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Ecole Normale Supérieure de Lyon



## **From Spin Ice to Kagomé Planes: The Kasteleyn Transition in kagomé spin ice**

1. The Kasteleyn Transition
2. Neutron scattering, simulation and experiment
3. Finite size scaling and worm commensurability



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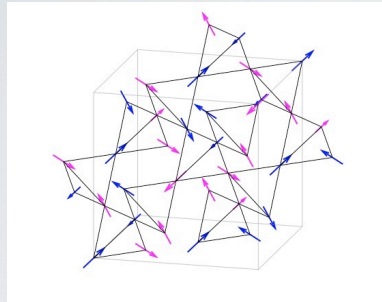


**From Spin Ice to Kagomé Planes:  
The Kasteleyn Transition in kagomé spin ice**

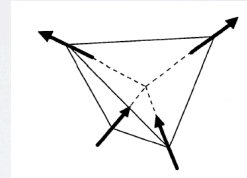
Adam Harman-Clarke, Tom Fennell,  
Jean-Yves Fortin, Steven Bramwell

## Ice rules in spin ice

Spin ice materials  $\text{Ho}_2\text{Ti}_2\text{O}_7$ ,  $\text{Dy}_2\text{Ti}_2\text{O}_7$

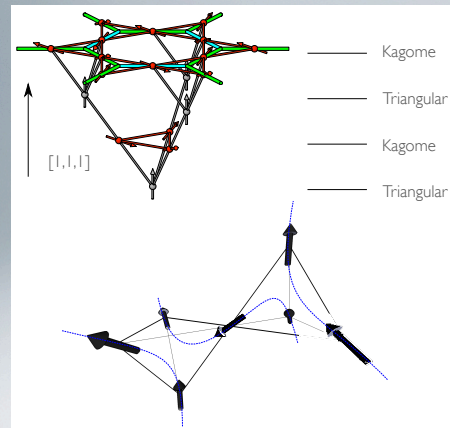


**Magnetic ice rules**  
**two-in two-out**



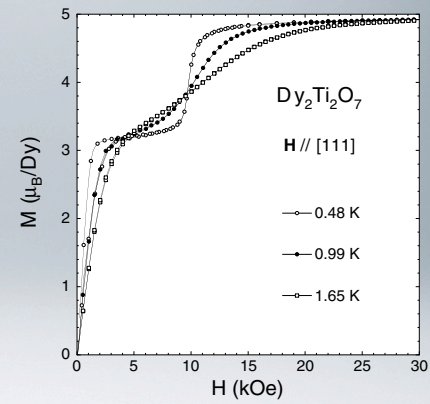
Harris et al, Phys. Rev. Lett. **79**, 2554-2557 (1997)

# KAGOME ICE



$$\nabla \cdot \mathbf{M}(\mathbf{r}) = 0$$

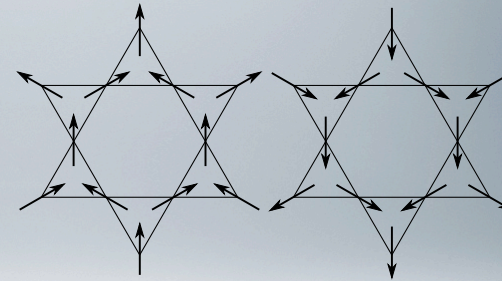
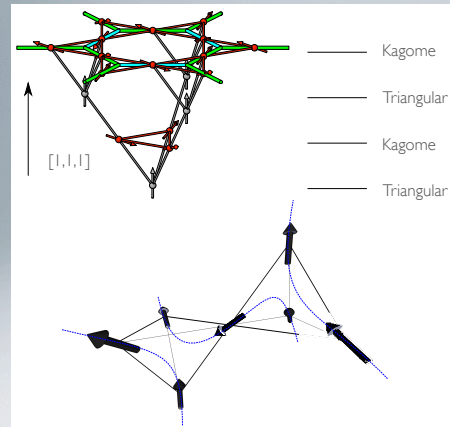
$$S_0 = \frac{3}{4} \frac{S_{\text{antiferro}}}{4} \approx 0.06R$$



Matsuhira *et al.* J o P: Cond. Mat., 2002  
 Udagawa *et al.* JPSJ, 2002  
 Wills *et al.* PRB, 2002  
 Isakov *et al.* PRB, 2004  
 Moessner and Sondhi, PRB, 2003



# KAGOME ICE



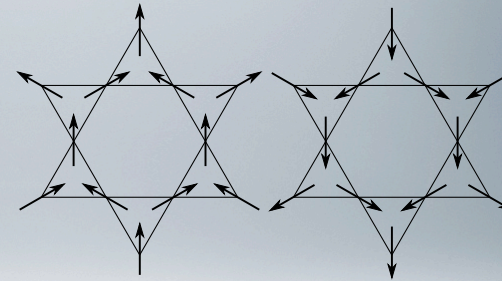
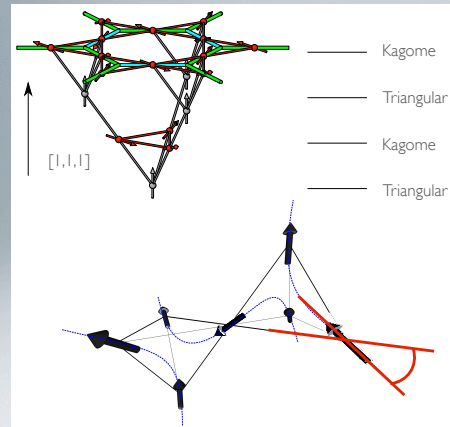
Broken  $Z_2$  symmetry

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# KAGOME ICE



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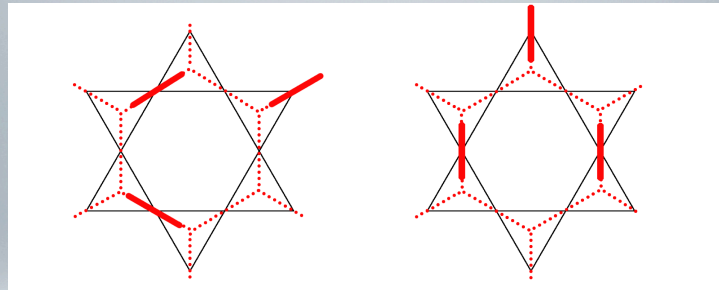
# THE KASTELEYN TRANSITION



Spin to dimer mapping

Kasteleyn, J. of Math. Phys. 1963  
Moessner and Sondhi, PRB, 2003

# THE KASTELEYN TRANSITION



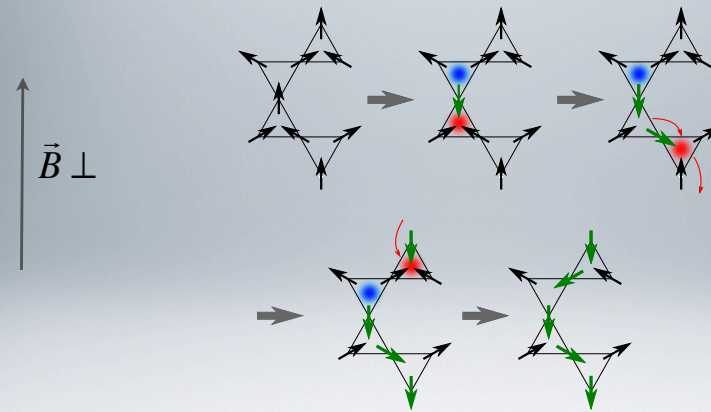
Disordered  
Finite entropy

Ordered  
Zero entropy

Kasteleyn, J. of Math. Phys. 1963  
Moessner and Sondhi, PRB, 2003

# WORM EXCITATIONS

(CLOSED LOOPS)



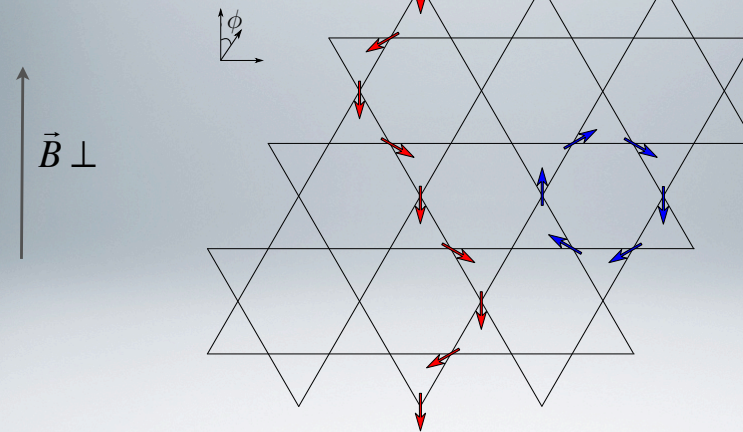
At transition  
 $\delta G = \delta \epsilon - T_k \delta S = 0$

energy loss  
 = entropy gain

Only long loops  
 change M

# WORM EXCITATIONS

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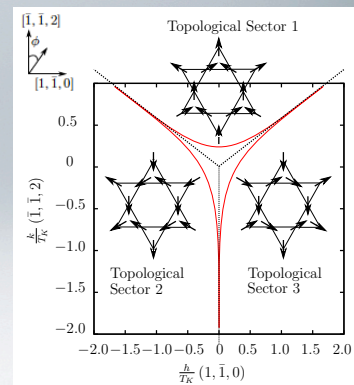
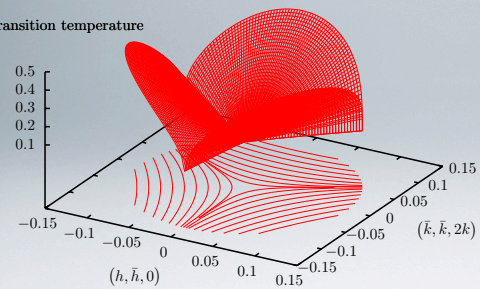
change M



# PHASE DIAGRAM

Temperature-Field Kagome Ice Phase Diagram

Transition temperature



## Thermodynamics of the K transition

internal energy  $U$  is constant for all (Pauling) states

Magnetic Helmholtz Free energy is pure Entropy!

$$F = -TS(m, N)$$

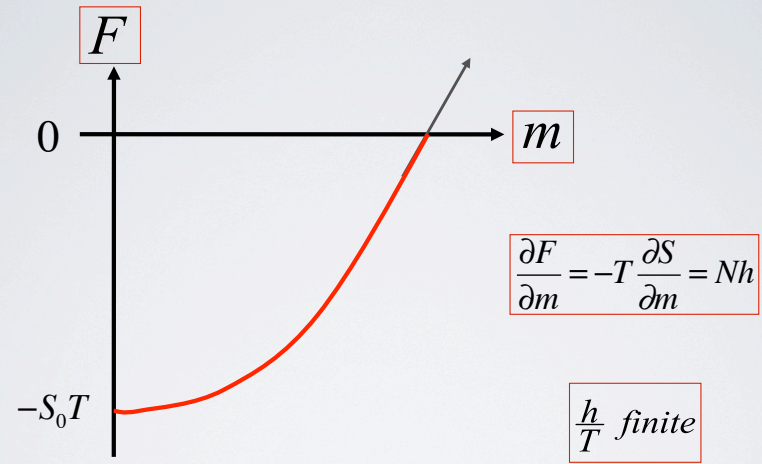
$$dF = -SdT + Nhdm$$

$$h = \frac{1}{N} \frac{\partial F}{\partial m} = -\frac{T}{N} \frac{\partial S}{\partial m}$$

$$\chi = \frac{\partial m}{\partial h} = -\frac{1}{T} \frac{N}{\partial^2 S / \partial m^2}$$

Kasteleyn transition:

$S \rightarrow 0$  for finite  $h/T$



KASTELEYN transition in collective paramagnet

# LANDAU FREE ENERGY

$$x = m_{sat} - m \quad \frac{G_L}{NT} = \frac{F - Nhm}{NT} = \frac{1}{T} (h - h_K)x + \frac{\alpha_2}{2} x^2 + \frac{\alpha_3}{3} x^3 \dots$$

Landau critical exponents:

$$\beta = 1, \gamma = \alpha = 0$$

Upper critical dimension is 3  
therefore mean field exponents will  
be subject to corrections in 2D.

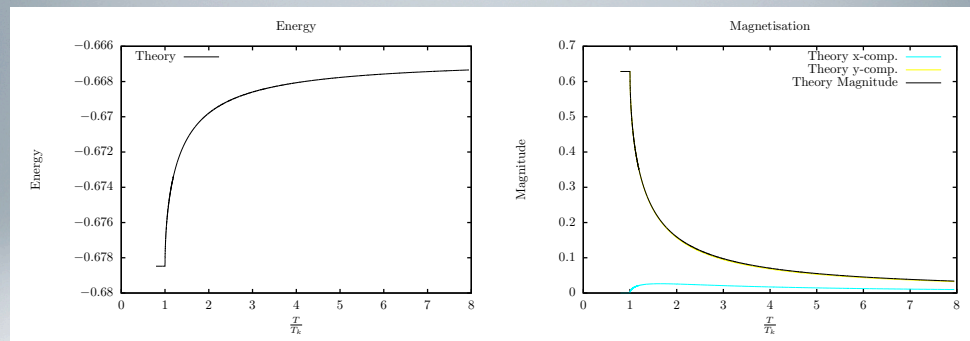
Fluctuation modified values:

$$\beta = 1/2, \gamma = \alpha = 1/2$$

$\alpha = 1/2$  for  $d = 2$  in agreement with the exact solution<sup>(3)</sup> and  
 $\alpha = (3 - d)/2$  more generally for  $1 < d < 3$ ;

Jaubert *et al.* J. Phys.: Conf. Ser. 2009  
Bhattacharjee *et al.* J. Stat. Phys. 1983

# THERMODYNAMICS



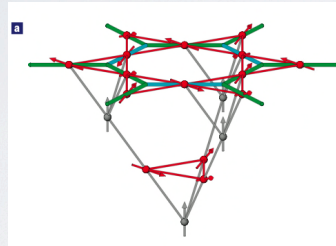
Asymmetric, 1st/2nd order character; biaxial magnetisation

# Neutron scattering - “in plane”, polarized, unpolarized

$$S(Q) = \left\langle \sum_R \vec{S}_\perp(R) \vec{S}_\perp(0) \exp(i\vec{Q} \cdot \vec{R}) \right\rangle$$

$\vec{S}_\perp(R)$  is component perp to  $Q$   
and parallel to  
neutron polarization

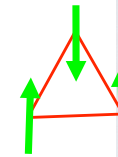
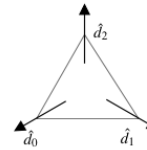
$\vec{B}$  ↑



Neutrons polarized along  
<111> could measure  
pseudo-spins

$$\begin{aligned} \hat{d}_0 &= [-\sqrt{3}/2, -1/2] \\ \hat{d}_1 &= [\sqrt{3}/2, -1/2] \\ \hat{d}_2 &= [0, 1] \end{aligned}$$

$$\sigma_i = \vec{S}_i \cdot \vec{d}_i$$

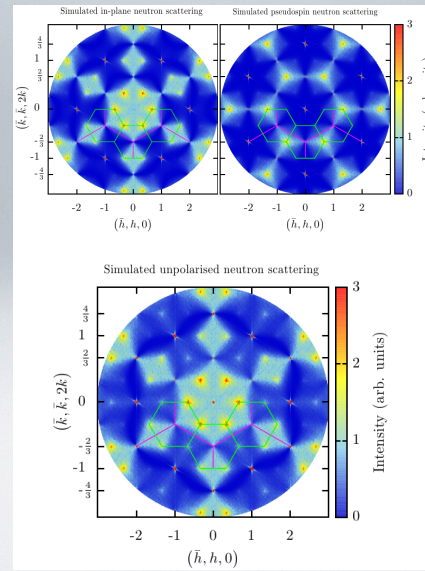


In plane <111>

Unpolarized is sum of both



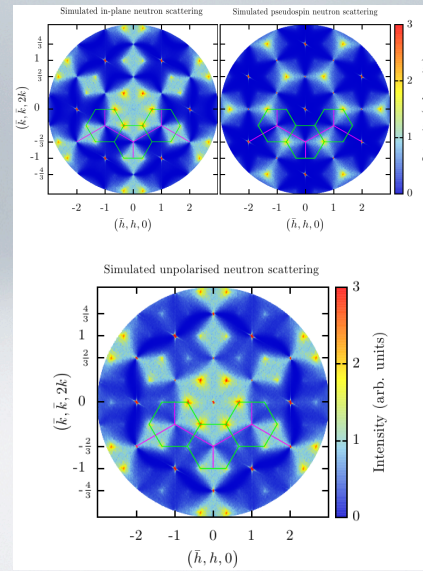
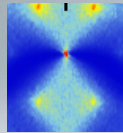
# ZERO FIELD NEUTRON SCATTERING



10800 spins,  
50 different spin  
configurations.

# ZERO FIELD NEUTRON SCATTERING

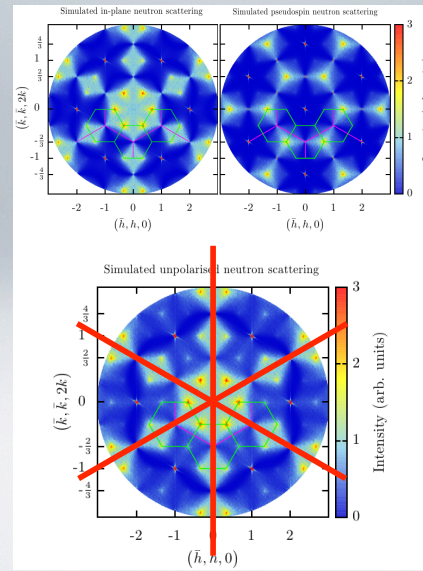
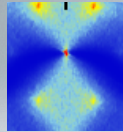
Pinch points



10800 spins,  
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# ZERO FIELD NEUTRON SCATTERING

Pinch points

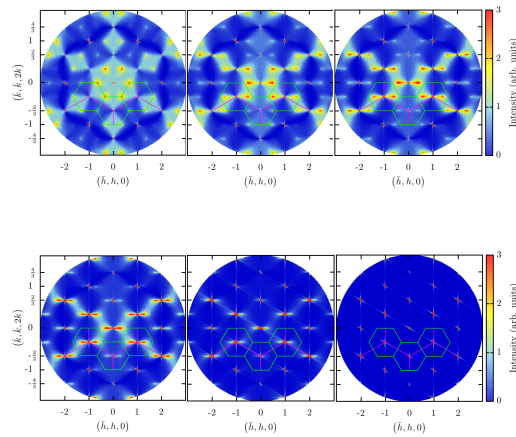


10800 spins,  
50 different spin  
configurations.

High symmetry

# NEUTRON SCATTERING FINITE FIELD

$$\phi=0$$



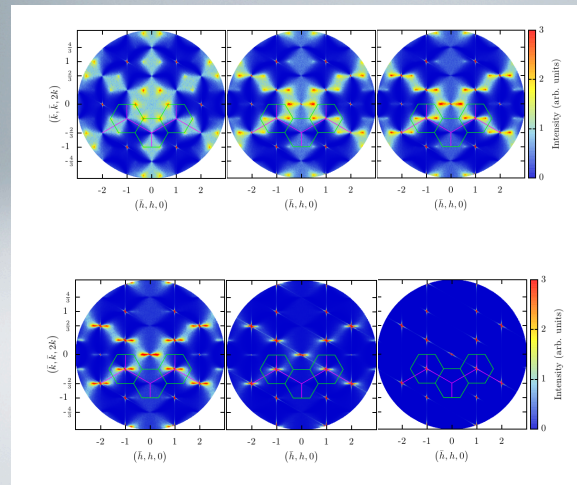
M.S. predictions

- Drifting peaks
- Reduced symmetry
- Different perpendicular correlation lengths
- Asymmetry of transition

Moessner and Sondhi, PRB, 2003

# NEUTRON SCATTERING FINITE FIELD

$$\phi=0$$



M.S. predictions

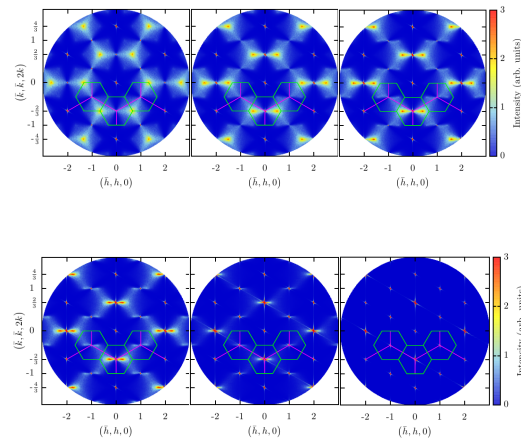
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Moessner and Sondhi, PRB, 2003



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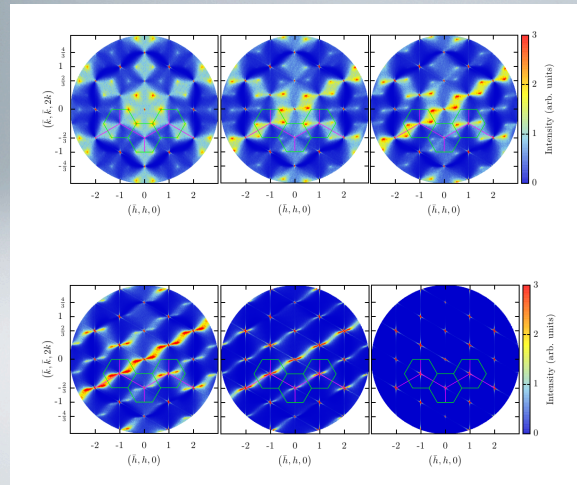
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# NEUTRON SCATTERING FINITE FIELD

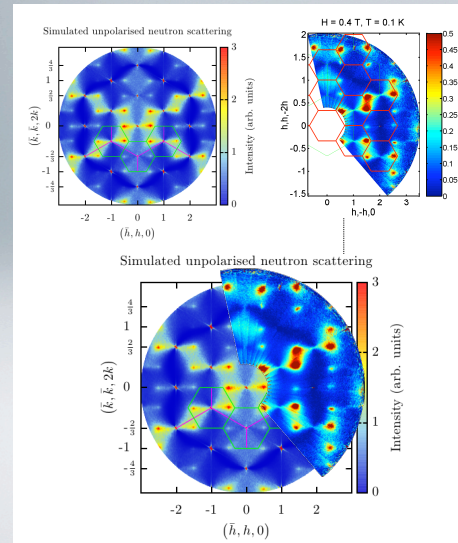
$$\phi \neq 0$$



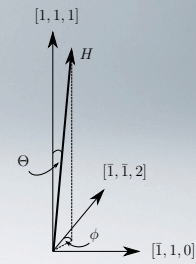
Note:

- Symmetry
- Peak shape
- Correlation lengths

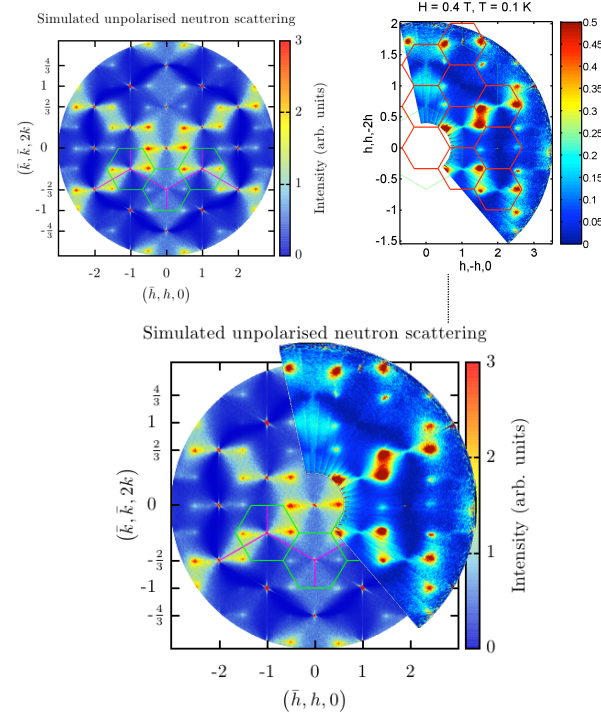
# COMPARISON WITH EXPERIMENT



$\text{Ho}_2\text{Ti}_2\text{O}_7$   
0.1 K, 0.4 T  
ILL



Fennell *et al.* Unpub.  
Fennell *et al.* Nat. Phys., 2007  
Morris *et al.* Science, 2009

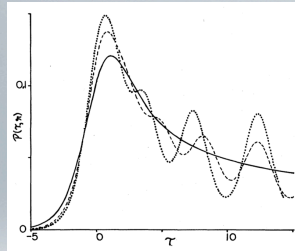


Agreement is qualitative

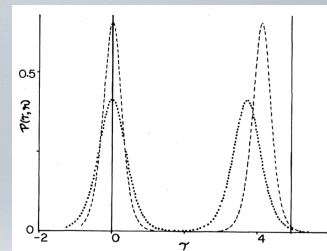
$$\frac{h}{T_{\text{exp}}} = \frac{10\mu_B H_{\text{exp}} \sin(3^\circ)}{k_B T_{\text{exp}}} \approx 1.4$$

$$\frac{h}{T_{th}} \approx 0.12$$

# FINITE SIZE SCALING



Short, wide,  $R \rightarrow \infty$



Tall, thin,  $R \rightarrow 0$

$$R = \frac{N^2}{M}$$

Specific heat of brick lattice

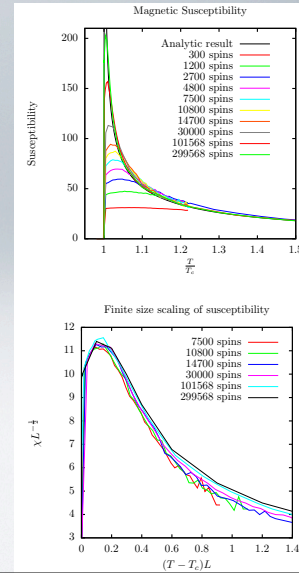
Bhattacharjee and Nagle, PRA, 1981

# COMMENSURATE FIELD BEHAVIOUR

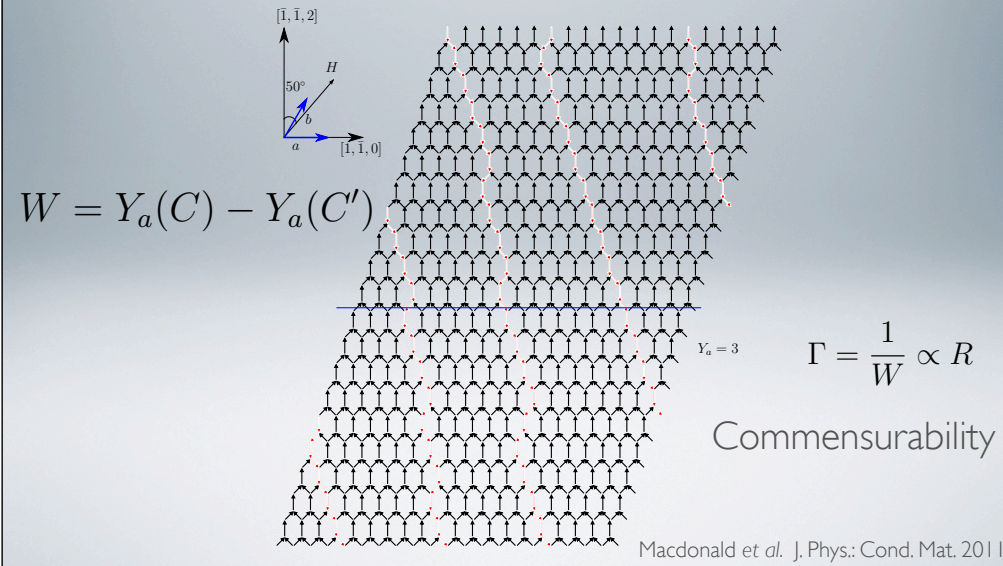
$$\begin{aligned}\chi &= t^{-\gamma} \mathcal{P} \left( \frac{\xi_{\perp}}{L_{\perp}}, \frac{\xi_{\parallel}}{L_{\parallel}} \right) \\ \chi &= t^{-\gamma} \mathcal{P} \left( \frac{1}{|t|^{\nu_{\perp}} L}, \frac{1}{|t|^{\nu_{\parallel}} L} \right) \\ &= t^{-\gamma} \times (|t|^{\nu_{\parallel}} L)^{\frac{\gamma}{\nu_{\parallel}}} \mathcal{Q} \left( \frac{1}{|t|^{\nu_{\perp}} L}, \frac{1}{|t|^{\nu_{\parallel}} L} \right) \\ &= L^{\frac{\gamma}{\nu_{\parallel}}} \mathcal{Q} \left( \frac{1}{|t|^{\nu_{\perp}} L}, \frac{1}{|t|^{\nu_{\parallel}} L} \right)\end{aligned}$$

$$\lim_{|t| \rightarrow 0} \chi = L^{\frac{\gamma}{\nu_{\parallel}}} \mathcal{Q} \left( \frac{1}{|t|^{\nu_{\perp}} L}, \frac{1}{|t|^{\nu_{\parallel}} L} \right)$$

$$\gamma = \frac{1}{2} \quad \nu_{\parallel} = 1 \quad \nu_{\perp} = \frac{1}{2}$$



# WINDING NUMBER





# INCOMMENSURATE FIELD BEHAVIOUR

$$\lim_{|t| \rightarrow 0} \chi = L^{\frac{\gamma}{\nu_{\parallel}}} \mathcal{Q} \left( \frac{1}{|t|^{\nu_{\parallel}} L} \right)$$

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# INCOMMENSURATE FIELD BEHAVIOUR

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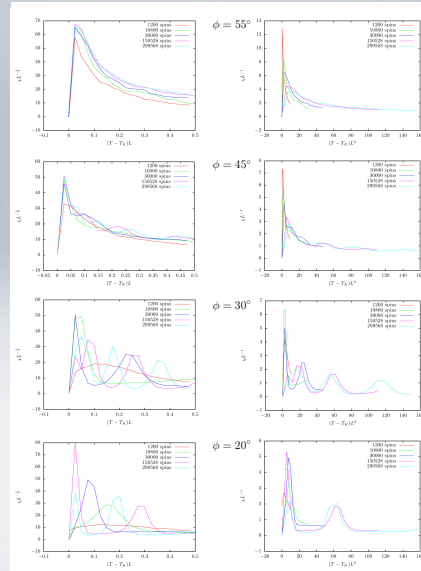
# INCOMMENSURATE FIELD BEHAVIOUR

$\nu_{\parallel}$  scaling

$\nu_{\perp}$  scaling

$$\lim_{|t| \rightarrow 0} \chi = L^{\frac{\gamma}{\nu_{\parallel}}} Q\left(\frac{1}{|t|^{\nu_{\parallel} L}}\right)$$

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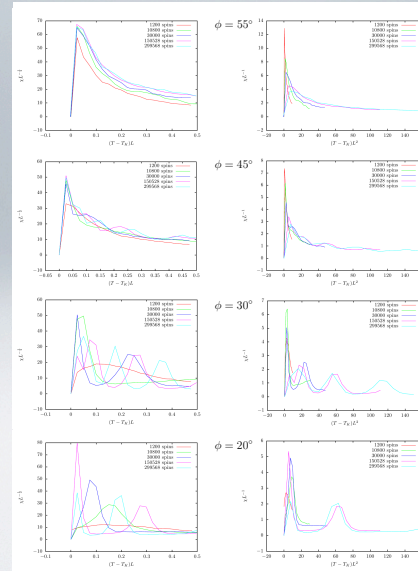
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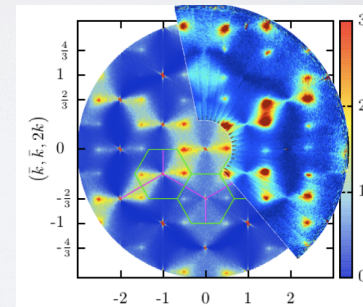
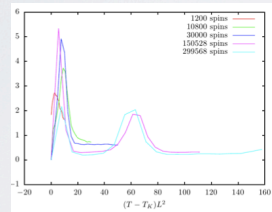
$$\gamma = \frac{1}{2} \quad \nu_{\parallel} = 1 \quad \nu_{\perp} = \frac{1}{2}$$



Quantised behaviour!

## Conclusions

1. The Kasteleyn Transition appears in model  $\langle 111 \rangle$  spin ice
2. A vestige of this transition can be observed in experiment
3. Finite size scaling exposes the topological nature of the K-transition



From Spin Ice to Kagomé Planes:  
Natal, December 2011