Title: Living on the edge: multiphase competition in $Yb_2Ti_2O_7$ and monopole crystal in $Tb_2Ti_2O_7$

Date: Jun 08, 2017 09:00 AM

URL: http://pirsa.org/17060039

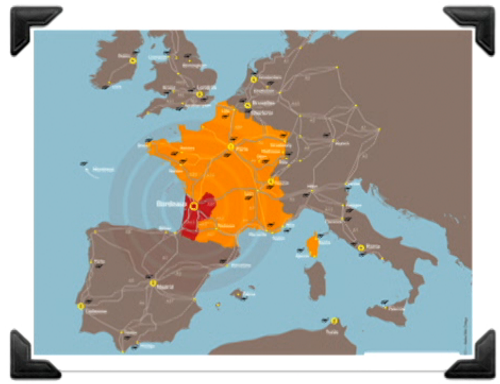
Abstract: $Yb_2Ti_2O_7$ and $Tb_2Ti_2O_7$ share the common point to sit at the edge between different phases. This multiphase competition makes the characterization of their low-temperature physics a challenge and, more generally, brings another degree of complexity to rare-earth pyrochlores. In this talk, we will take two different approaches to study these materials. For $Yb_2Ti_2O_7$, we explicitly investigate the influence of thermal and quantum fluctuations in this competition, with finite-temperature order by disorder and quantum shifting of the phase boundaries. For $Tb_2Ti_2O_7$, we will step away from the puzzling zero-field physics, and explain the undisputed order observed experimentally in a high [110] field. This order strongly supports the presence of magneto-electric coupling in $Tb_2Ti_2O_7$, and offers a rare example of long-range order of magnetic monopoles.

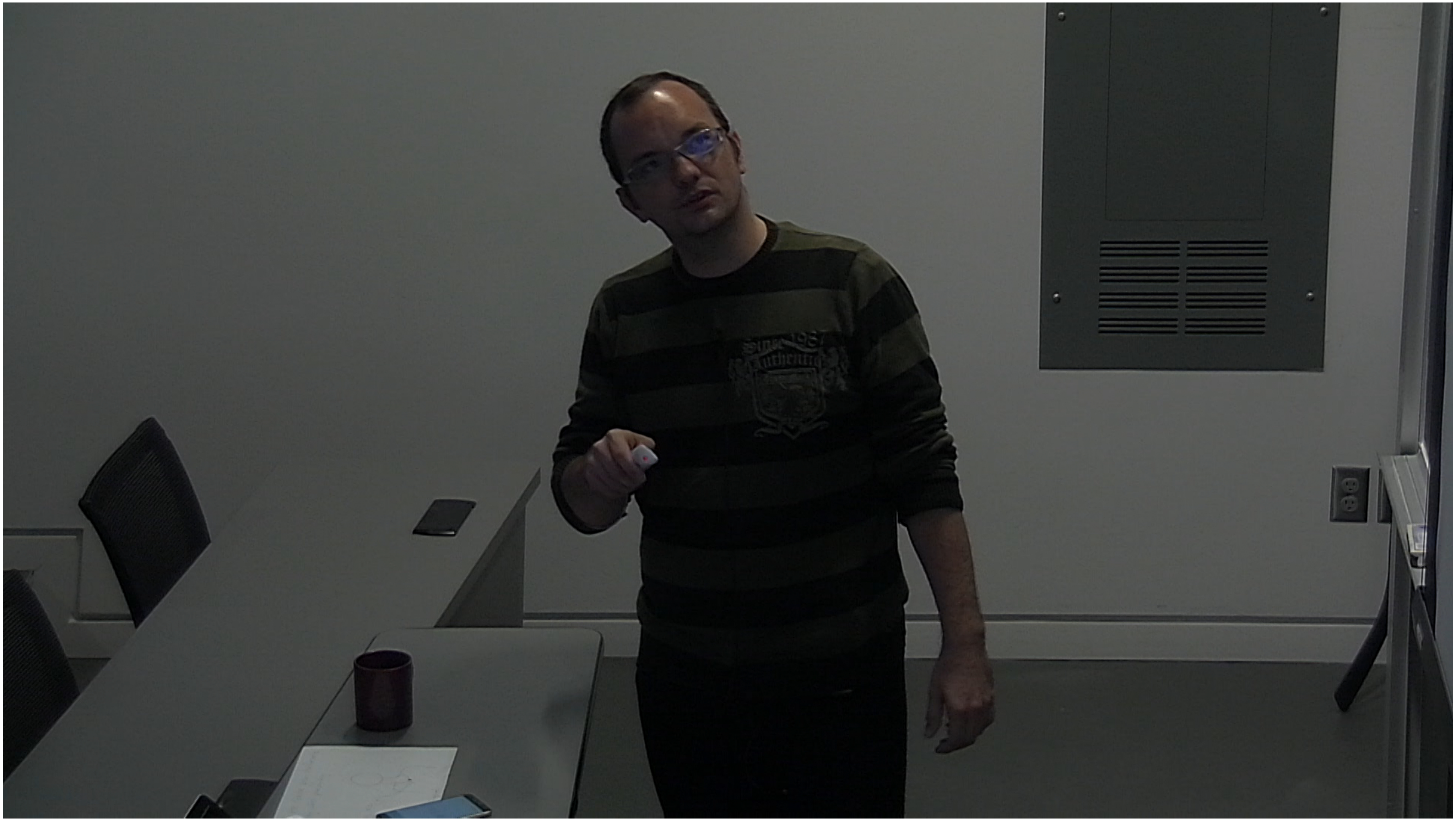
Living on the edge

Multiphase competition in $Yb_2Ti_2O_7$
Monopole crystal in $Tb_2Ti_2O_7$

QSI workshop
Perimeter Institute
June 8th, 2017

université de BORDEAUX





Influence of boundaries in $Yb_2Ti_2O_7$

Generic nearest-neighbour Hamiltonian

Curnoe PRB 2007

$$\mathcal{H} = \sum_{\langle ij \rangle} \vec{S}_i \, \bar{\mathcal{J}}_{ij} \, \vec{S}_j \quad \text{with} \quad \bar{\mathcal{J}} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix}$$

$Yb_2Ti_2O_7$

Ross et al PRX 2011

Robert et al PRB 2015

Thompson et al arXiv 2017

$Er_2Ti_2O_7$

Savary et al PRL 2012

$Er_2Sn_2O_7$

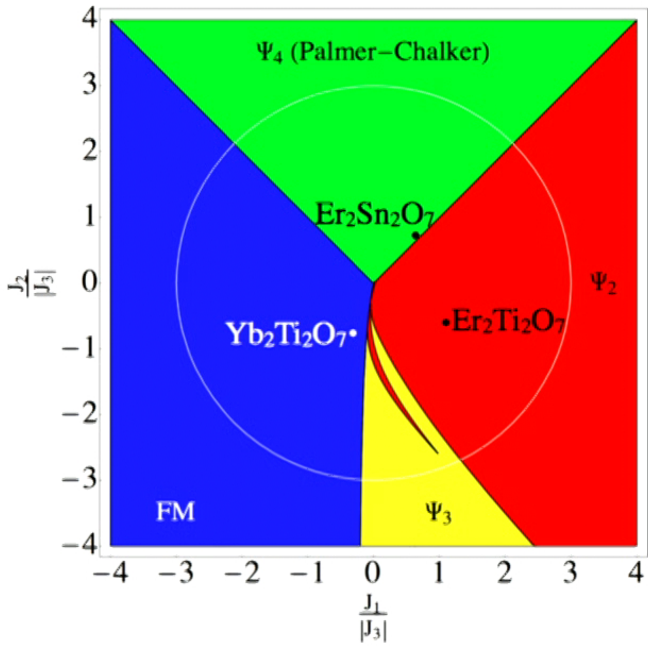
Guitteny et al PRB 2013

Petit et al arXiv 2017

Phase diagram at $T = 0$

for classical Heisenberg spins

$J_3 < 0$ & $J_4 = 0$



Yan, Benton, Jaubert, Shannon PRB 2017

Influence of boundaries in $Yb_2Ti_2O_7$

Parameters of $Yb_2Ti_2O_7$ (Ross et al PRX 2011)

$\{J_{i=1,2,3,4}\} = \{-0.09(3), -0.22(3), -0.29(2), 0.01(2)\}$ meV

Jaubert, Benton, Rau, Oitmaa, Singh, Shannon & Gingras PRL 2015

We will consider

$J_1 \in [-0.09 : 0] \quad \{J_{i=2,3,4}\} = \{-0.22, -0.29, 0\}$

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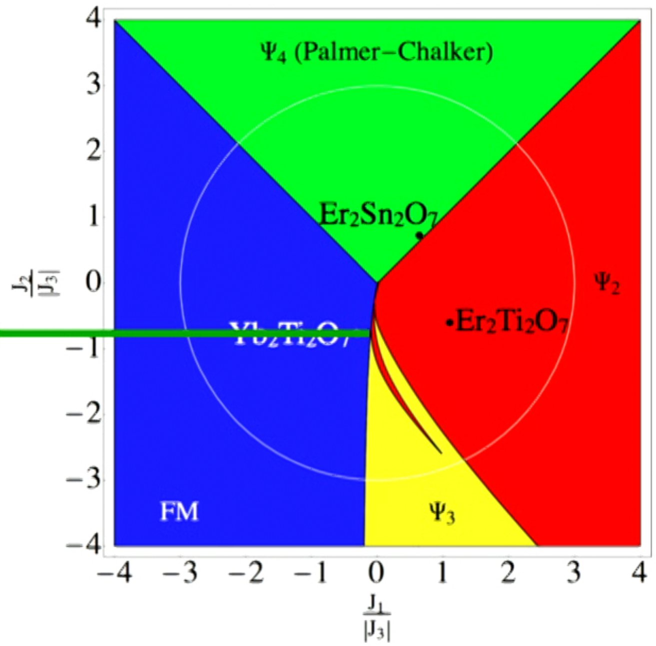

Yan, Benton, Jaubert, Shannon PRB 2017

Influence of boundaries in $Yb_2Ti_2O_7$

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We will consider

$J_1 \in [-0.09 : 0]$ $\{J_{i=2,3,4}\} = \{-0.22, -0.29, 0\}$

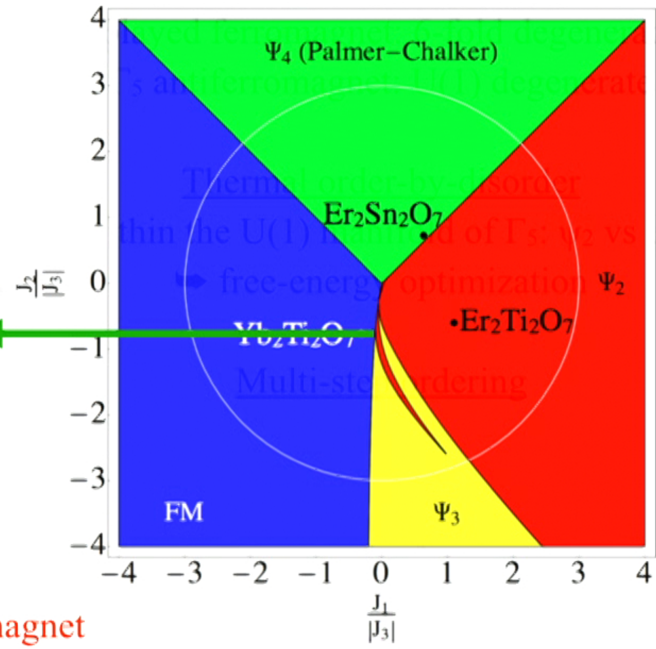
splayed ferromagnet (SFM) | Γ_5 antiferromagnet

J_1: -0.09 ... -0.029 ... 0

Phase diagram at $T = 0$

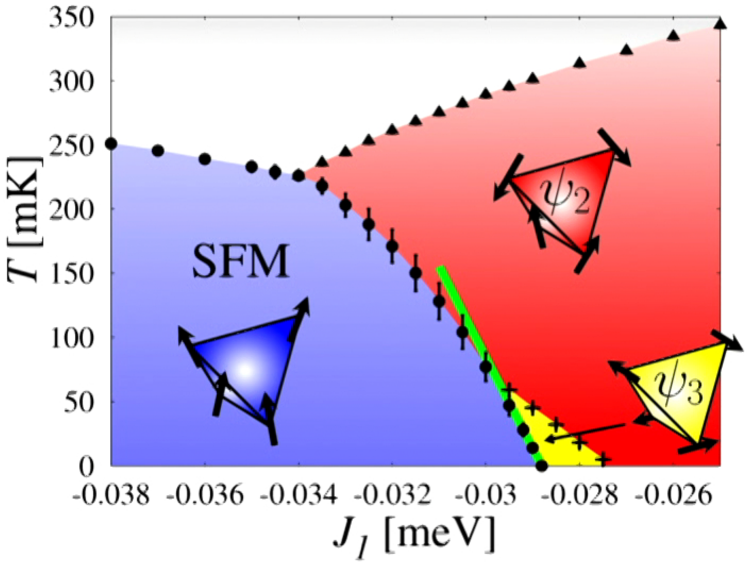
for classical Heisenberg spins

$J_3 < 0$ & $J_4 = 0$



Yan, Benton, Jaubert, Shannon PRB 2017

Classical phase diagram (Monte Carlo)



<u>Multiphase competition</u>

splayed ferromagnet: 6-fold degenerate

Γ_5 antiferromagnet: U(1) degenerate

<u>Thermal order-by-disorder</u>

within the U(1) manifold of Γ_5: ψ_2 vs ψ_3

➡ free-energy optimization

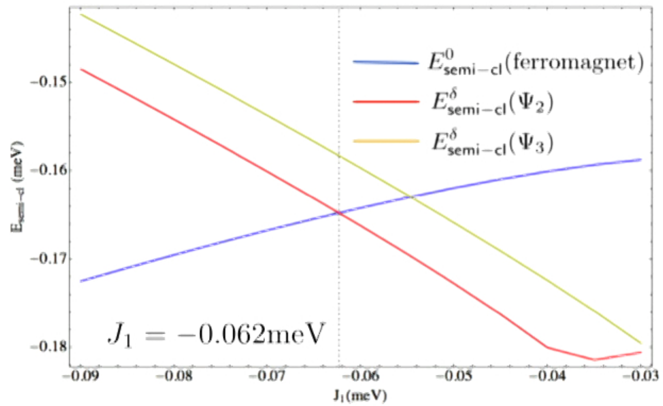
<u>Multi-step ordering</u>

Jaubert, Benton, Rau, Oitmaa, Singh, Shannon & Gingras PRL 2015

Robert, Lhotel, Remenyi, Sahling, Mirebeau, Decorse, Canals & Petit PRB 2015

Quantum fluctuations at zero temperature

Semiclassical (linear spin wave theory - LSWT):
We compare the stability of the classical phases (SFM, ψ_2, ψ_3) using LSWT.
To study the stability of a classically *excited* state, we use the method of [Coletta et al PRB 2013]
which provides an upper-bound of the semiclassical energy of the ψ_2 and ψ_3 states.



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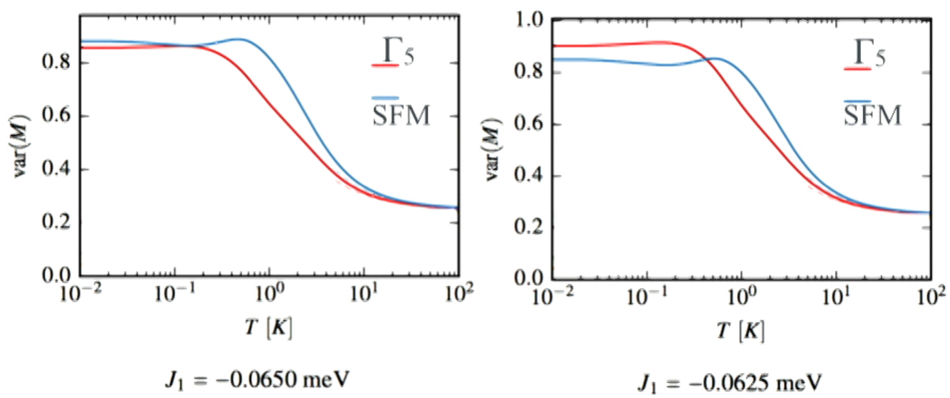
which provides an upper-bound of the semiclassical energy of the ψ_2 and ψ_3 states.
The frontier is at J_1 = -0.062 meV.

Quantum (exact diagonalization with 4 and 16 sites - ED):
We compare the correlators (variance) of the corresponding order parameters.
The frontier is at J_1 = -0.064(2) meV.



Quantum fluctuations at finite temperature

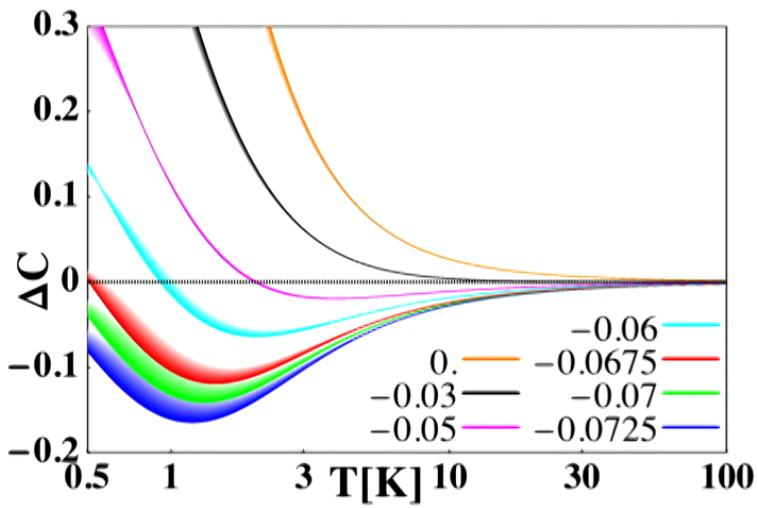
Numerical-linked-cluster calculations (NLC)

We compare the correlators (variance) of the corresponding order parameters:

$\Delta C = C_{\Gamma 5} - C_{SFM}$

At high temperature, we recover the classical frontier. Below ~ 3 K, quantum fluctuations modify the classical physics (upturn of ΔC).

The frontier is at J_I = -0.070(3) meV.



Quantum fluctuations at finite temperature

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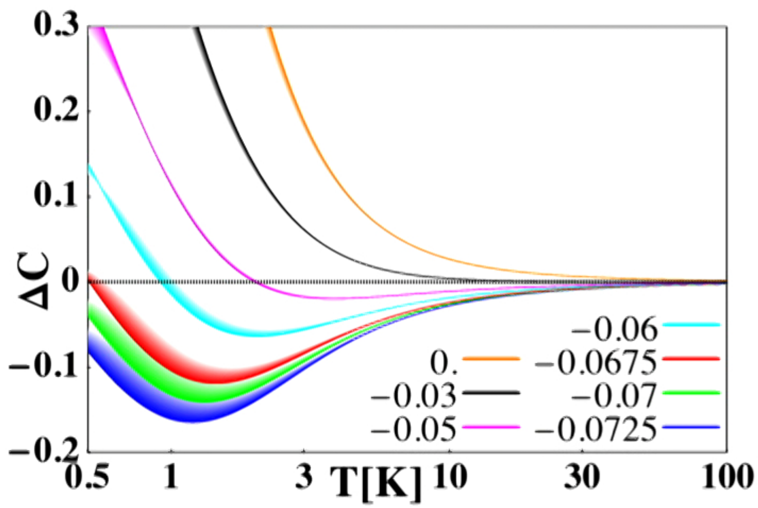
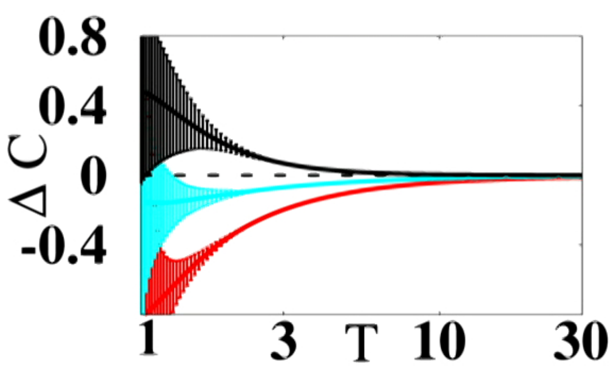




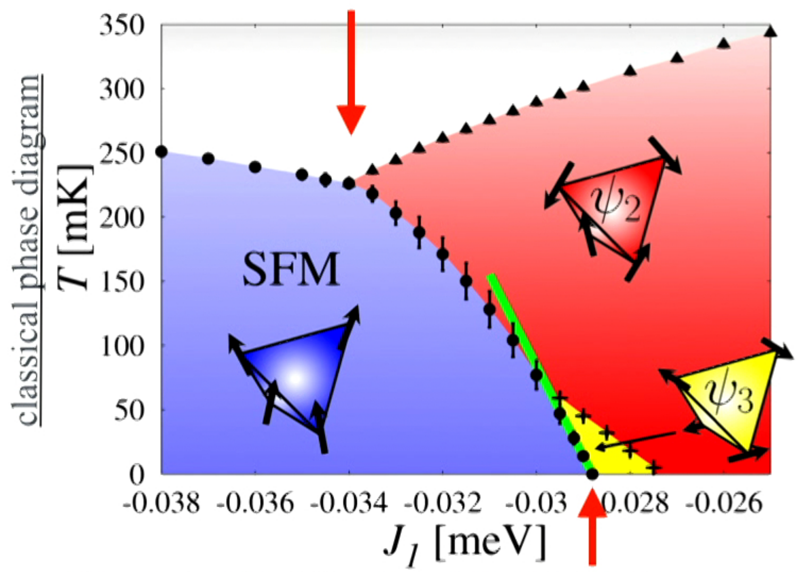
High-temperature-expansion (HTE)

The determination of the boundary is more difficult, but its quantum shifting is confirmed.

The frontier is at J_l = -0.06(3) meV.

Quantum shifting of the phase diagram

quantum fluctuations coming from high temperature
NLC [-0.070(3) meV], HTE [-0.06(3) meV]

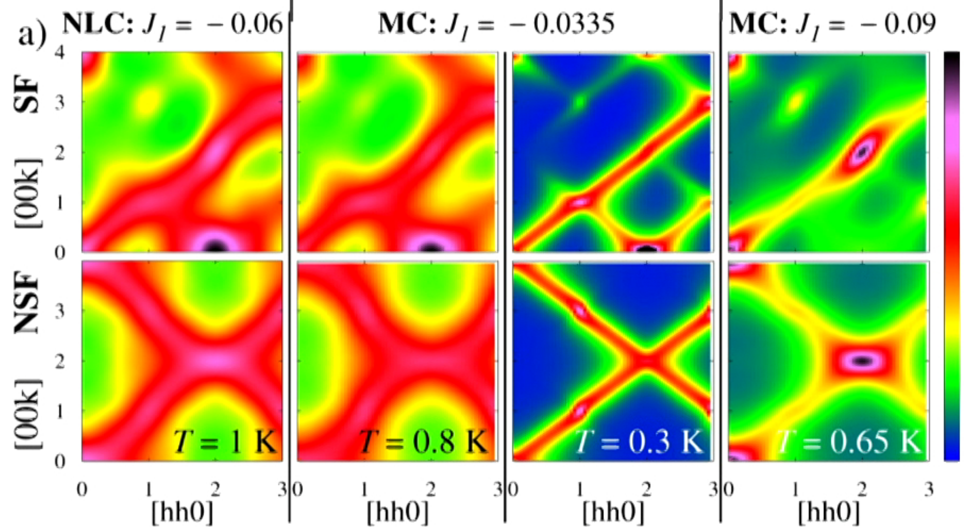


quantum fluctuations at T = 0: LSWT [-0.062 meV], ED [-0.064(2) meV]

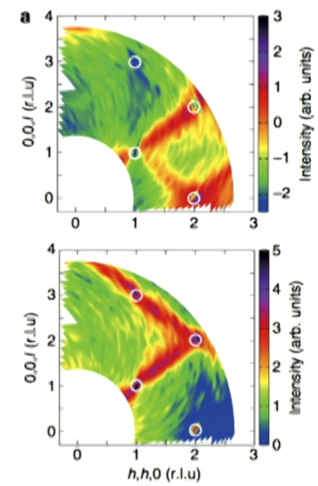
The Γ_5 manifold is favored by quantum fluctuations.
➥ the classical boundary is shifted to more negative values of J_1 by quantum fluctuations.
Our results suggest the same shape of the phase diagram.

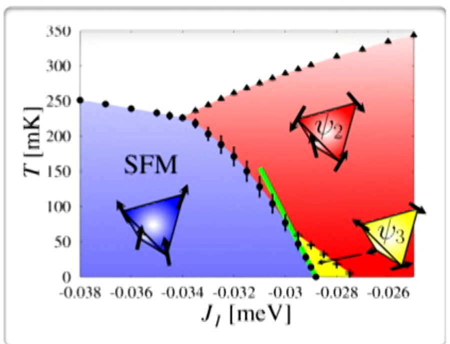
Neutron scattering of $Yb_2Ti_2O_7$

close to the quantum boundary | close to the classical boundary | Ross et al parameters



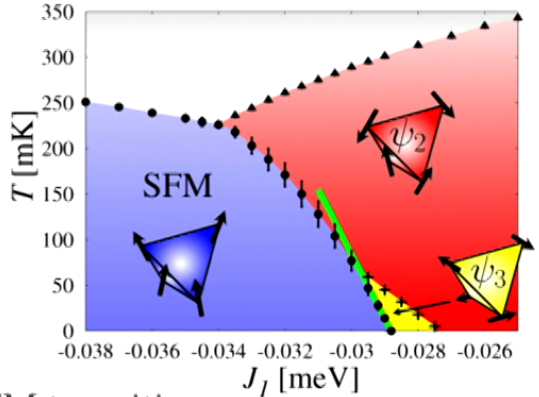
Chang et al
Nature Comm. 2014





The boundary shifts with quantum fluctuations.
➥ different theoretical methods might give
slightly different coupling parameters near the boundary.

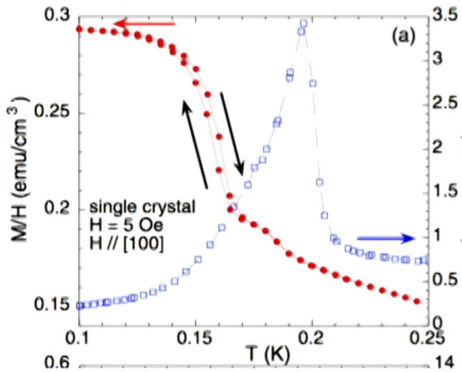
Bulk measurements: double transition



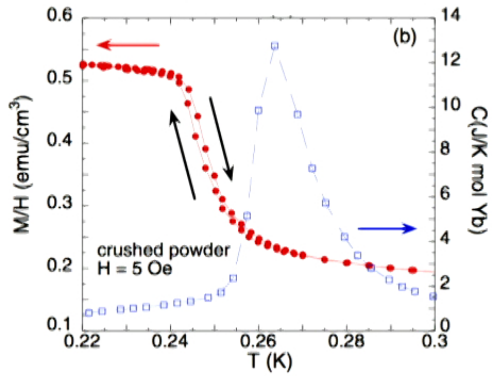
1st order SFM transition

Lhotel et al PRB 2014

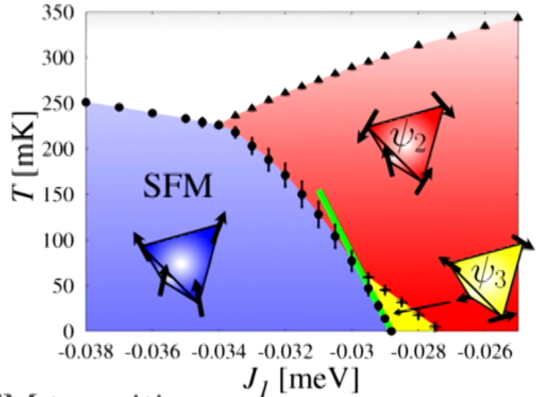
T_c = 150 mK and 195 mK

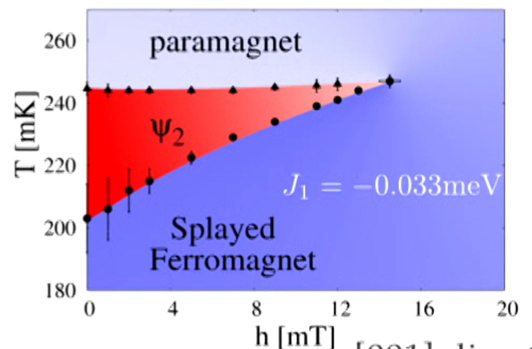


T_c = 245 mK and 265 mK



Bulk measurements: double transition



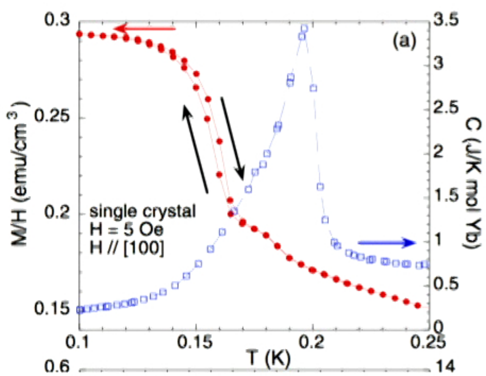


1st order SFM transition

[001] direction

Lhotel et al PRB 2014

T_c = 150 mK and 195 mK



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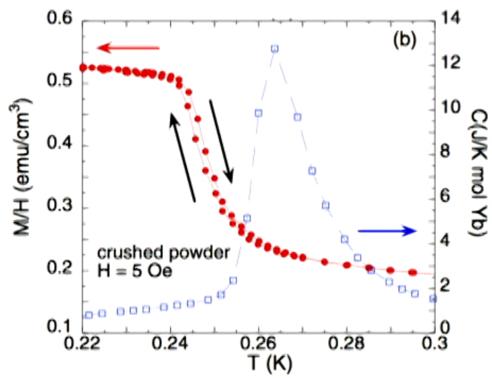
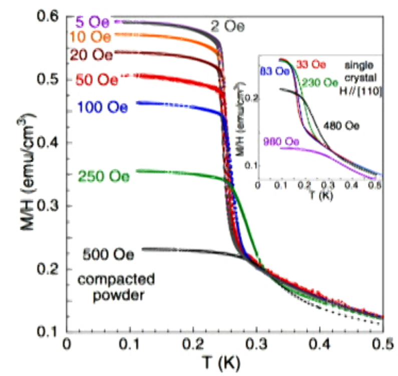
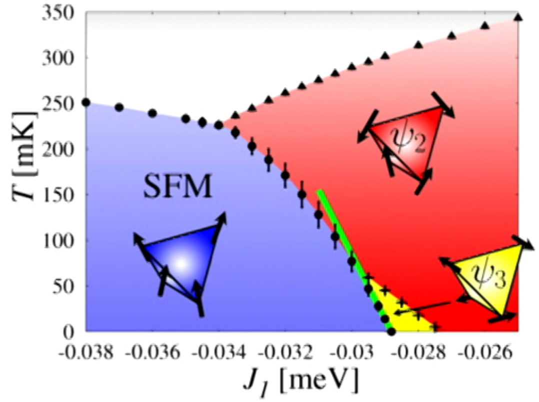
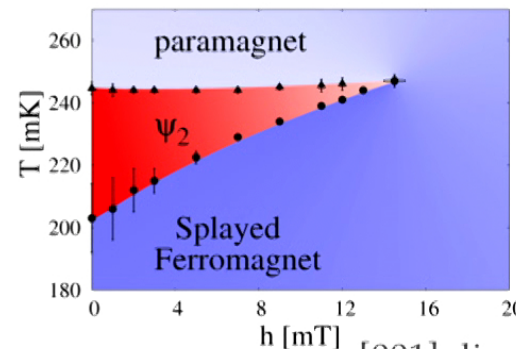


$h_c \approx 20$ mT



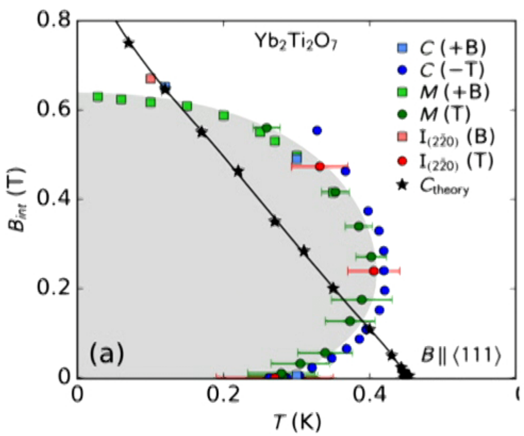
Bulk measurements: reentrance in a field





[001] direction

Scheie et al arXiv 2017



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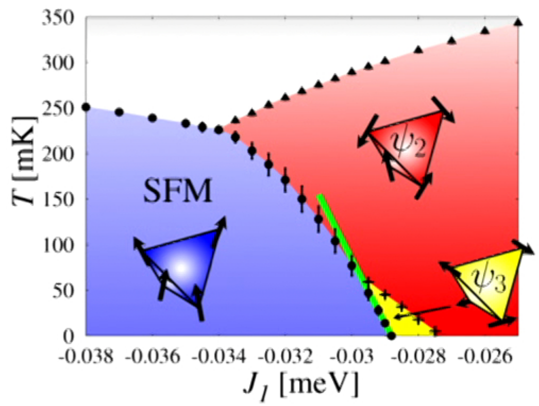
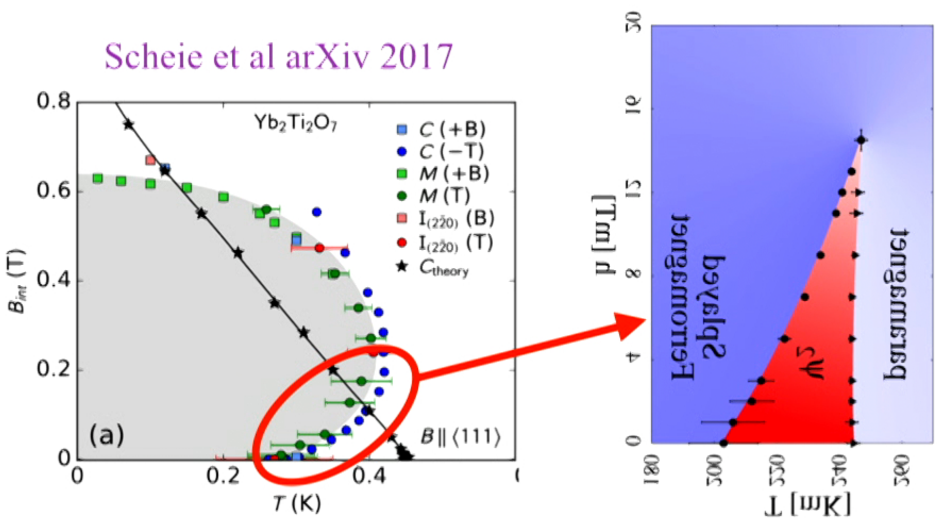


[001] direction

Scheie et al arXiv 2017



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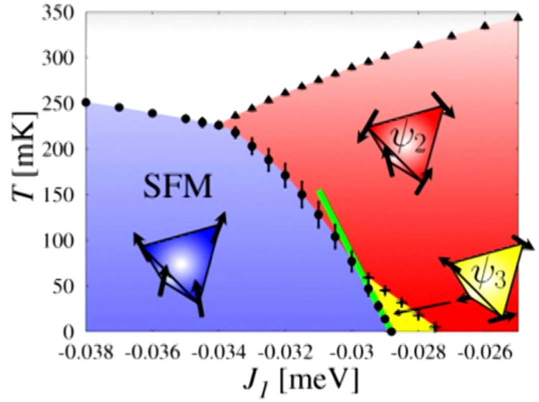
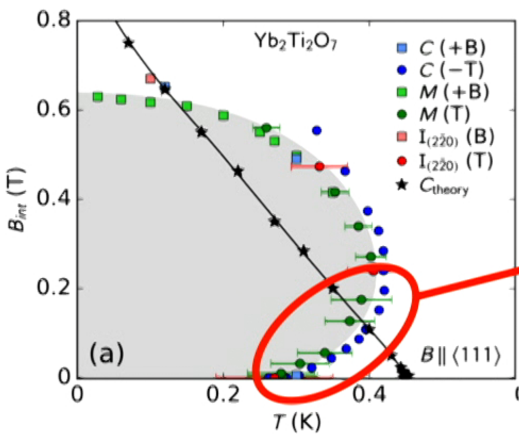
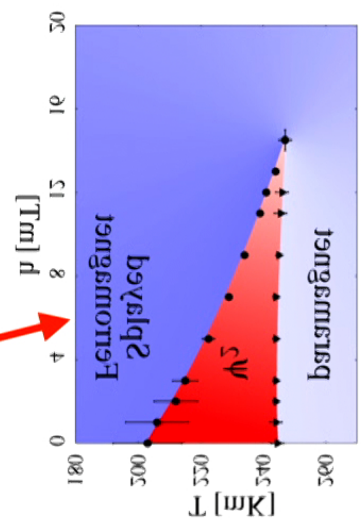


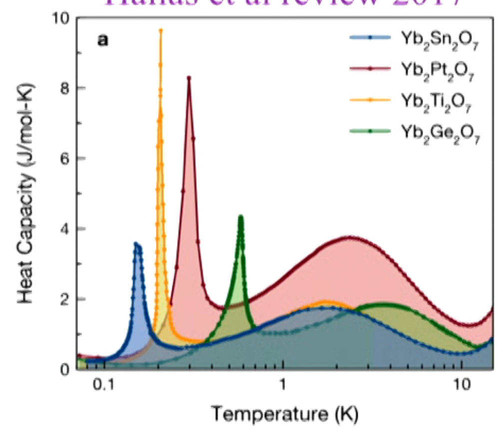
[001] direction

Scheie et al arXiv 2017





Hallas et al review 2017

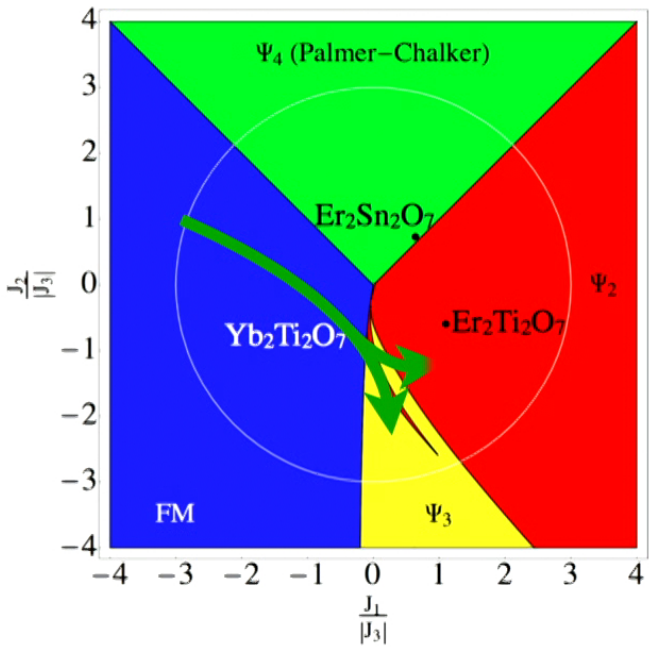


Applegate et al PRL 2012

Chemical pressure

$Yb_2Sn_2O_7$
splayed ferromagnet → $Yb_2Ti_2O_7$ → Γ_5 antiferromagnet
Yaouanc et al PRL 2013
Dun et al PRB 2013

$Yb_2Ge_2O_7$
Γ_5 antiferromagnet
Dun et al PRB 2014
Dun et al PRB 2015
Hallas et al PRB 2016



Monopole crystal in $Tb_2Ti_2O_7$

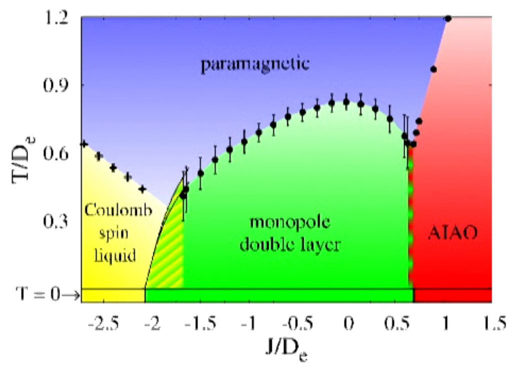
Han Yan
OIST
Japan

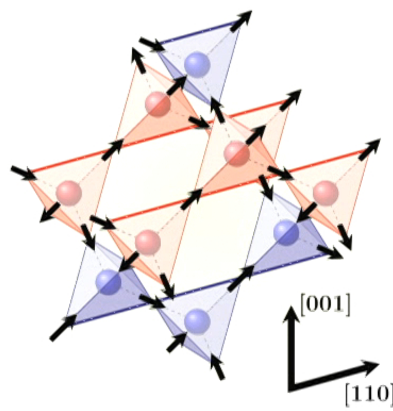
Nic Shannon
OIST
Japan

Owen Benton
RIKEN
Japan

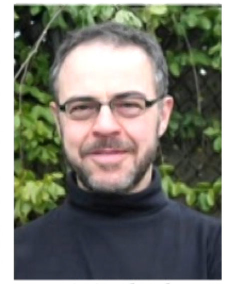
Roderich Moessner
MPI-PkS
Dresden
Germany

Jaubert & Moessner PRB 2015





Jeff Rau
U. Waterloo
Canada



Michel Gingras
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Rajiv Singh
UC Davis
USA

Jaan Oitmaa
UNSW
Australia

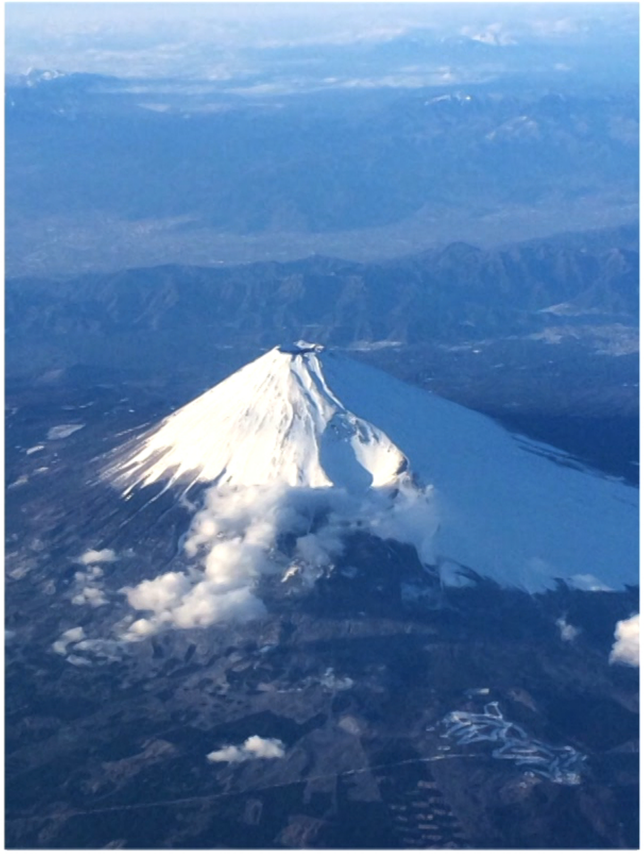
$Tb_2Ti_2O_7$

VOLUME 82, NUMBER 5 PHYSICAL REVIEW LETTERS 1 FEBRUARY 1999

Cooperative Paramagnetism in the Geometrically Frustrated Pyrochlore Antiferromagnet $Tb_2Ti_2O_7$

J. S. Gardner,[1] S. R. Dunsiger,[2] B. D. Gaulin,[1] M. J. P. Gingras,[3] J. E. Greedan,[4] R. F. Kiefl,[2] M. D. Lumsden,[1] W. A. MacFarlane,[2] N. P. Raju,[4] J. E. Sonier,[2] I. Swainson,[5] and Z. Tun[5]

Benton, Yan, Jaubert & Shannon, Nature Comm. 2016



$Tb_2Ti_2O_7$ in a [110] magnetic field

PHYSICAL REVIEW B **82**, 100401(R) (2010)

Superlattice correlations in $Tb_2Ti_2O_7$ under the application of [110] magnetic field

J. P. C. Ruff,[1] B. D. Gaulin,[1,2,3] K. C. Rule,[4] and J. S. Gardner[5,6]
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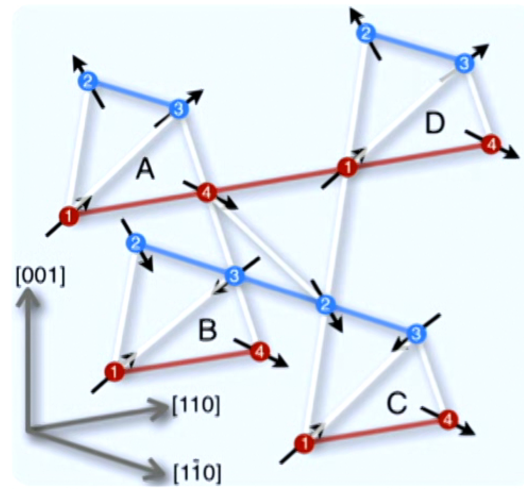
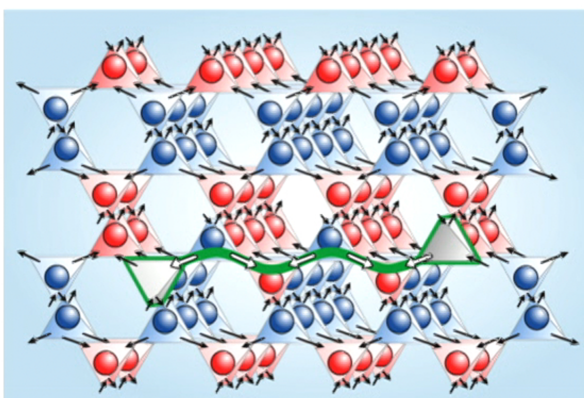
[6]*Department of Physics, Indiana University, 2401 Milo B. Sampson Lane, Bloomington, Indiana 47408-1398, USA*





PHYSICAL REVIEW B **85**, 214420 (2012)

Double-layered monopolar order in the $Tb_2Ti_2O_7$ spin liquid

A. P. Sazonov,* A. Gukasov, and I. Mirebeau
CEA, Centre de Saclay, DSM/IRAMIS/Laboratoire Léon Brillouin, F-91191 Gif-sur-Yvette, France

P. Bonville
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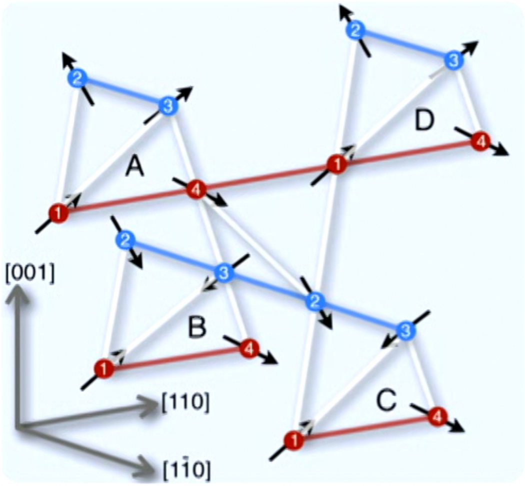

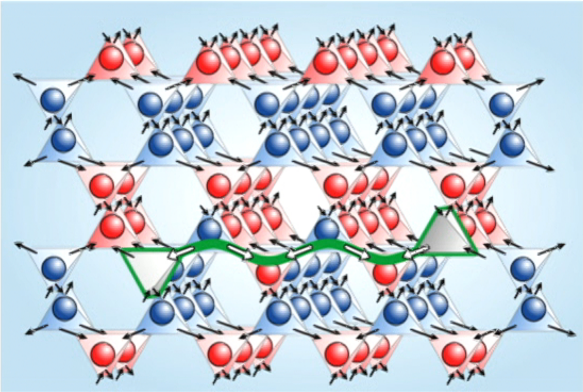

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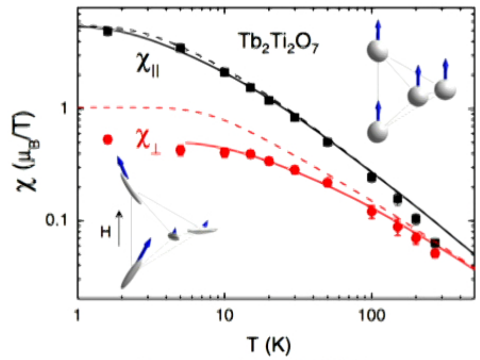
$Tb_2Ti_2O_7$: spin ice & magneto-elastic

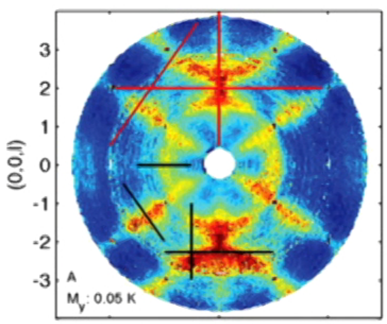
<u>Spin Ice physics</u>

Ising, Coulomb phase



Cao et al. PRL 2009

Gingras *et al.* PRB 2000 (CEF)



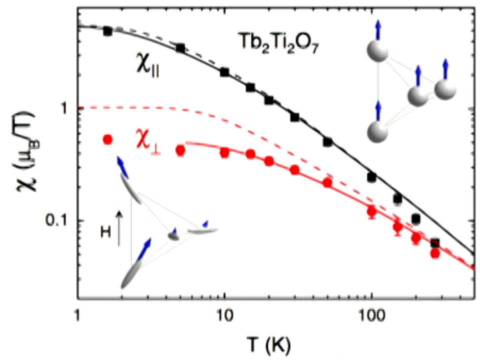
Fennell et al. PRL 2012

Guitteny *et al.* PRL 2013

$Tb_2Ti_2O_7$: spin ice & magneto-elastic

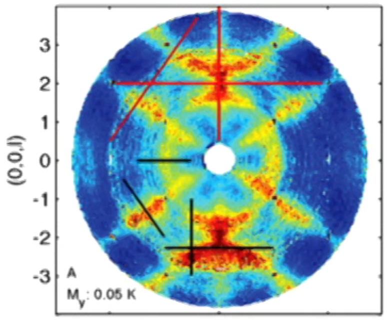
Spin Ice physics

Ising, Coulomb phase



Cao et al. PRL 2009

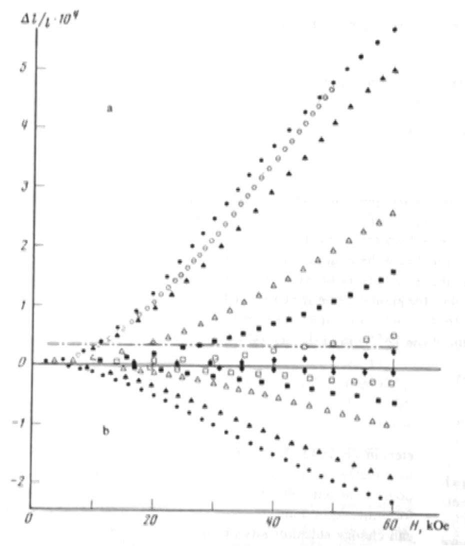
Gingras *et al.* PRB 2000 (CEF)

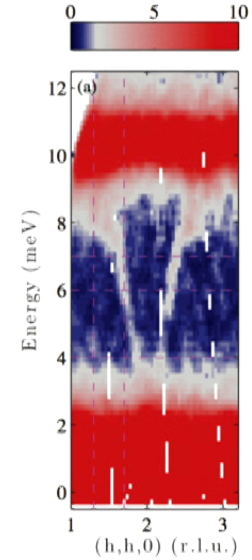


Fennell et al. PRL 2012

Guitteny *et al.* PRL 2013

Magneto-striction





Aleksandrov et al. JETP 1985

Rule et al. JPCS 2009

Ruff et al. PRL 2010

Klevkovkina et al. JPCS 2011

Fennell et al. PRL 2014

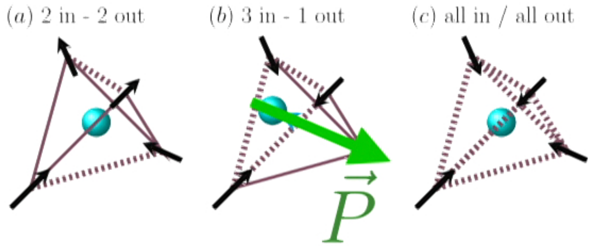
Bonville et al. PRB 2014

Constable et al. PRB 2017

Magneto-electric coupling in spin ice

Electric dipoles on
magnetic monopoles

Khomskii Nature Comm. 2012



Spin-current model

$$\vec{P} \propto \vec{e}_{ij} \times (\vec{S}_i \times \vec{S}_j)$$

Katsura *et al.* PRL 2005
Sarkar *et al.* PRB 2014

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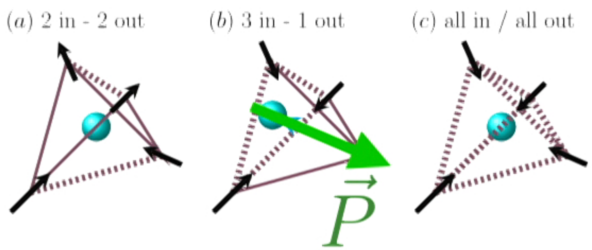


Spin-current model

$$\vec{P} \propto \vec{e}_{ij} \times (\vec{S}_i \times \vec{S}_j)$$

Katsura *et al.* PRL 2005

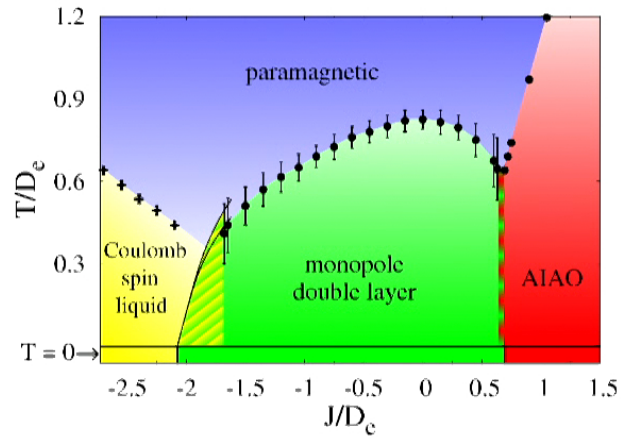
Sarkar *et al.* PRB 2014

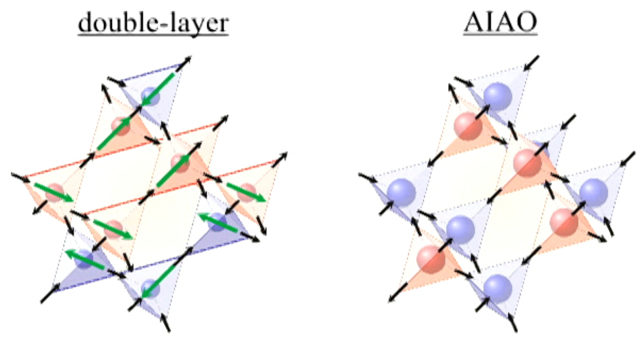
$$\mathcal{H} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \;\; \text{~~} - h \sum_i \vec{S}_i \text{~~}$$

~~$+ D_m r^3 \sum_{i>j} \frac{\vec{S}_i \cdot \vec{S}_j - 3(\vec{S}_i \cdot \vec{e}_{ij})(\vec{S}_j \cdot \vec{e}_{ij})}{r_{ij}^3}$~~

$$+ D_e r_e^3 \sum_{\alpha > \beta} \frac{\vec{P}_\alpha \cdot \vec{P}_\beta - 3(\vec{P}_\alpha \cdot \vec{e}_{\alpha\beta})(\vec{P}_\beta \cdot \vec{e}_{\alpha\beta})}{r_{\alpha\beta}^3}$$

nearest neighbour + *electric* dipolar interaction

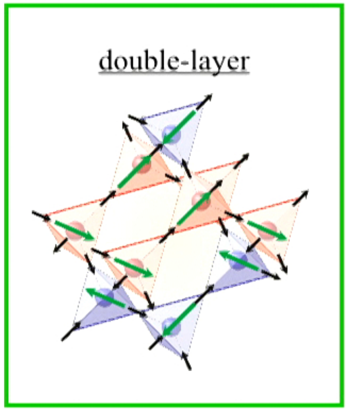


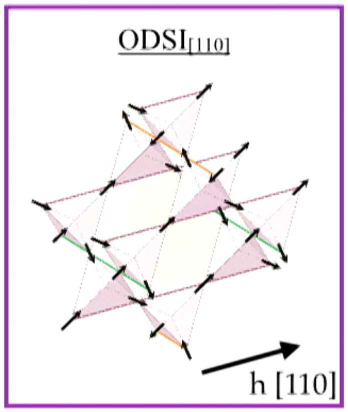


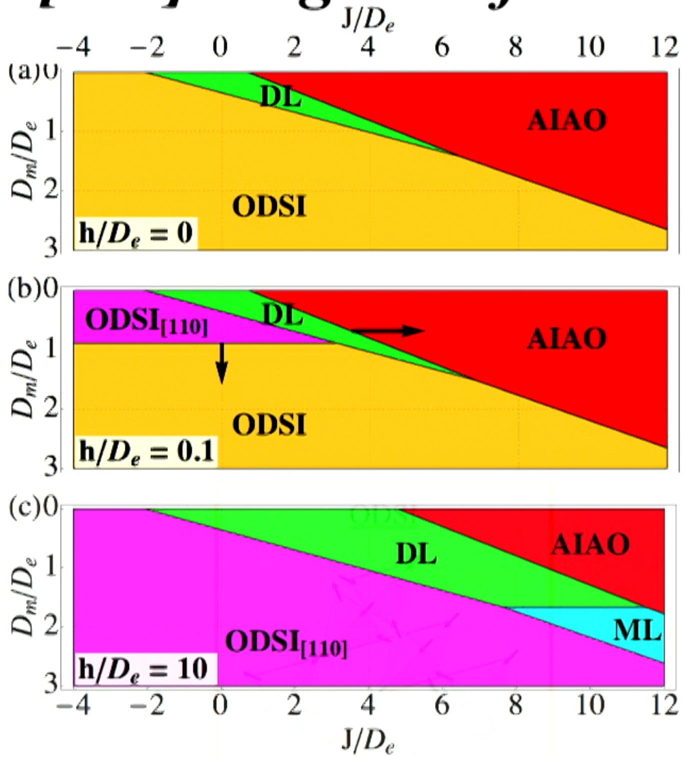
magnetic crystallography

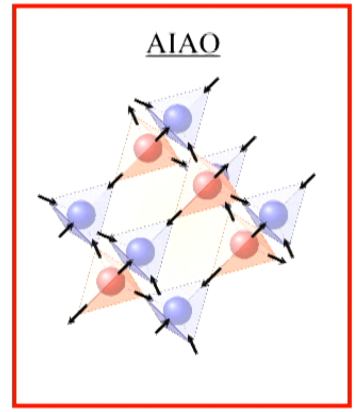
Electric & Magnetic dipolar interactions

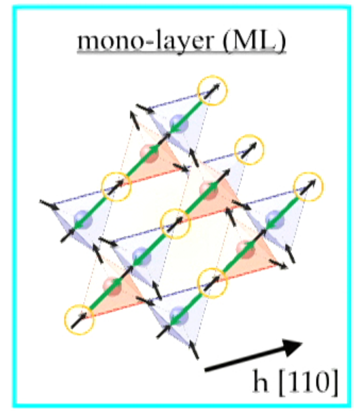
[110] magnetic field





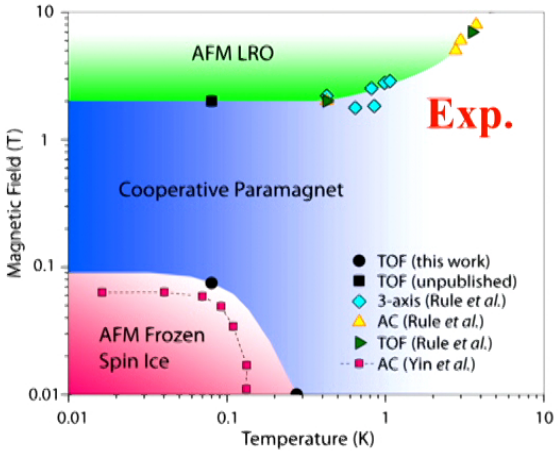






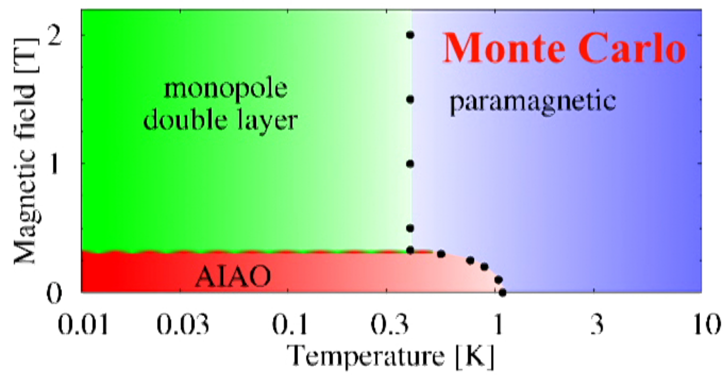
Magneto-electric coupling in $Tb_2Ti_2O_7$

Double-layer observed in a [110] magnetic field



Ruff et al. PRB 2010
Sazonov et al. PRB 2010
Sazonov et al. PRB 2012
Fritsch et al. PRB 2014

$$\mathcal{H} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - \vec{h} \cdot \sum_i \vec{S}_i + D_m r_m^3 \sum_{i>j} \frac{\vec{S}_i \cdot \vec{S}_j - 3(\vec{S}_i \cdot \vec{e}_{ij})(\vec{S}_j \cdot \vec{e}_{ij})}{r_{ij}^3} + D_e r_e^3 \sum_{\alpha>\beta} \frac{\vec{P}_\alpha \cdot \vec{P}_\beta - 3(\vec{P}_\alpha \cdot \vec{e}_{\alpha\beta})(\vec{P}_\beta \cdot \vec{e}_{\alpha\beta})}{r_{\alpha\beta}^3}$$



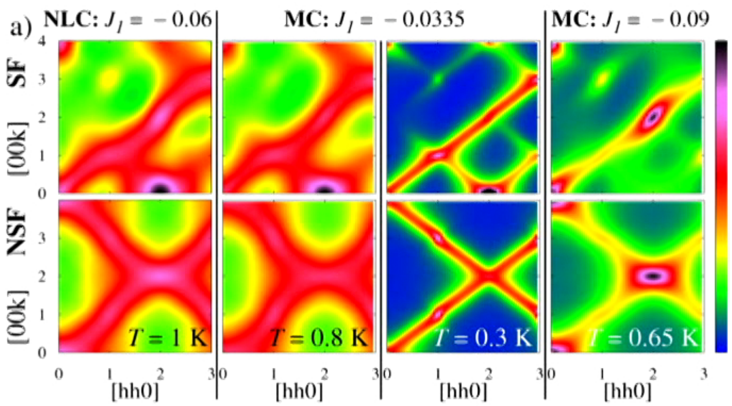
$$J = -2.7K \quad D_m = 0.48K \quad D_e = 0.32K$$

$$P \sim 2.10^{-31}\text{Cm} \quad \delta r \sim 0.6 \text{ pm}$$

Multiphase competition in $Yb_2Ti_2O_7$

Order-by-disorder responsible for multi-step ordering and field-reentrance in $Yb_2Ti_2O_7$. Thermal and quantum fluctuations work together to favour the Γ_5 antiferromagnet.

Jaubert, Benton, Rau, Oitmaa, Singh, Shannon & Gingras PRL 2015
Yan, Benton, Jaubert & Shannon, PRB 2017



Multiferroic spin ice

- crystal of magnetic charges(double-layer)
- enhanced by a [110] magnetic field
- observed in $Tb_2Ti_2O_7$

Jaubert & Moessner PRB 2015