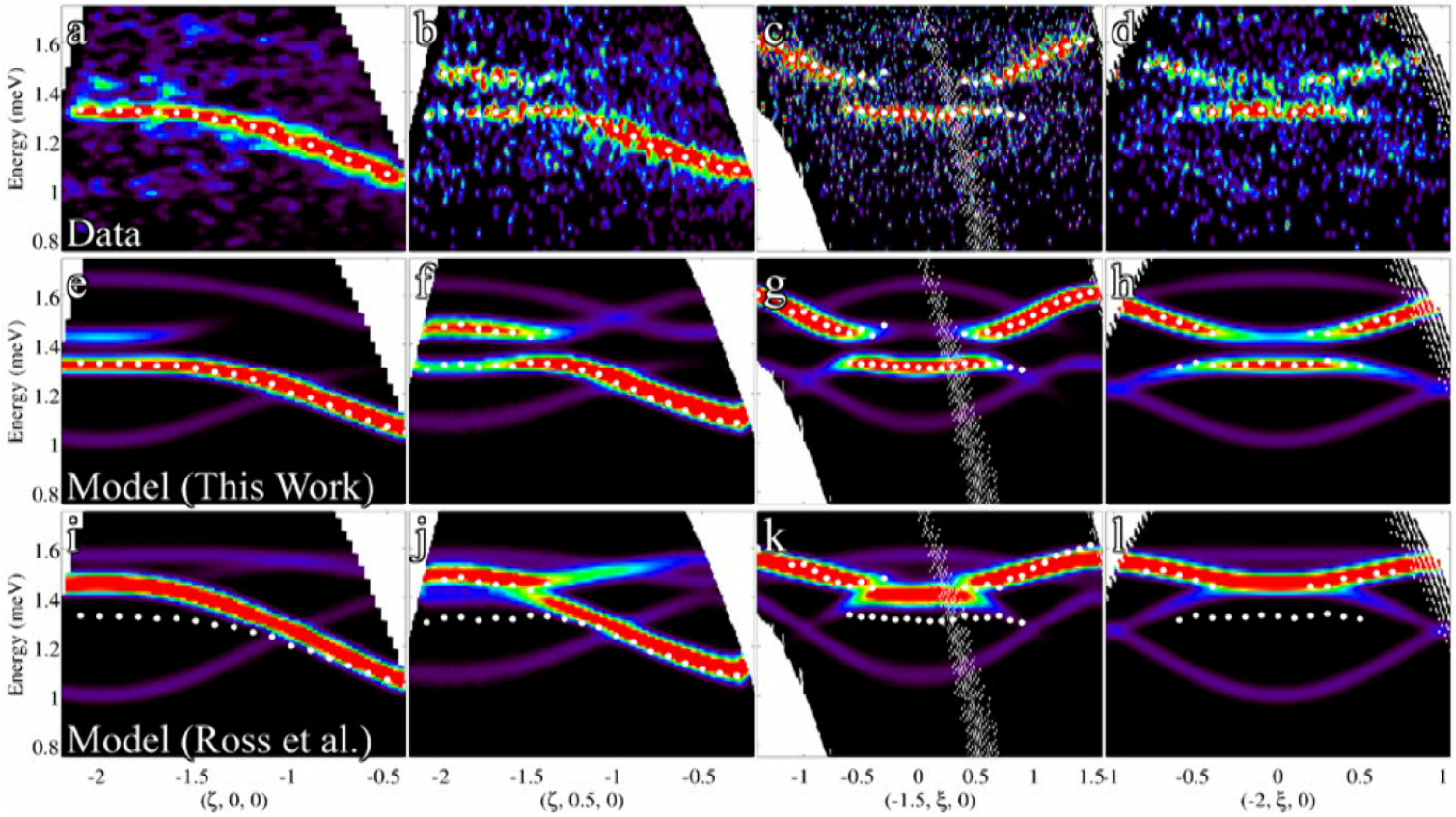
$$J_{zz} = 0.026(3)\ \text{meV}$$
$$J_{\pm} = 0.074(2)\ \text{meV}$$
$$J_{\pm\pm} = 0.048(2)\ \text{meV}$$
$$J_{z\pm} = -0.159(2)\ \text{meV}$$
$$g_{\parallel} = 2.14(3)$$
$$g_{\perp} = 4.17(2).$$

Parameterization of dispersions at B=5T // [-1,1,0]



This work	*Ross et al (2011)*
$J_{zz} = 0.026(3)$ meV	$J_{zz} = 0.17 \pm 0.04$,
$J_{\pm} = 0.074(2)$ meV	$J_{\pm\pm} = 0.05 \pm 0.01$,
$J_{++} = 0.048(2)$ meV	$J_{\pm} = 0.05 \pm 0.01$,
$J_{z\pm} = -0.159(2)$ meV	$J_{z\pm} = -0.14 \pm 0.01$
$g_{\parallel} = 2.14(3)$	$g_z = 1.80$
$g_{\perp} = 4.17(2)$.	$g_{xy} = 4.32$
(see also Robert et al PRB 2015)	$g_{xy}/g_z = 2.4$ fixed

Parameterization of dispersions at B = 5T //[001]



- earlier parameterization does not fit data in [001] field

Convergence of refinement of Hamiltonian parameters

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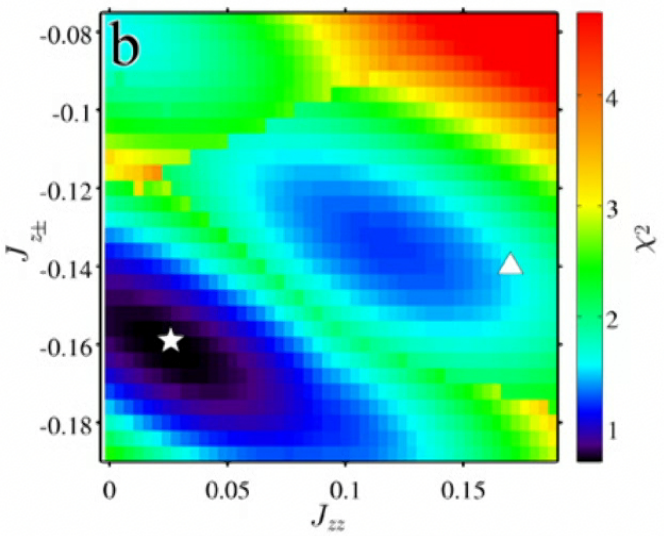
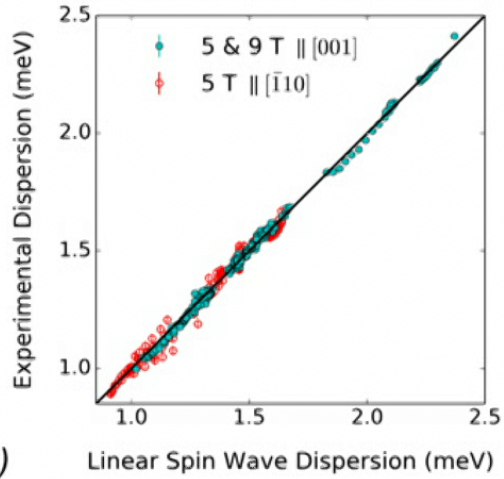


- unique solution explains **all existing dipersions data (2 field orientations) + saturation magnetization**
- refined g-factor ratio agrees with recent crystal field parameterization 1.96 +/- 0.13 *J. Gaudet et al (2015)*
- agrees with parameterization of diffuse scattering at 0.4 K Roberts et al PRB (2015) *DiLong et al (2014)*
- agrees with THz data (energies &polarization)



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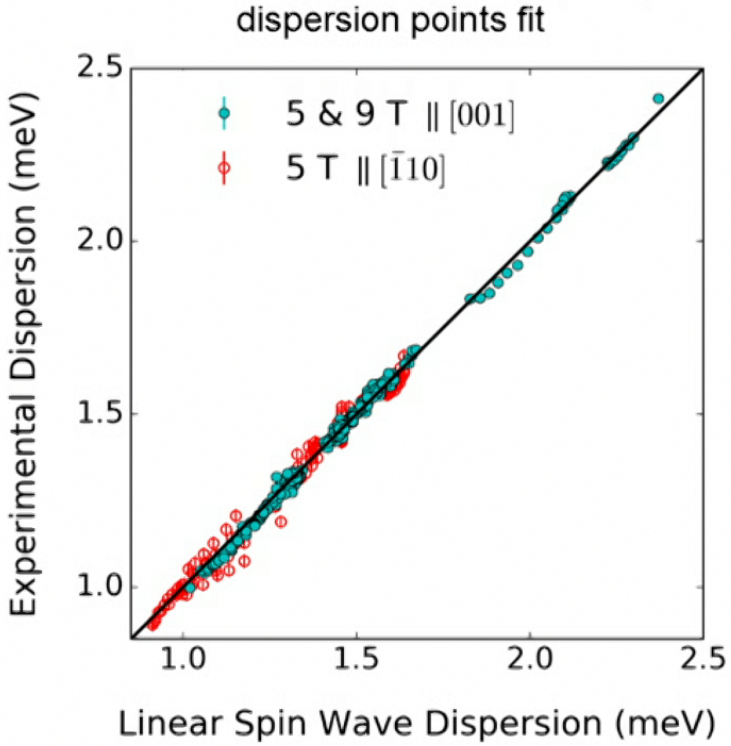

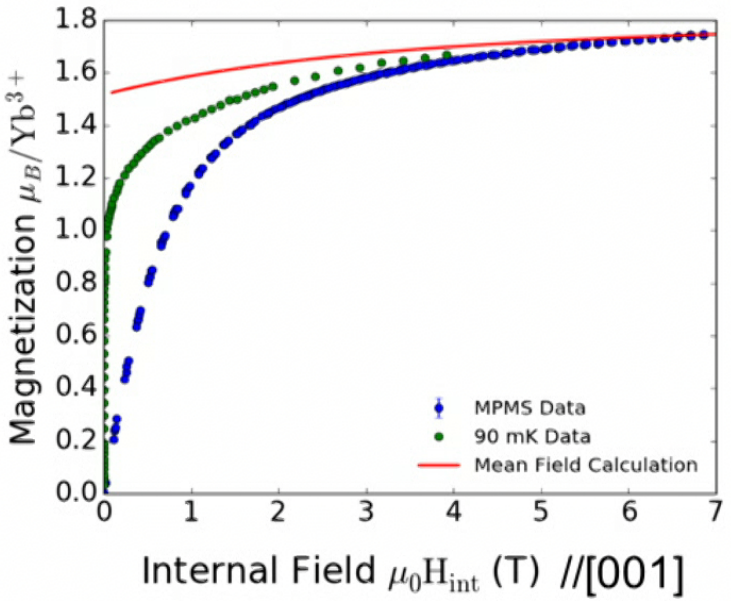

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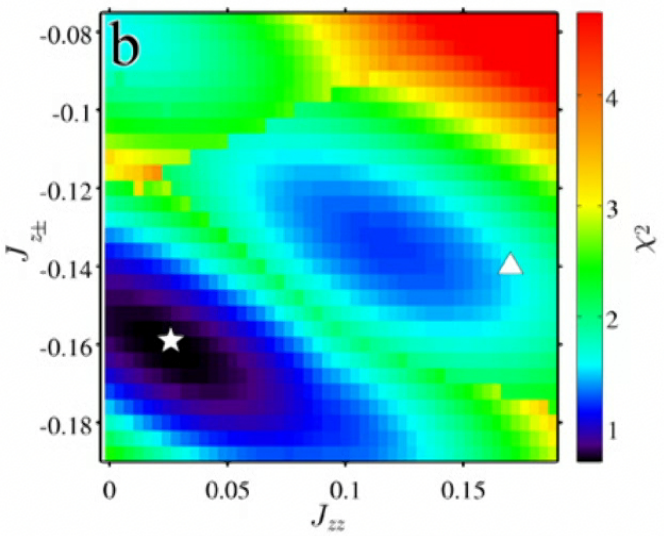

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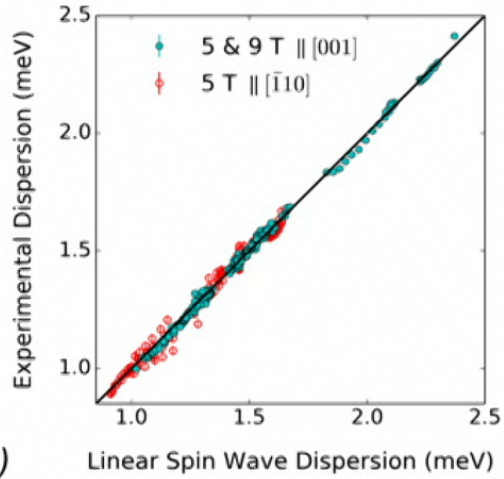
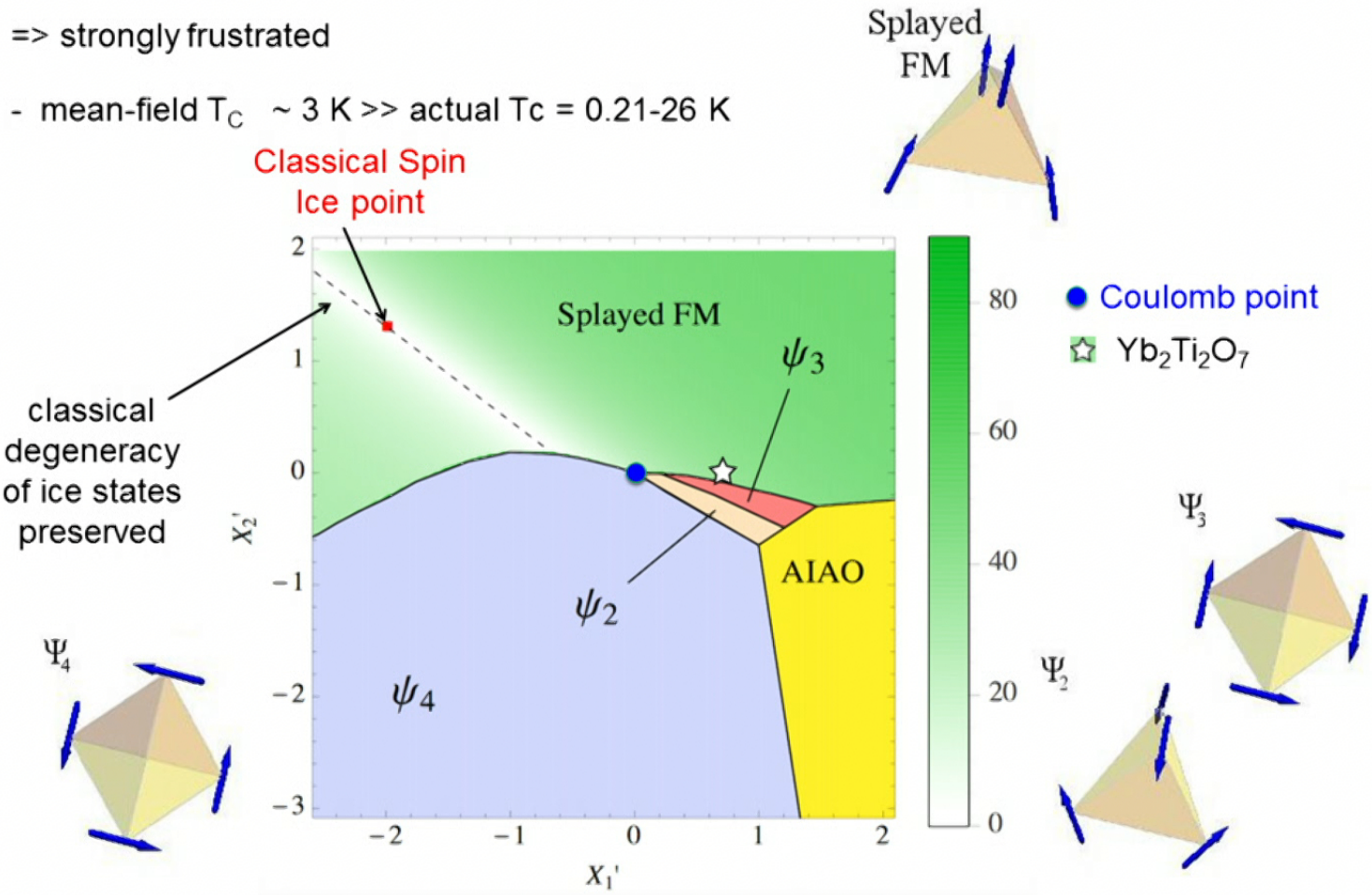


Semi-classical Phase Diagram

- revised parameters put system **almost on phase boundary** Splayed FM – AFM $\Psi_{2,3}$

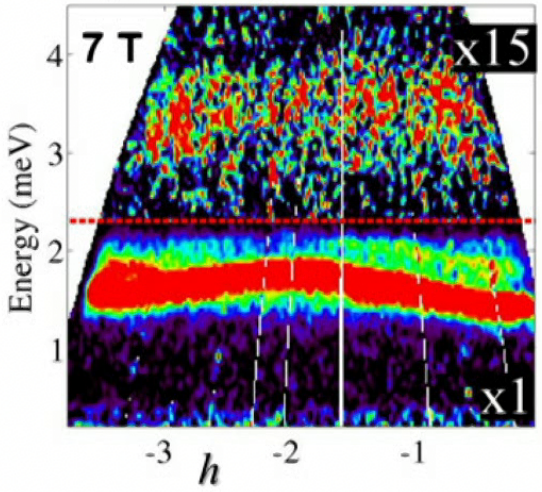
=> strongly frustrated

- mean-field T_C ~ 3 K >> actual Tc = 0.21-26 K



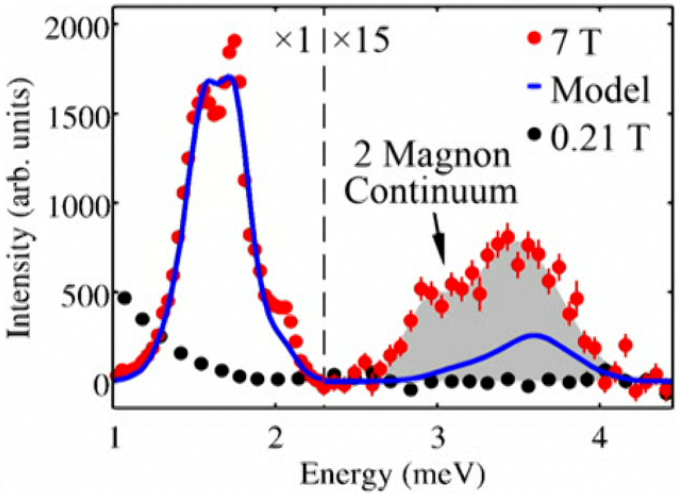
Two-magnon scattering continuum

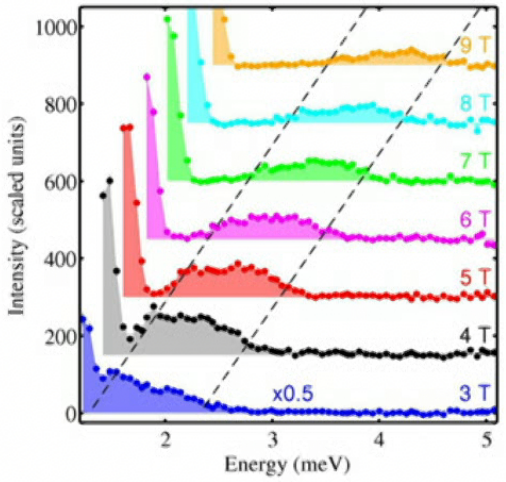
- at higher energies see additional weak continuum scattering (1-2% of one-magnon weight)

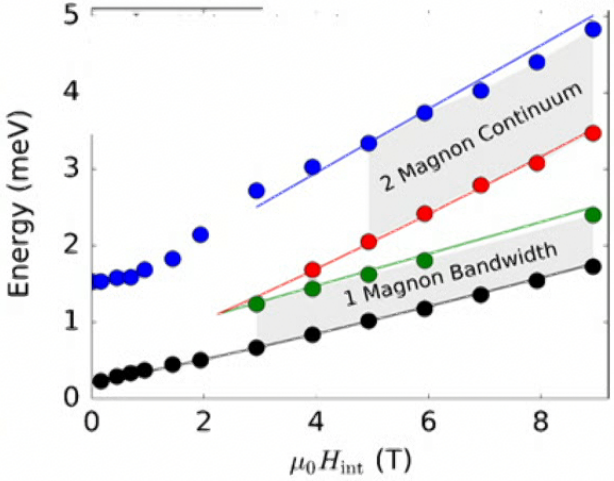


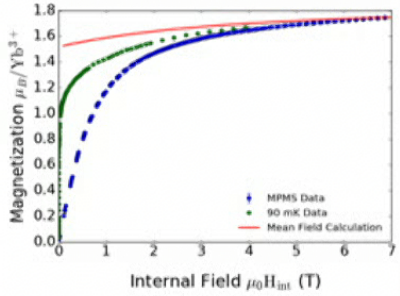
2 magnon continuum

1 magnon dispersions

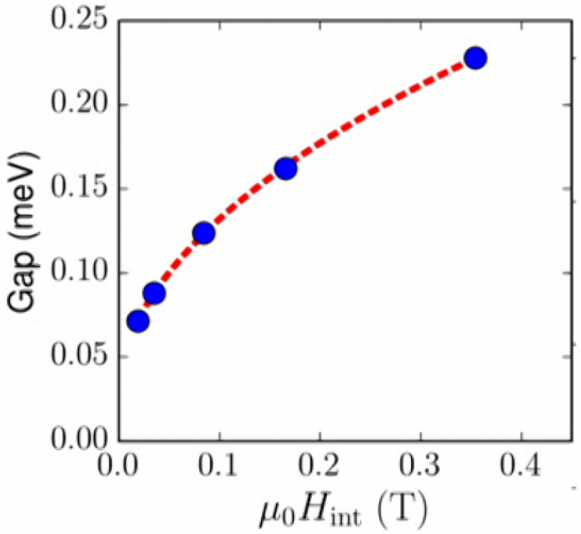


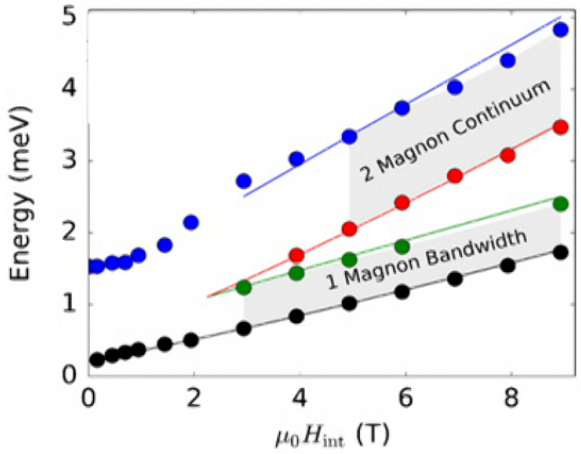


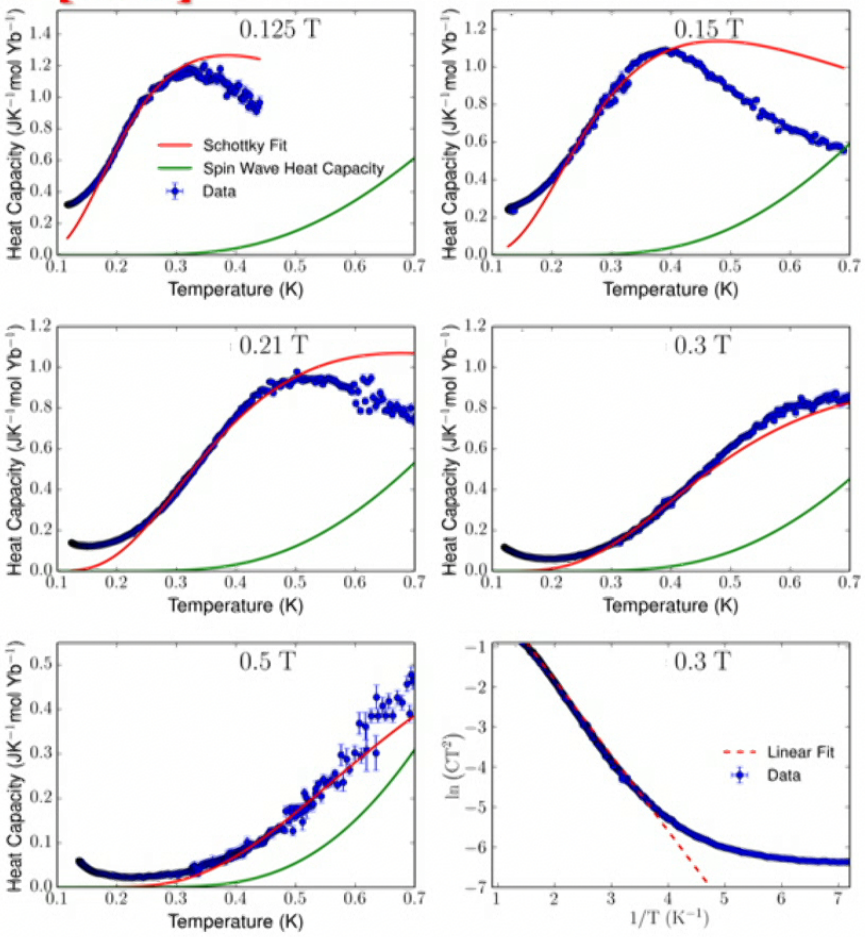




Gap vs magnetic field // [001]





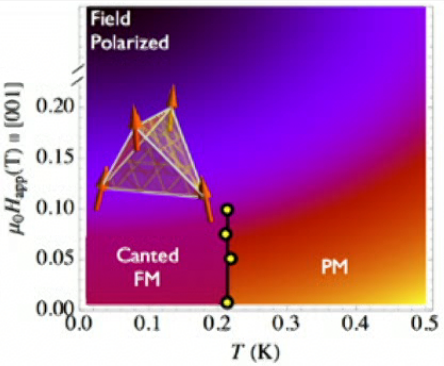


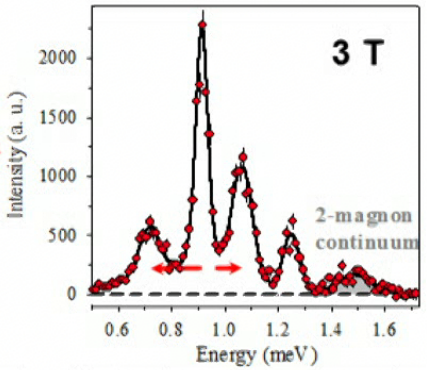
- gap increases in field, cross-over canted FM-> field-polarized

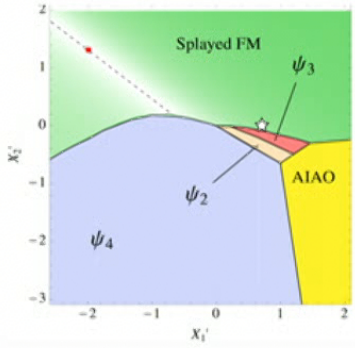
Conclusions

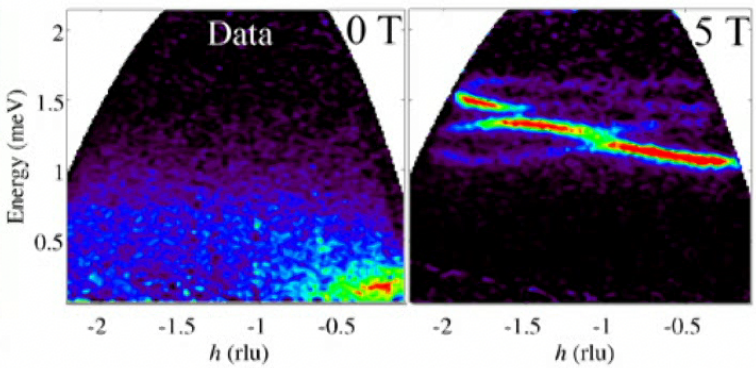
- in [001] field Canted FM and Field-Polarized are smoothly connected, no phase transition, **gap grows in field**
- at high field see sharp magnons + **2-magnon continuum** that grows rapidly upon lowering field, when overlap occurs top **magnon decays** and lower magnon dispersions are strongly renormalized; continuum dominates at zero field
- at high fields sharp magnons captured well by spin waves of nn Hamiltonian with revised parameters, **negligible J_{zz}** & **dominant $J_{z\pm}$** almost on (mean-field) phase boundary between Canted FM and AFM $\Psi_{2,3}$, strongly frustrated

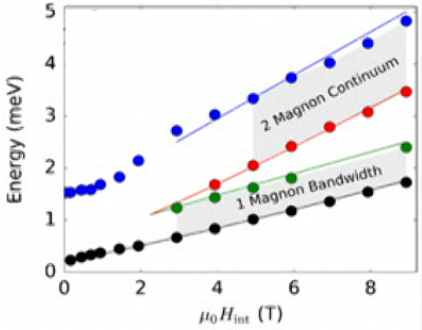
arxiv: 1703:04506









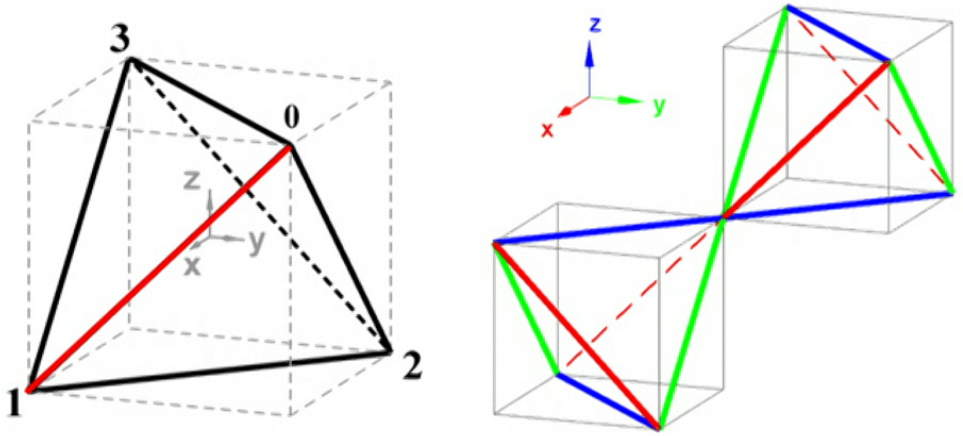


Exchange Hamiltonian – global cubic axes

$$\mathbf{J}_{01} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix}$$

$[J_1\, J_2\, J_3\, J_4] = [\,-0.028 \quad \mathbf{-0.326} \quad \mathbf{-0.272} \quad 0.049]$ meV

FM Ising coupling $J_2\, S_x S_x$ ("Kitaev"-type)
+ "pseudo-dipolar" symmetric exchange + $J_3(\, S_y S_z + S_z S_y)$ Γ-term



- for spins //z 4/6 Kitaev bonds + 6 Γ bonds create quantum dynamics