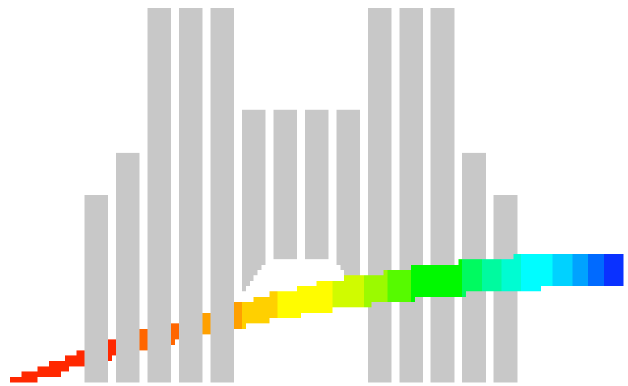
Topological phases and the Kasteleyn transition



Peter Holdsworth

Ecole Normale Supérieure de Lyon

1. Ice and Spin-Ice, collective paramagnets
2. Topologically constrained states
3. Monopole excitations out of them
4. The Kasteleyn transition in spin ice
5. Mapping to a quantum phase transtion

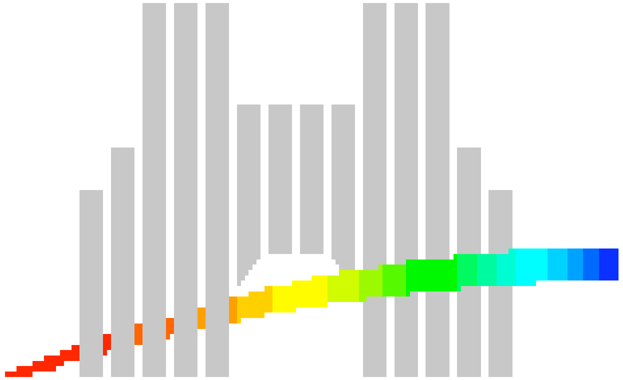
Collaboration

Ludovic Jaubert
John Chalker
Roderich Moessner

Thanks

Steven Bramwell Mark Harris
Tom Fennell Des McMorrow

Financial support: ESF-HFM network, Royal Society, ANR 05 BLAN 0105, London Centre for Nanotechnology



Hexagonal and cubic ice maintain proton disorder to T=0

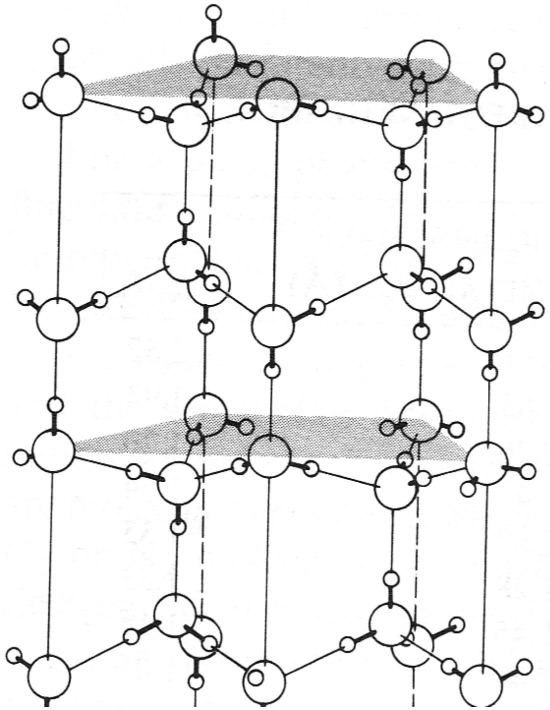


Figure 19.11
The crystal structure of one of the many phases of ice. The large circles are oxygen ions; the small circles are protons. Ice is an example in which hydrogen bonding plays a crucial role. (After L. Pauling, *The Nature of The Chemical Bond*, 3rd. ed., Cornell University Press, Ithaca, New York, 1960.)

Image from « Solid State Physics »
Ashcroft and Mermin

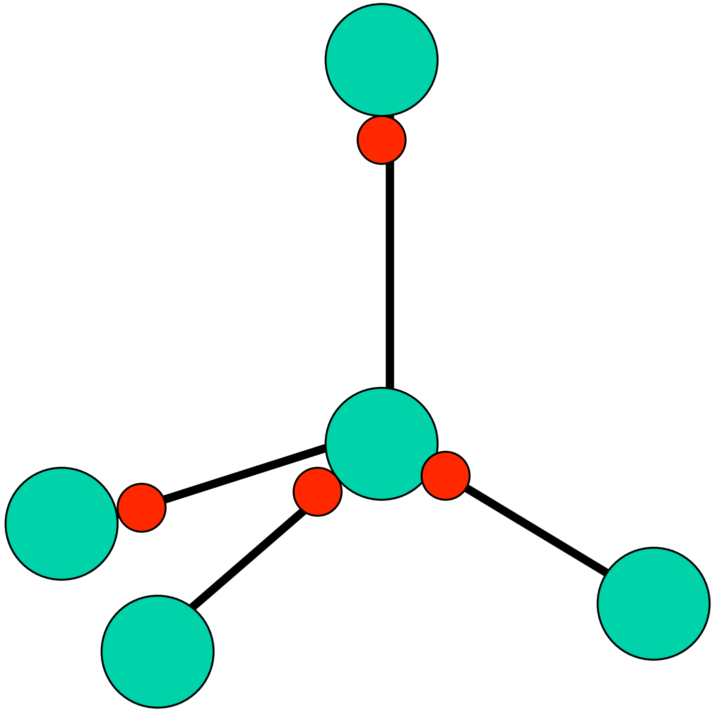
The Entropy of Water and the Third Law of Thermodynamics. The Heat Capacity of Ice from 15 to 273°K.

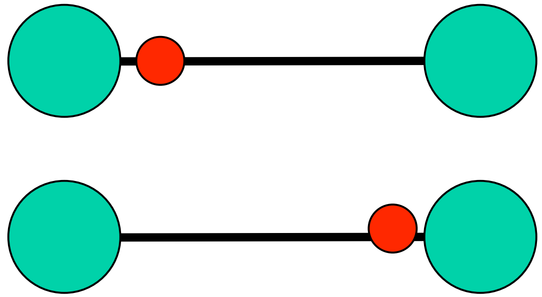
By W. F. Giauque and J. W. Stout

Berkeley, Calif.
Received March 30, 1936

J. Am. Chem. Soc, 58, 1144, 1936

Bernal-Fowler rules and Pauling Entropy





Each Hydrogen takes 2 positions.
For 1 mole of $H_2 0$

$$\boxed{\Omega^0 = 2^{2N}}$$

$2^4=16$ configs for each O^{2-}, 6/16 satisfy Bernal Fowler rules:

$$\boxed{\Omega \approx 2^{2N}\left(\frac{3}{8}\right)^N = \left(\frac{3}{2}\right)^N} \quad \Rightarrow \quad \boxed{S \approx R \ \log\left(\frac{3}{2}\right)} \quad \text{Per mole}$$

A magnetic analogue of ice-
Spin ice

Harris, Bramwell, McMorrow, Zeiske and Godfrey, *Phys. Rev. Lett.* **79**, 2554 (1997)

In $Ho_2Ti_2O_7$ and $Dy_2Ti_2O_7$ Ho and Dy ions sit on corners of an open Pyrochlore structure.

Ising like spins along body centres of the tetrahedra.

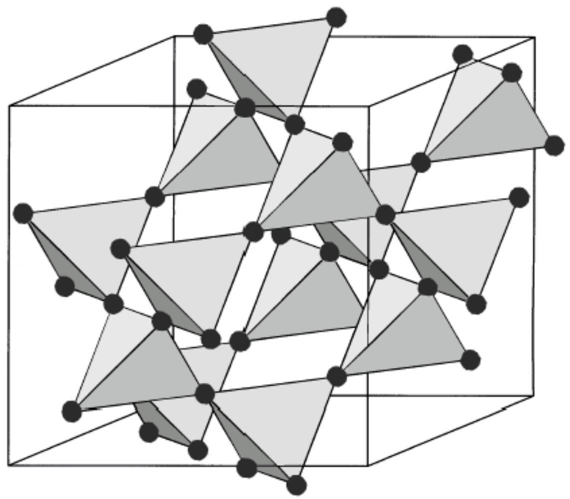
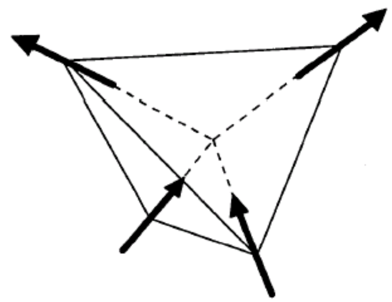


FIG. 1. The pyrochlore lattice.

$$H = -J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$$

$$\vec{S}_i = \pm \begin{matrix} <1,1,1> \\ <1,-1,-1> \\ <-1,1,-1> \\ <-1,-1,1> \end{matrix}$$

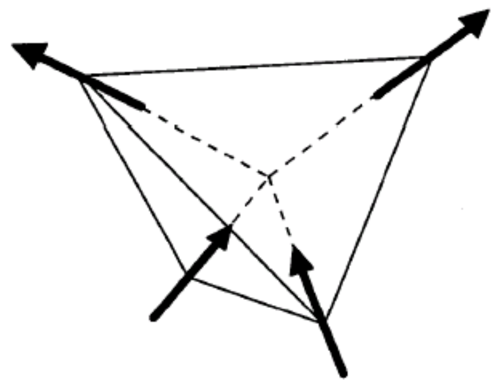


Pyrochlore lattice

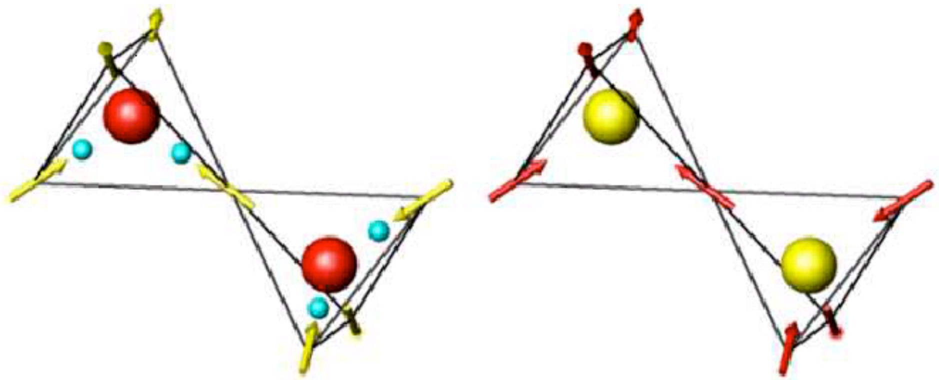
Here we study NN model-

(dipole interaction den Hertog and Gingras, PRL.84, 3430 (2000).)

Frustrated ferromagnet with two spins "in" and two "out on each tetrahedron



Magnetic ice rules => Pauling ground state Entropy. Violation of third law.

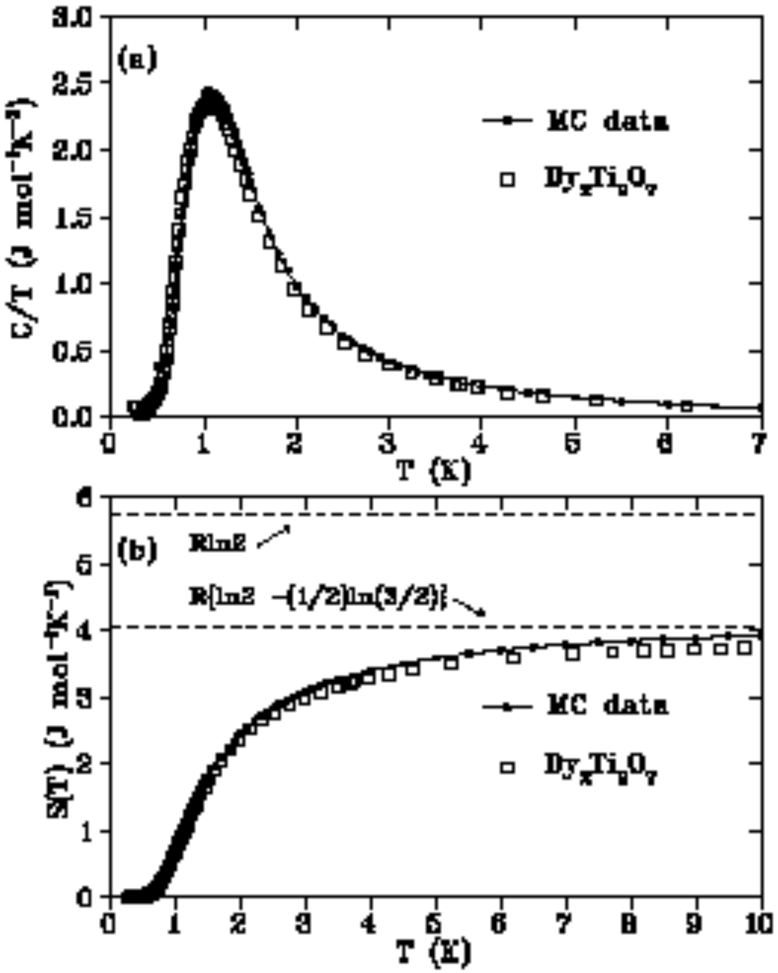


$$\boxed{S_P = Nk_B \frac{1}{2} \ln \frac{3}{2}}$$

Pyrochlore is the duel of a diamond lattice as appears in the cubic ice phase

Magnetic « Giauque and Stout » experiment:

Ramirez et al, Nature399,333, (1999)



Life on the « constrained » manifold of Pauling states:

Like a paramagnet the internal energy $U = -\frac{NJ}{\sqrt{3}}$ is constant for all Pauling states

Differences between a paramagnet and this « collective » paramagnet (Villain, *Z. Phys. B*, 33, 31 (1979)):

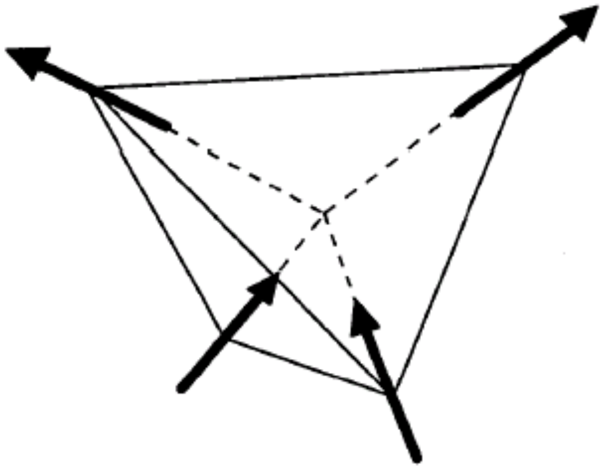
1. **Long range correlations**

2. **Topological excitations back to paramagnetic phase space**

3. **(Kasteleyn) phase transition in presence of magnetic field**

Topological constraints and divergence free condition:

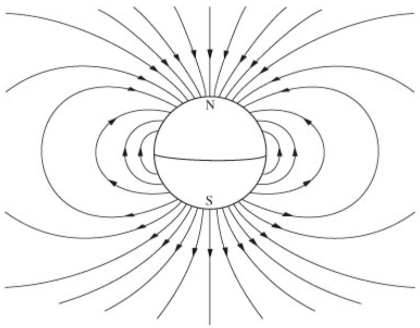
The ice rules impose local constraints



Two spins in two spins out
=> A divergence free field

$$\vec{\nabla}.\vec{S}=0$$

$$<\vec{S}(\vec{r}).\vec{S}(0)>\sim\frac{1}{r^3}$$



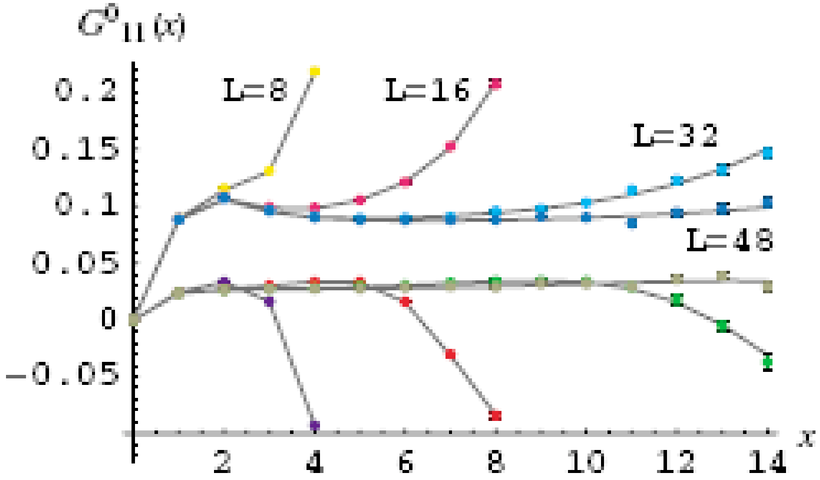
Like a dipolar magnetic field
⇒Power law correlations
Henley Phys. Rev. B **71**, 014424, 2005

Dipolar magnetic fields and spin ice:

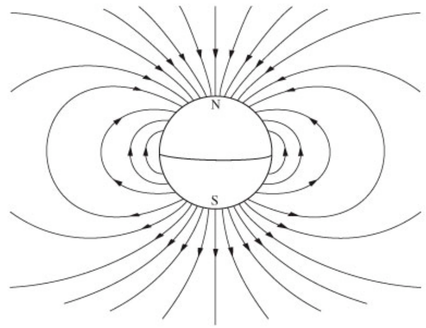
Izakov et al, PRL 93, 167204, 2004

$$\vec{B} = \vec{S}_{spin-ice}$$

$$r^3 < \vec{B}(\vec{r}).\vec{B}(0) >$$



Critical phase ? No
Coupling between spin and space
ensures correlations are not divergent.



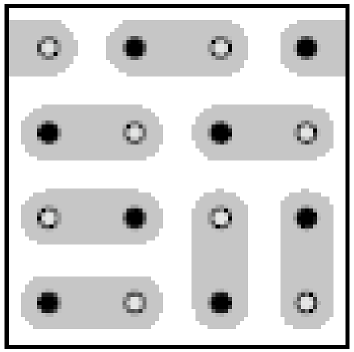
$$\int r^2 < \vec{B}(\vec{r}).\vec{B}(0) > dr d\Omega = const.$$

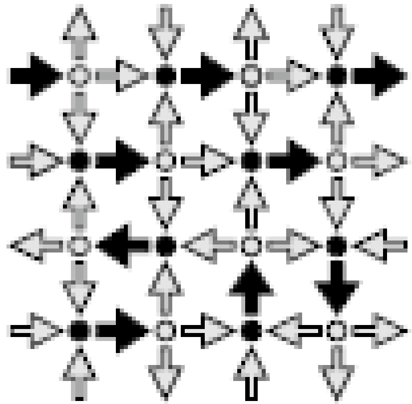
For ice see: Castro Neto, Pujol, and Fradkin, PRB, 74, 024302, 2006

Constraints for dimers on bipartite lattice:

Constraint written as divergenceless field: |B| = 1 along dimer, 1/(z-1) between dimers

Huse et. al. PRL 91, 167004, 2003

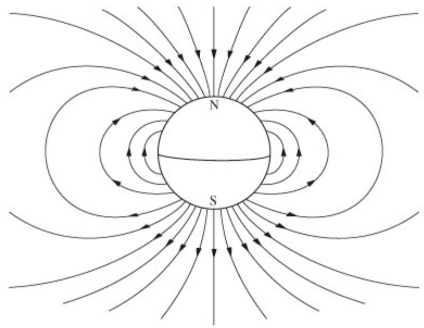




$$\vec{\nabla}.\vec{B}=0$$

Dipolar fields – power law correlations

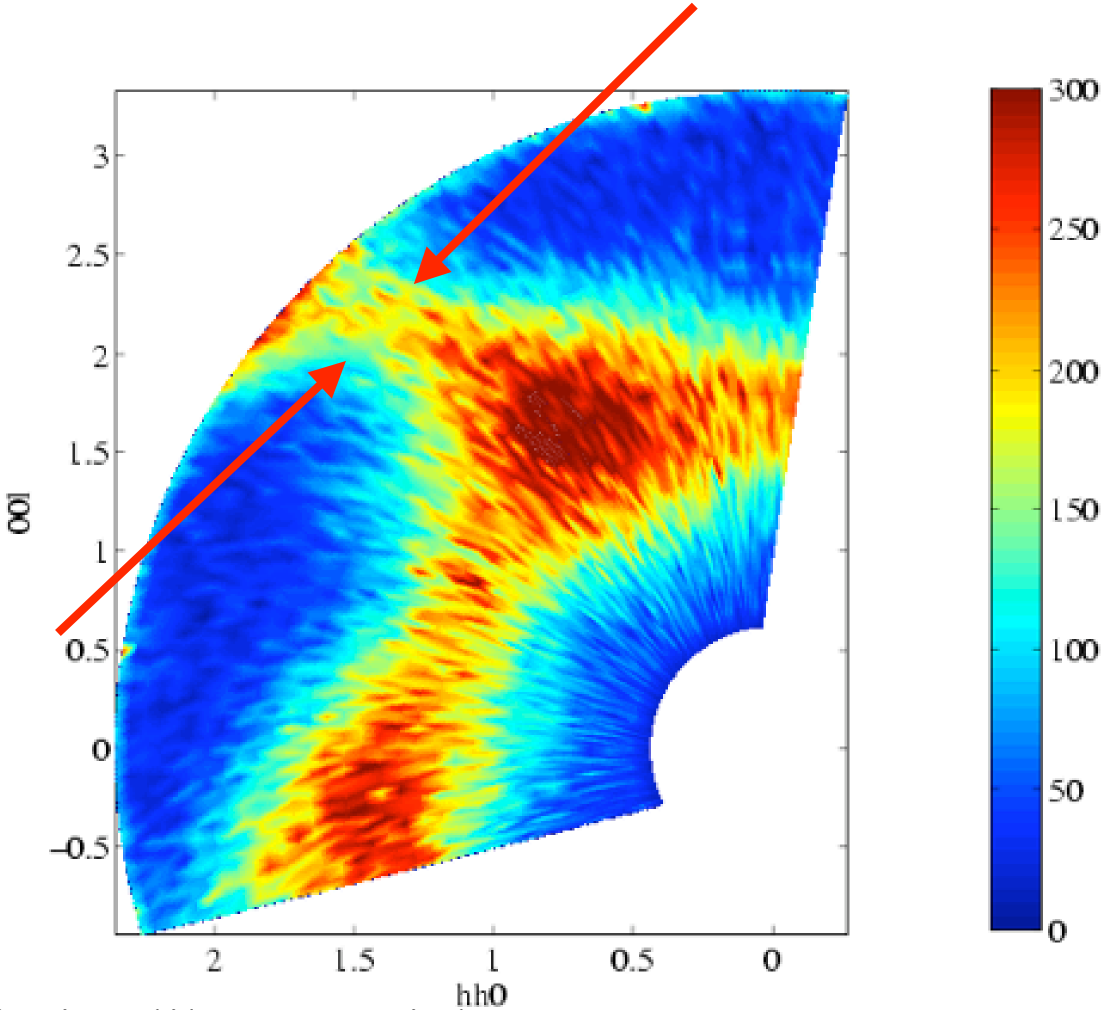
$$<\vec{B}(\vec{r}).\vec{B}(0)>\sim\frac{1}{r^3}$$



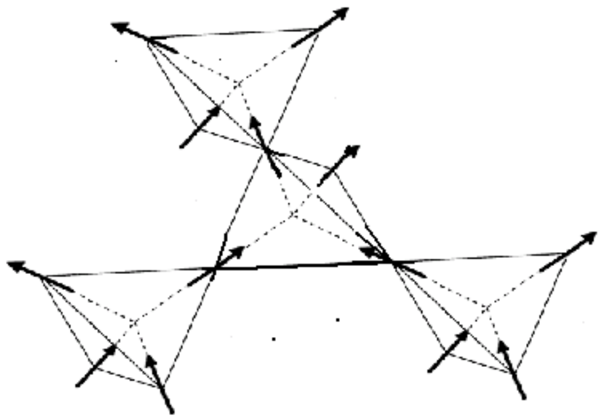
However, long range correlations do appear as « pinch » points in reciprocal space. (Youngblood and Axe, Phys. Rev. B 23, 232 (1981)).

Regions of intense diffuse scattering.

Narrowing=> correlations over large length scales

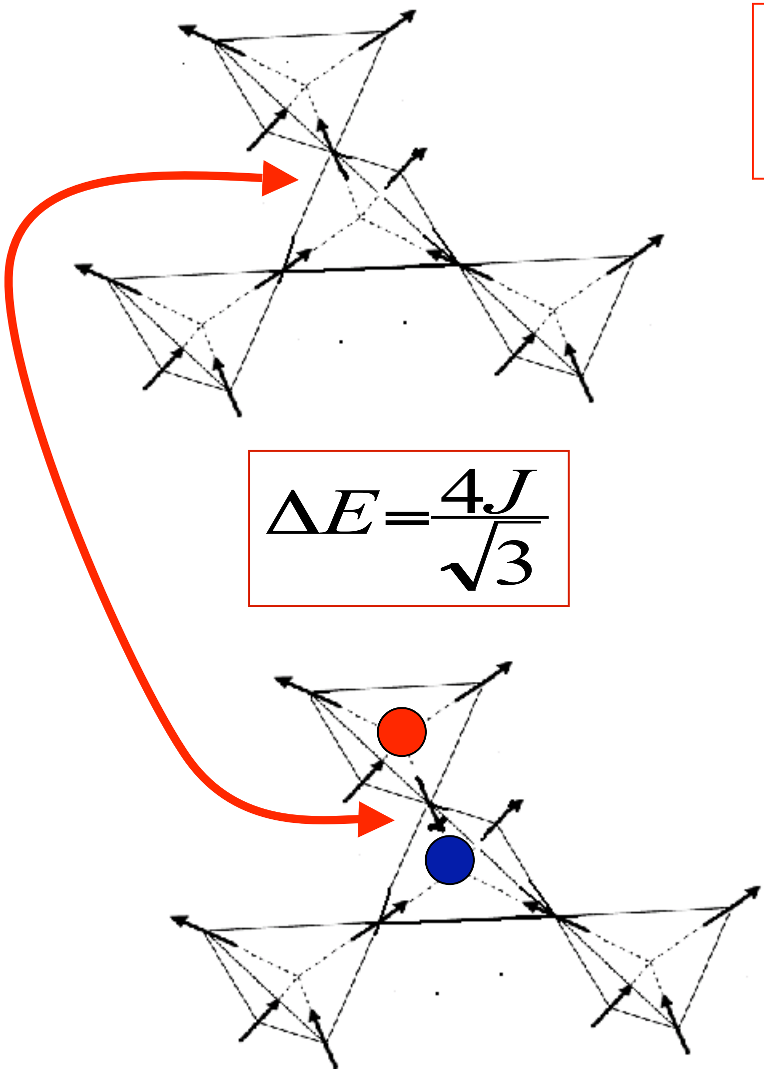


Single crystal of a spin ice like material (Fennell, Bramwell, Harris 2007)



Topological constraints
Excitations back to paramagnet….

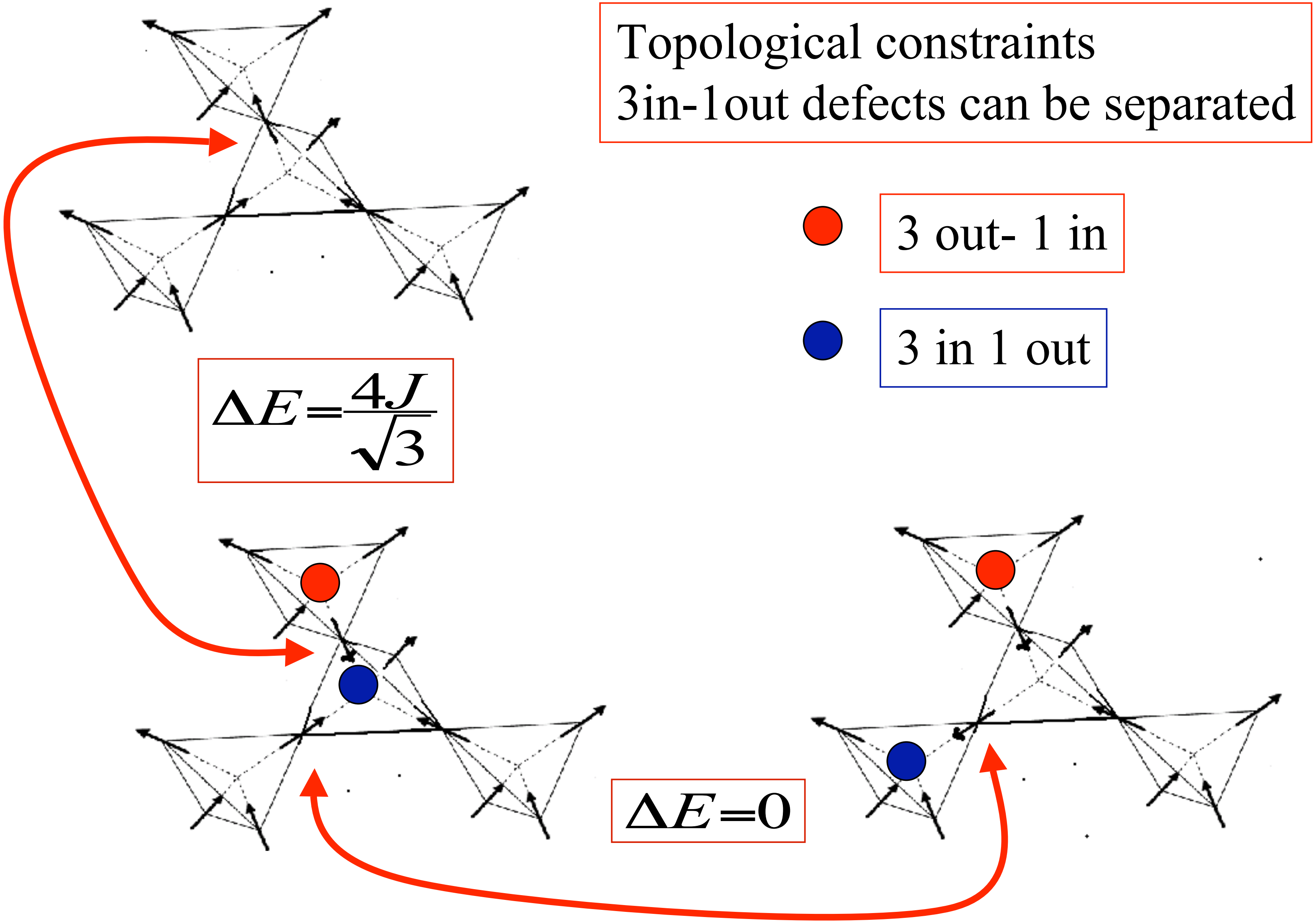
Topological constraints
3in-1out defects can be created

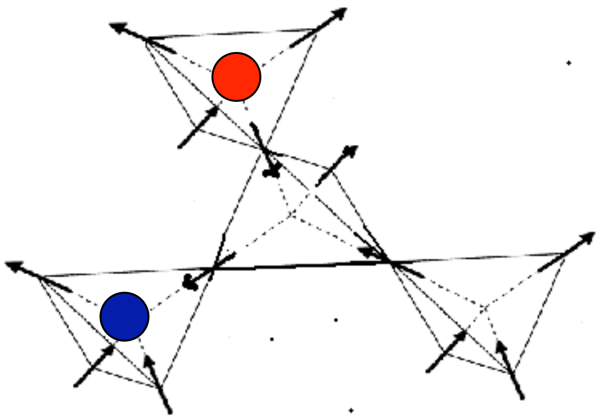


$$\Delta E = \frac{4J}{\sqrt{3}}$$

3 out- 1 in

3 in 1 out


Topological constraints
3in-1out defects can be separated
3 out- 1 in
3 in 1 out
$\Delta E = \frac{4J}{\sqrt{3}}$
$\Delta E = 0$



Topological defects (monopoles)
can only be created/destroyed in pairs

In our NN model the defects move freely

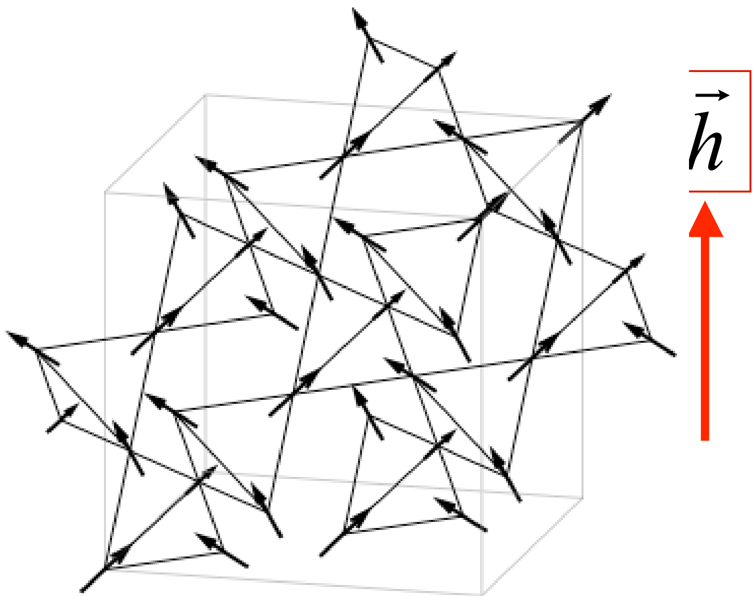
Including dipole spin-spin
interactions the defects interact
(monopoles)

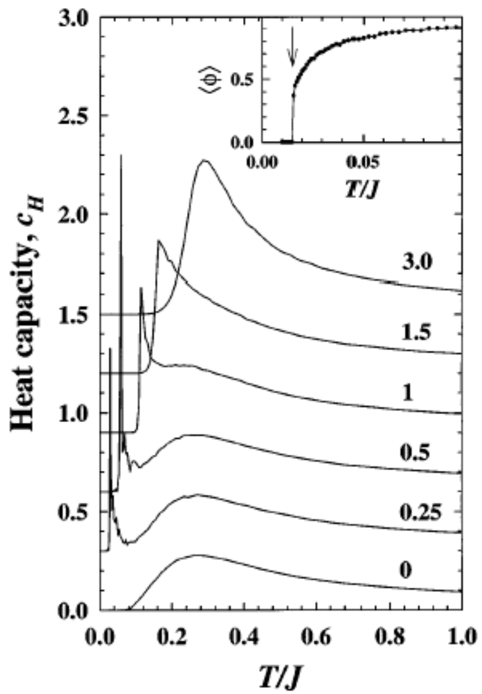
Castelnovo, Moessner, Sondhi,
Nature, 451, 42, 2008

Spin ice in a [100] field

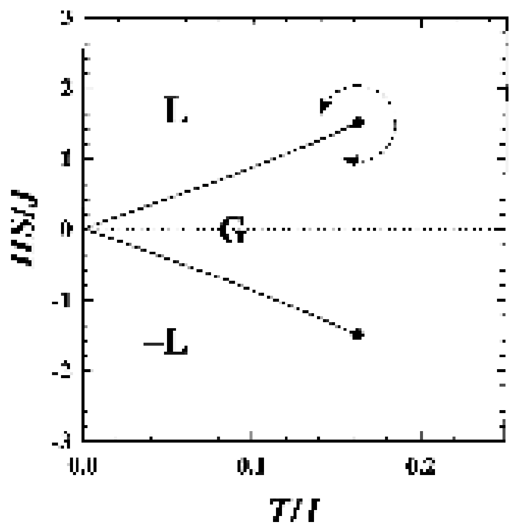
Degeneracy lifted in favour of a unique long range ordered ground state

Evidence of singular behaviour
(Symmetry sustaining phase transition)

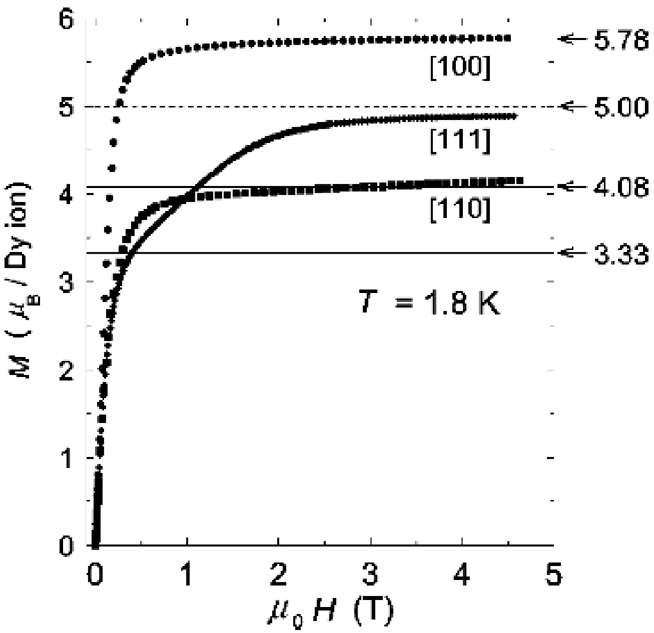




Harris , Bramwell, Holdsworth, Champion
PRL 81,4496, 1998

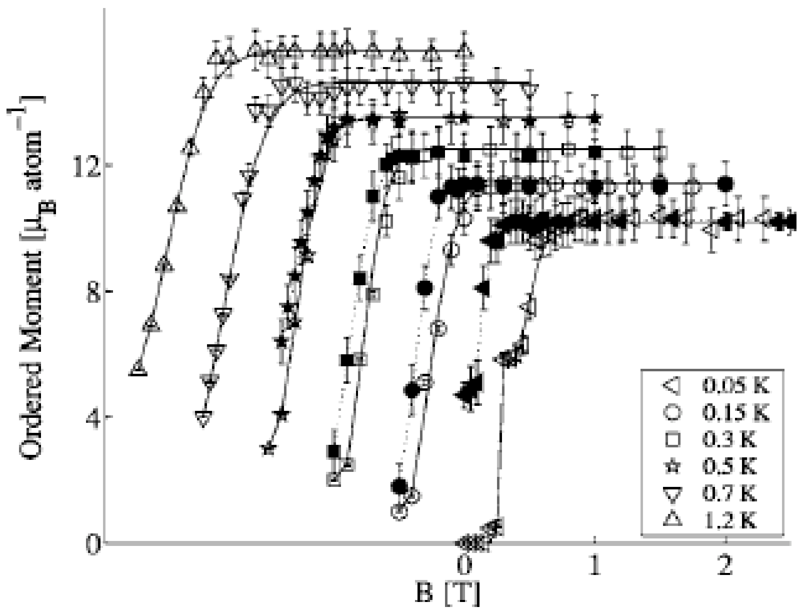


Experimentally, M vs B_{ex} is very different from that of a Paramagnet (Brillouin function)



$Dy_2Ti_2O_7$ in [100] field

Fukazawa et al, Phys. Rev. B. 65, 054410, 2002



$Ho_2Ti_2O_7$ in [100] field

Fennell et al, PRB 72, 224411, 2005

Thermodynamics of a (collective) paramagnet

internal energy U is constant for all states

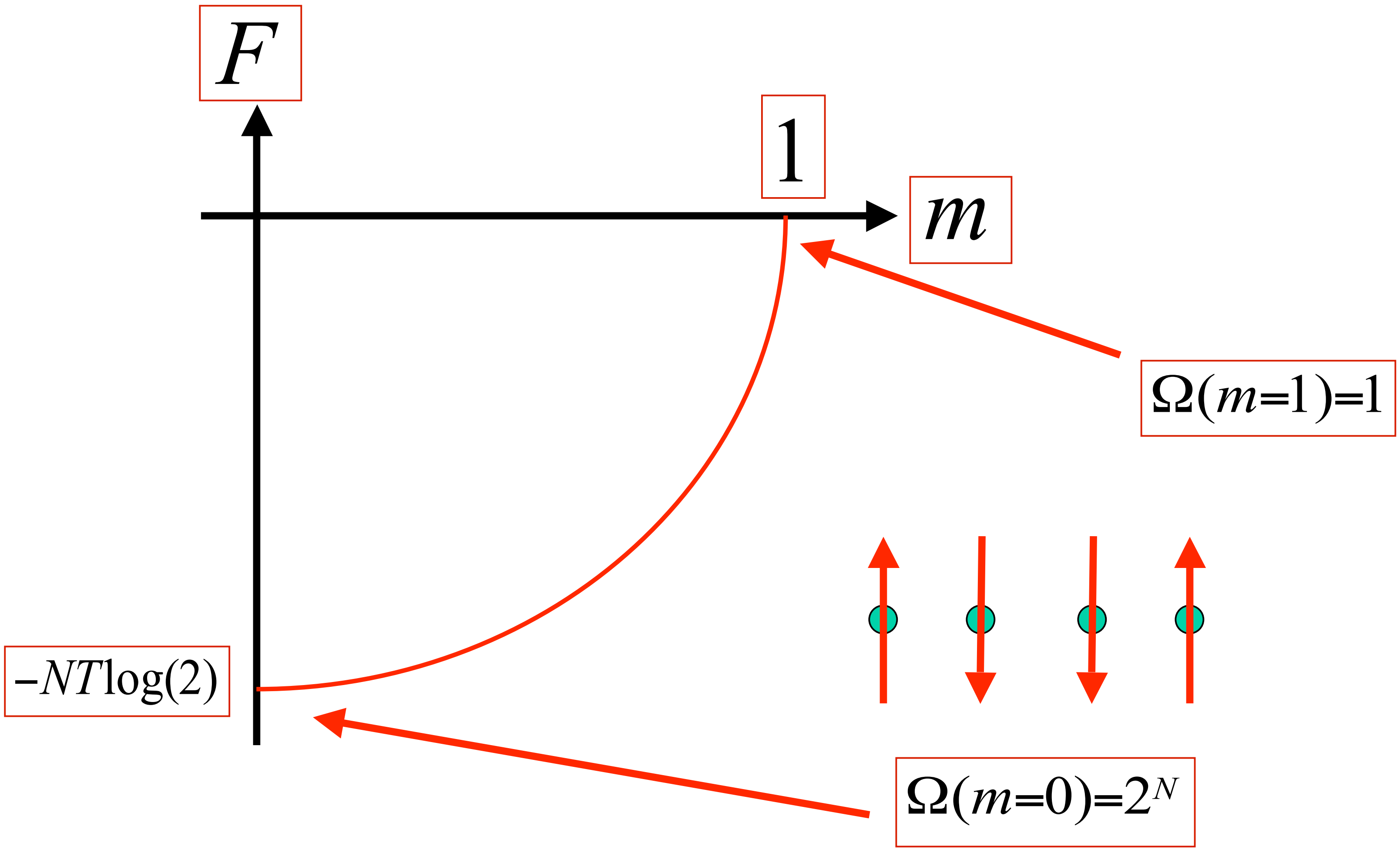
Magnetic Helmholtz Free energy is pure Entropy!

$$\boxed{F = -TS(m,N)} \qquad \boxed{dF = -SdT + Nhdm}$$

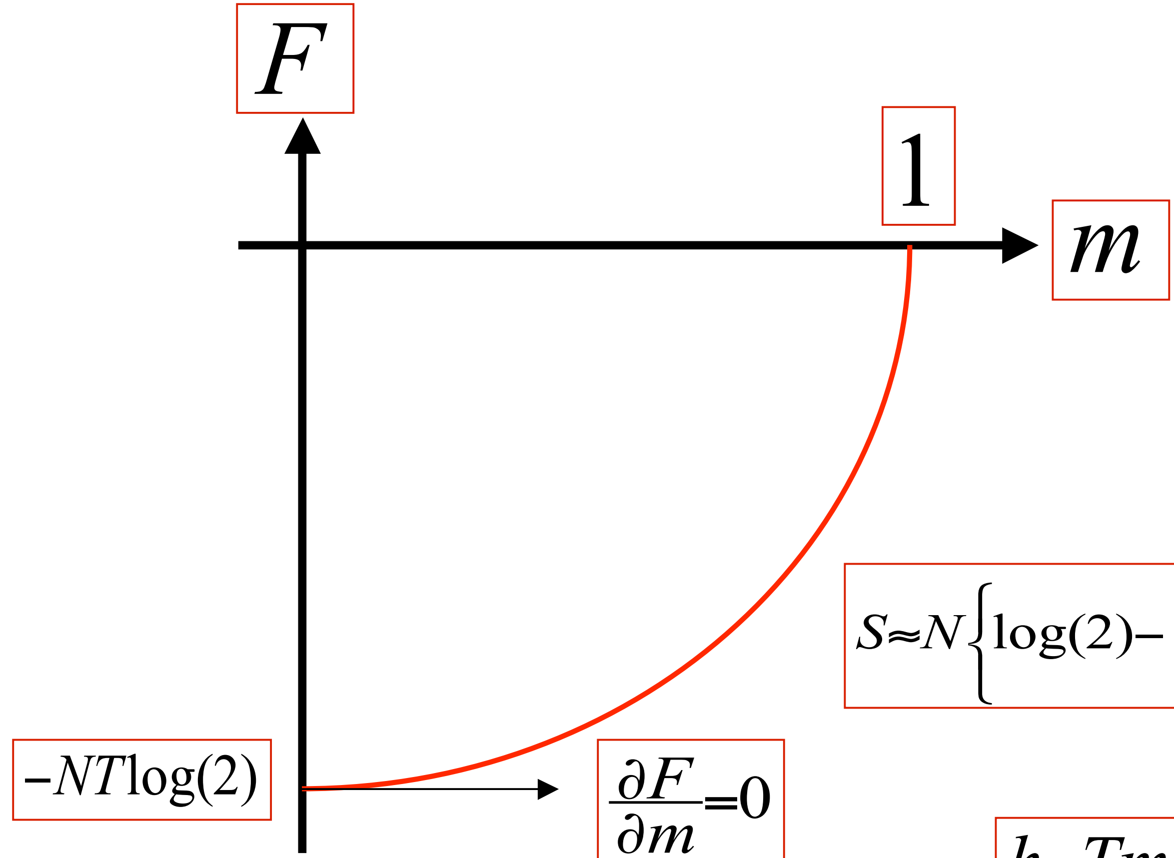
$$\boxed{h = \frac{1}{N}\frac{\partial F}{\partial m}} \qquad \boxed{\chi = \frac{\partial m}{\partial h} = \frac{N}{\partial^2 F / \partial m^2}}$$

How do the Entropy and m disappear in presence of a field ?

A simple paramagnet: $S = -N\left\{\frac{(1+m)}{2}\log\left(\frac{1+m}{2}\right) + \frac{(1-m)}{2}\log\left(\frac{1-m}{2}\right)\right\}$



A simple paramagnet: $\boxed{S=-N\left\{\frac{(1+m)}{2}\log\left(\frac{1+m}{2}\right)+\frac{(1-m)}{2}\log\left(\frac{1-m}{2}\right)\right\}}$



$$m\approx 0$$

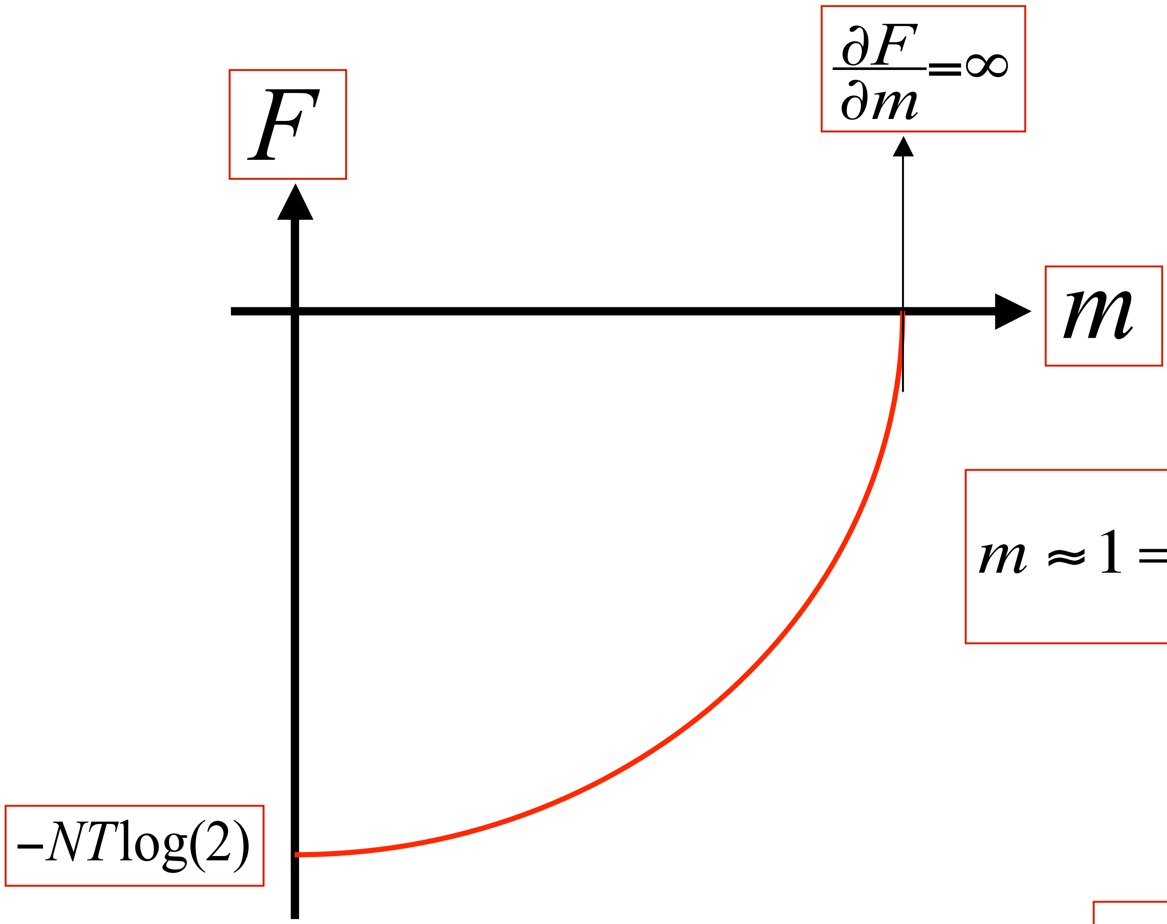
$$S\approx N\left\{\log(2)-\frac{m^2}{2}\right\}$$

$$\frac{\partial F}{\partial m}=0$$

$$h=Tm$$

$$\chi=\frac{1}{T}$$

A simple paramagnet: $\boxed{S = -N\left\{\frac{(1+m)}{2}\log\left(\frac{1+m}{2}\right) + \frac{(1-m)}{2}\log\left(\frac{1-m}{2}\right)\right\}}$



$\boxed{m \approx 1}$

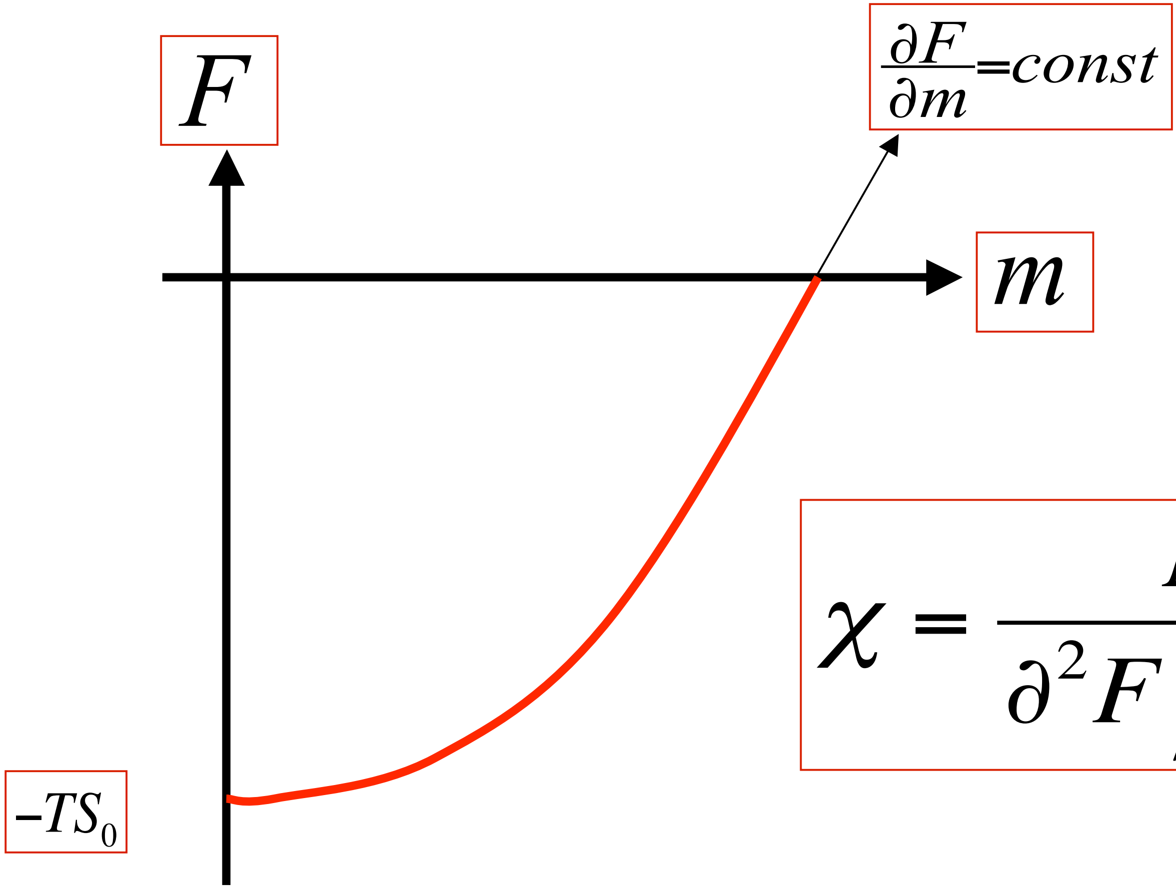
$$\boxed{m \approx 1 \Rightarrow \frac{h}{T} = -\frac{1}{2}\log\left(\frac{1-m}{2}\right)}$$

$$\boxed{\frac{h}{T} \Rightarrow \infty}$$

$$\boxed{\chi \approx (1-m) \Rightarrow 0}$$

No phase transition!

BUT- if the slope were finite at F=-TS=0 ?



$\frac{h}{T}$ *finite*

$$\frac{\partial^2 F}{\partial m^2} = 0$$

$$\chi = \frac{N}{\partial^2 F / \partial m^2} = \infty$$

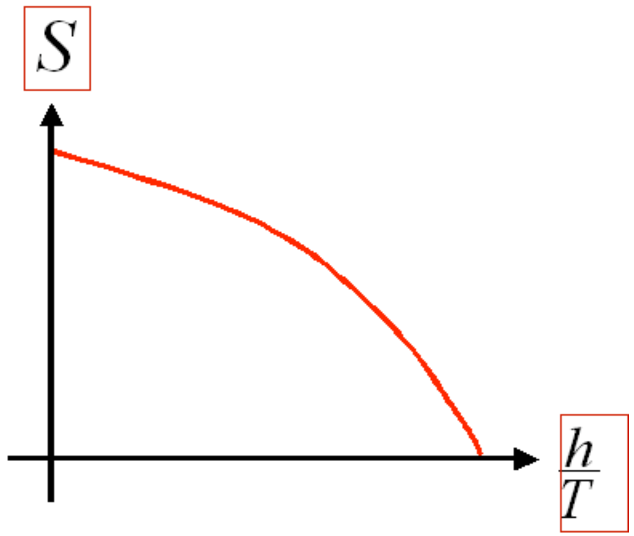
KASTELEYN transition in collective paramagnet

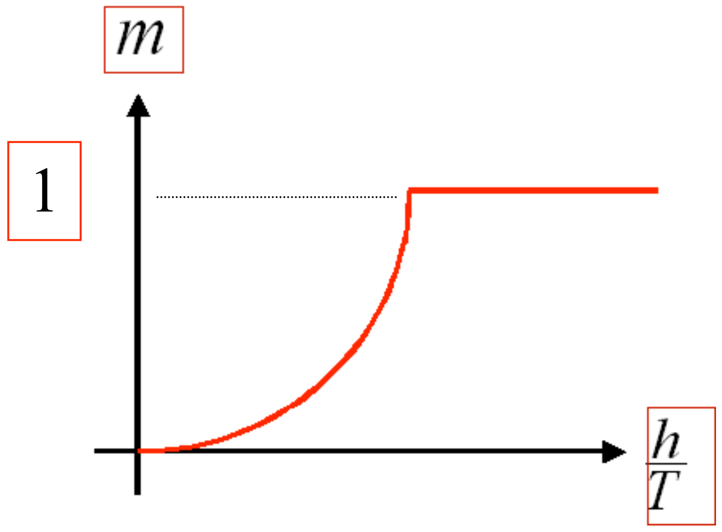
KASTELEYN transition in collective paramagnet

P.W. Kasteleyn, J.Math. Phys. 4, 287, 1963

Moessner and Sondhi PRB 68, 064411, 2003

Bhattacharjee, Nagle, Huse and Fisher, J. Stat. Phys, 32, 361, 1983



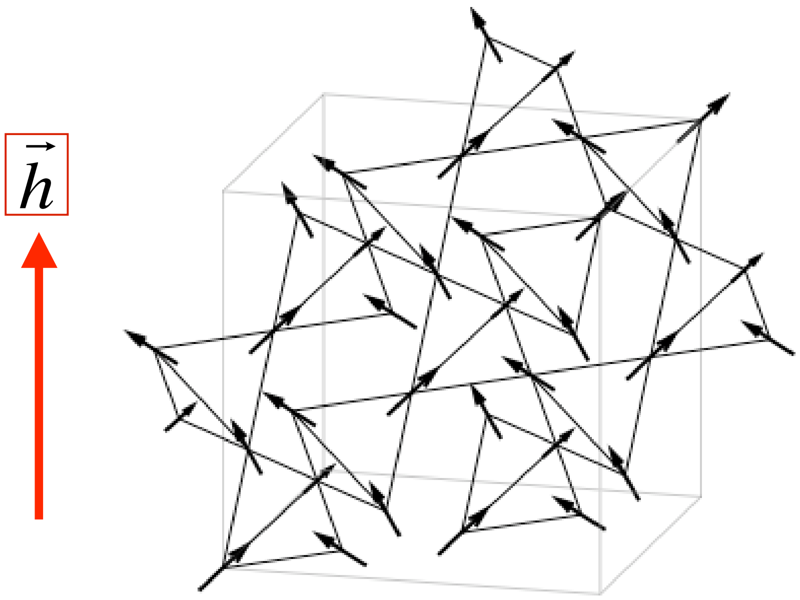


S(T)=0 implies extensively gapped excitations…..

Spin ice in field-leaving the ordered state at low T:

The lowest energy excitations are closed lines of spin flips:

Jaubert, Chalker, Holdsworth and Moessner, Phys. Rev. Lett., 100, 067207, 2008



At each step black-red

$$\boxed{\delta\varepsilon_{Zeeman} = \frac{2h}{\sqrt{3}}}$$

$$\boxed{\delta S = \log(2)}$$

Free energy of line

$$\boxed{\Delta G = L\left(\frac{2h}{\sqrt{3}} - T\log(2)\right)}$$ => Lines at $$\boxed{T_K = \frac{2h}{\log(2)\sqrt{3}}}$$

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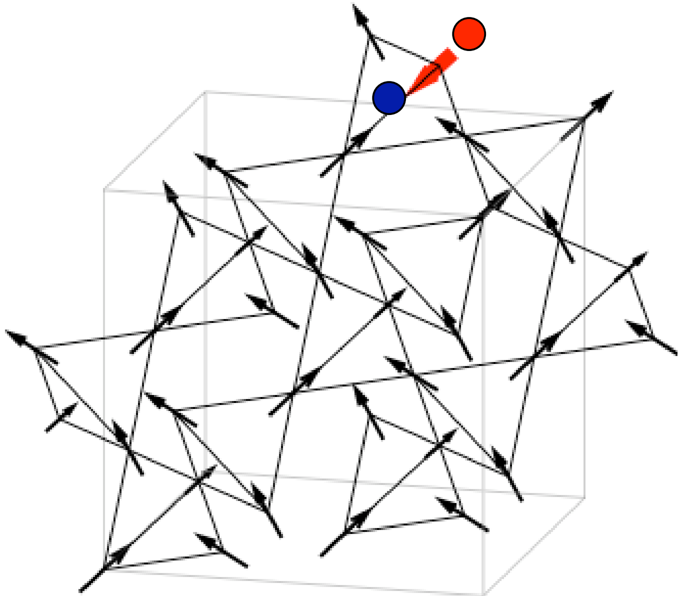
$\vec{h}$



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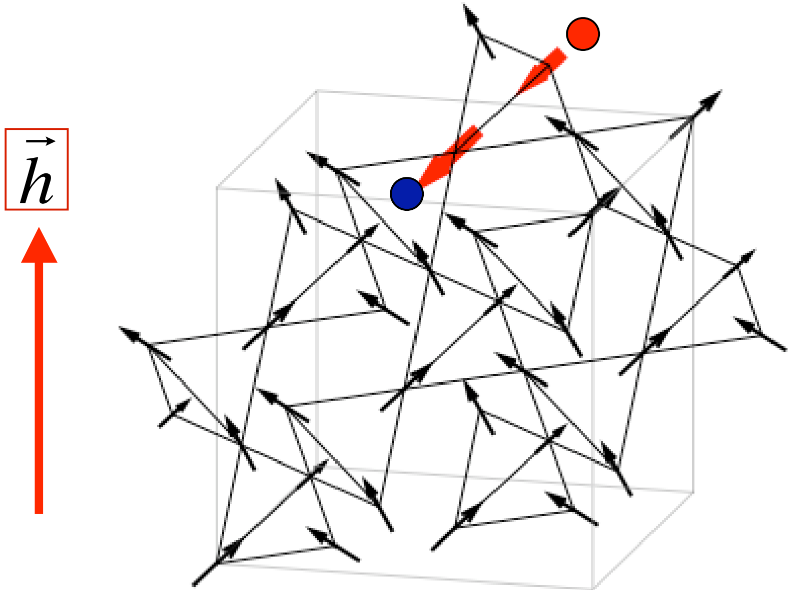

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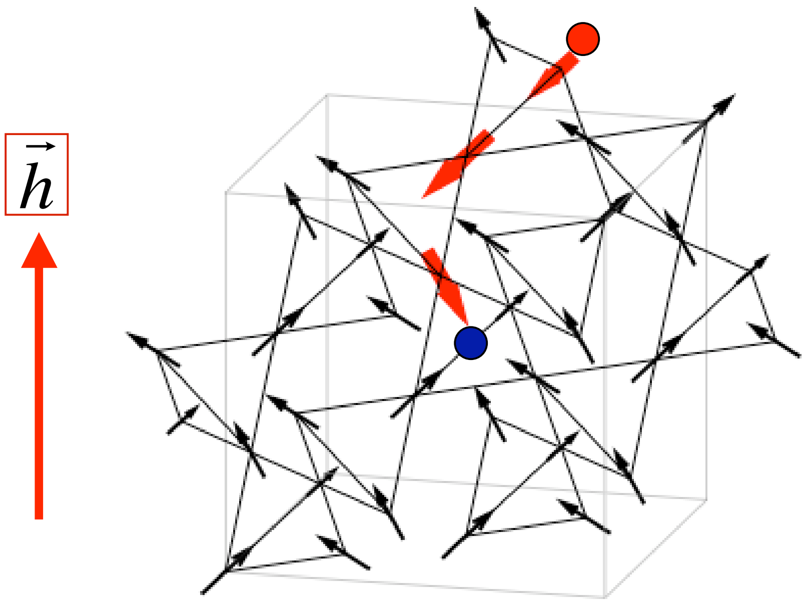

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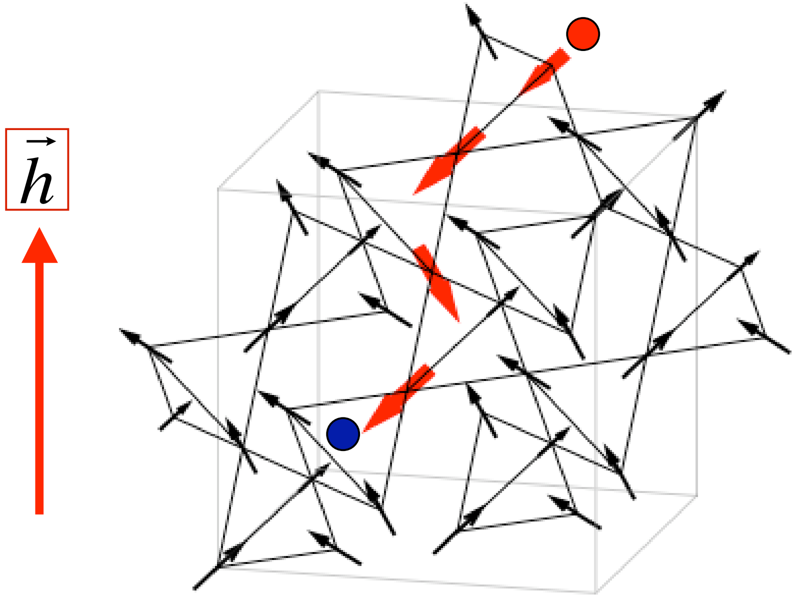

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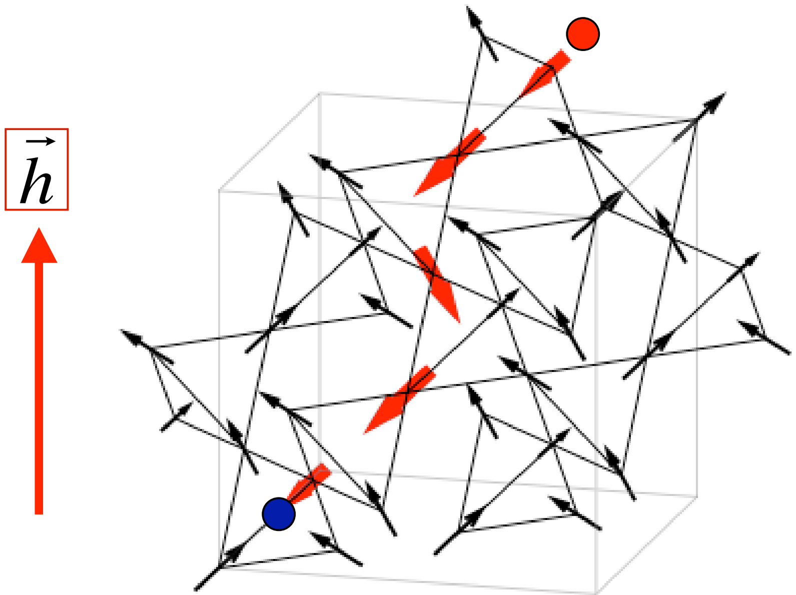

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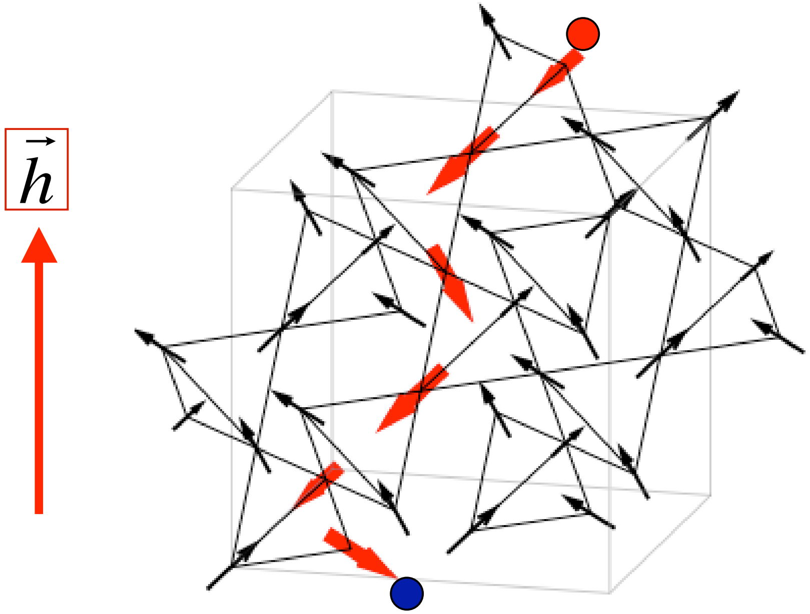

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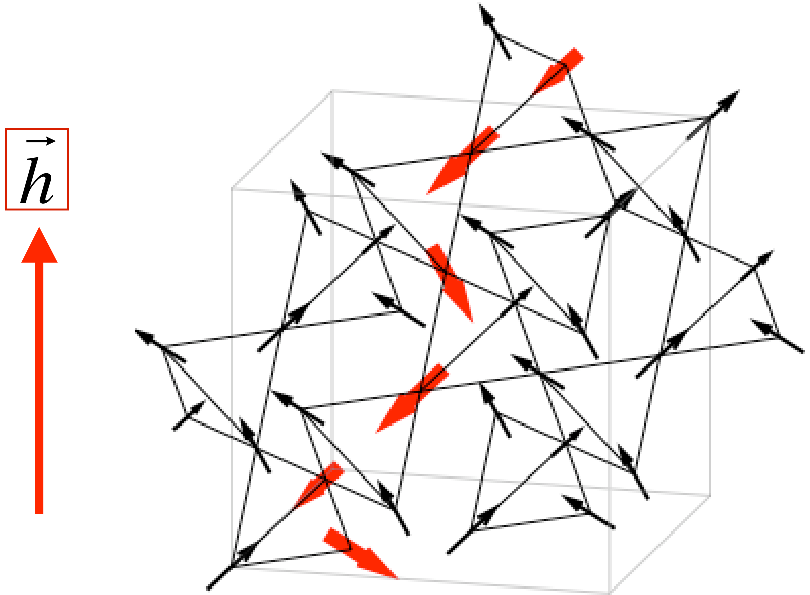

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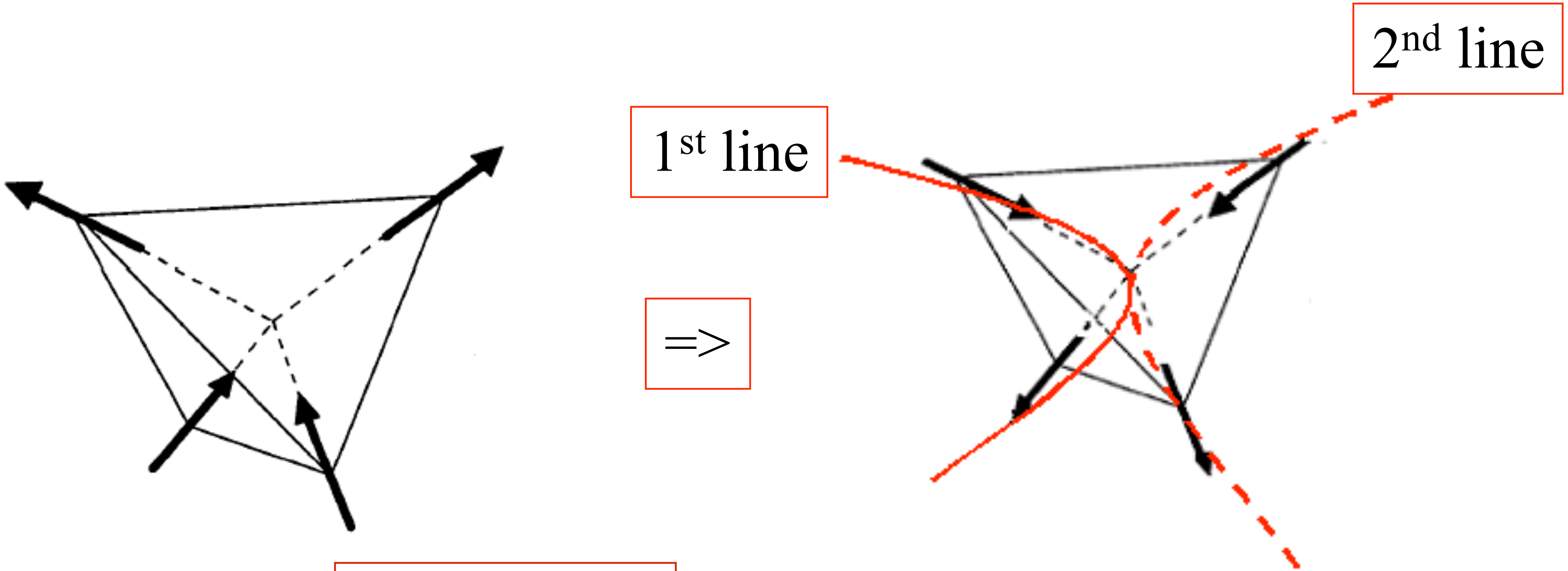
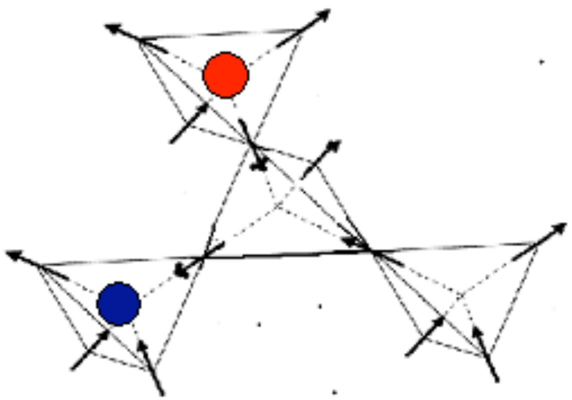


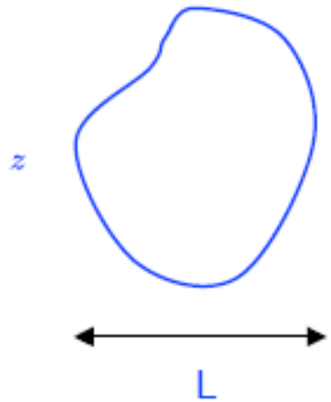
Cost $\boxed{2\delta\varepsilon_{Zeeman} = \frac{4h}{\sqrt{3}}}$ No entropy

2 lines indistinguishable inside a tetrahedron
-repulsion-continuous Kasteleyn transition.
Test by simulation…..

Non-local loop Monte Carlo algorithm: create a paire of topological defects and follow them in a virtual move. A closed loop keeps system on constrained subspace

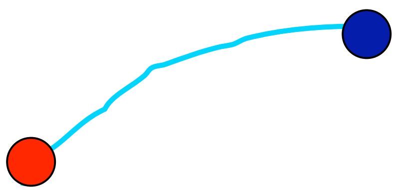


=>



$$W = \exp(-\beta \Delta \varepsilon_{Zeeman})$$

Can also terminate on a defect:

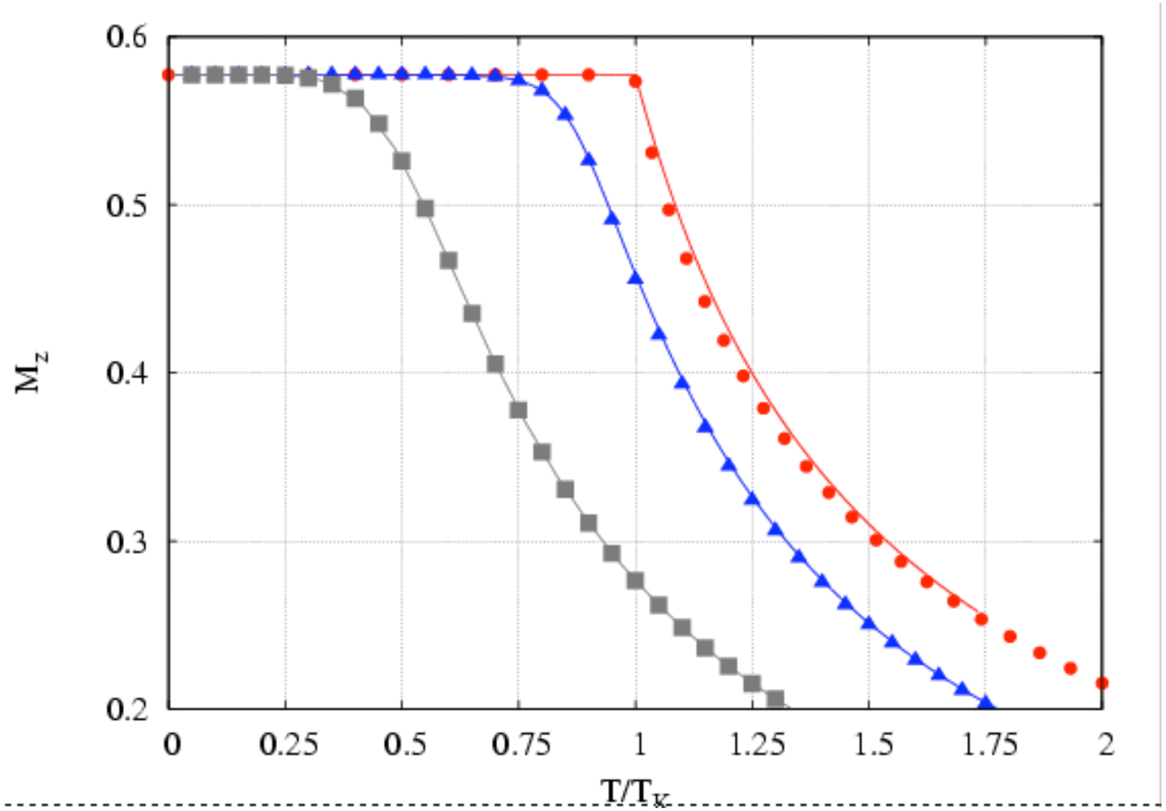


$$W = \exp(-\beta \Delta \varepsilon_{Zeeman} - \beta \Delta \varepsilon_{J})$$

Melko et. al. PRL 87, 067203 (2001)
Isakov et. al. PRB 70, 104418 (2004)

h/J => 0 sharp but continuous (Kasteleyn) transition

Jaubert, Chalker, Holdsworth and Moessner, Phys. Rev. Lett., 100, 067207, 2008



● $\frac{h}{J}=0.01$

▲ $\frac{h}{J}=0.2$

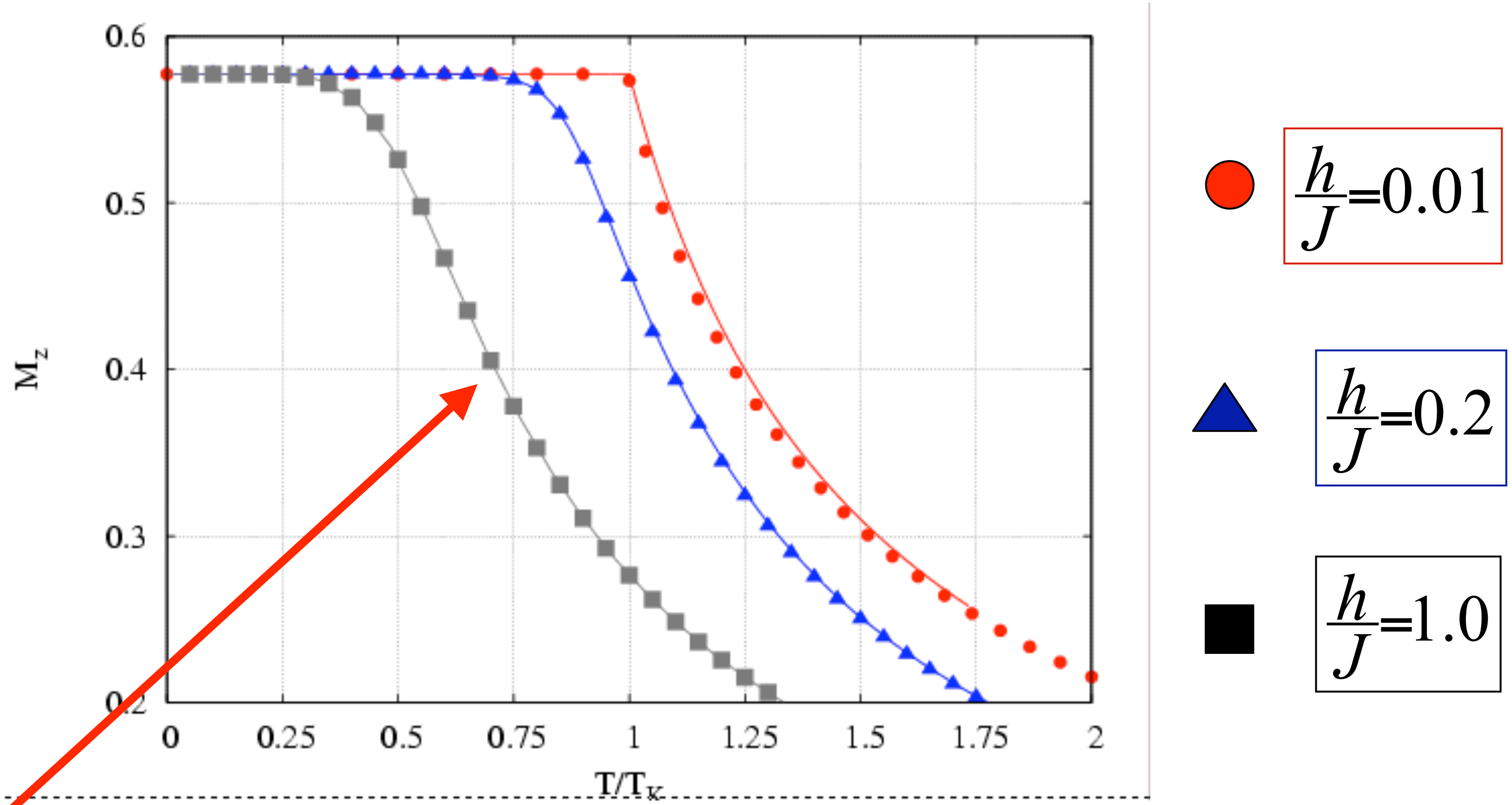
■ $\frac{h}{J}=1.0$

$N=10^6$

$N_{MCS}=10^5$

h/J => 0 sharp but continuous (Kasteleyn) transition

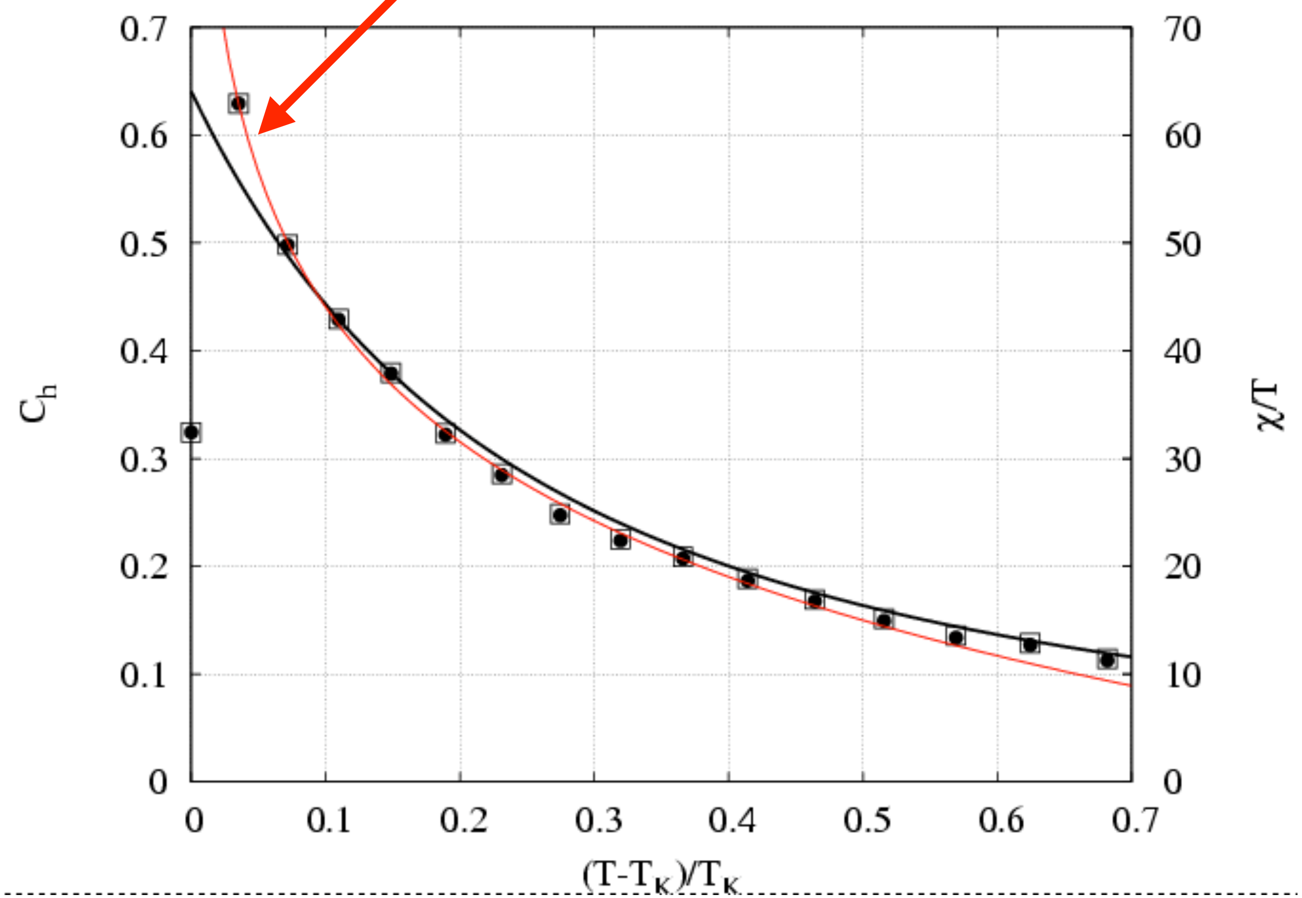
Jaubert, Chalker, Holdsworth and Moessner, Phys. Rev. Lett., 100, 067207, 2008



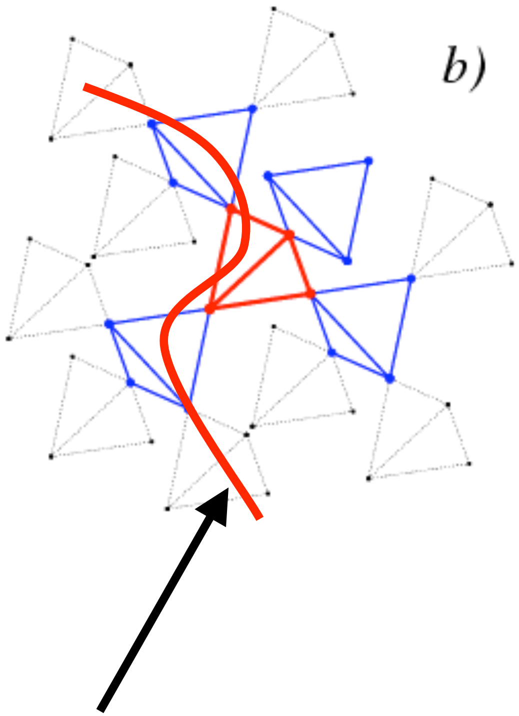
Transition rounded as topological defects appear

Specific heat and susceptibility diverge as $-\log(T-T_K) \Rightarrow d_c=3$

Bhattacharjee et al, JSP, 32, 361, 1983



Analytic calculation on related system;



n-level Cayley tree-fix spins on outside-either free or mean field $[S_i^n]$

$$\boxed{Z_n([S_i])}$$

Through recursion relation

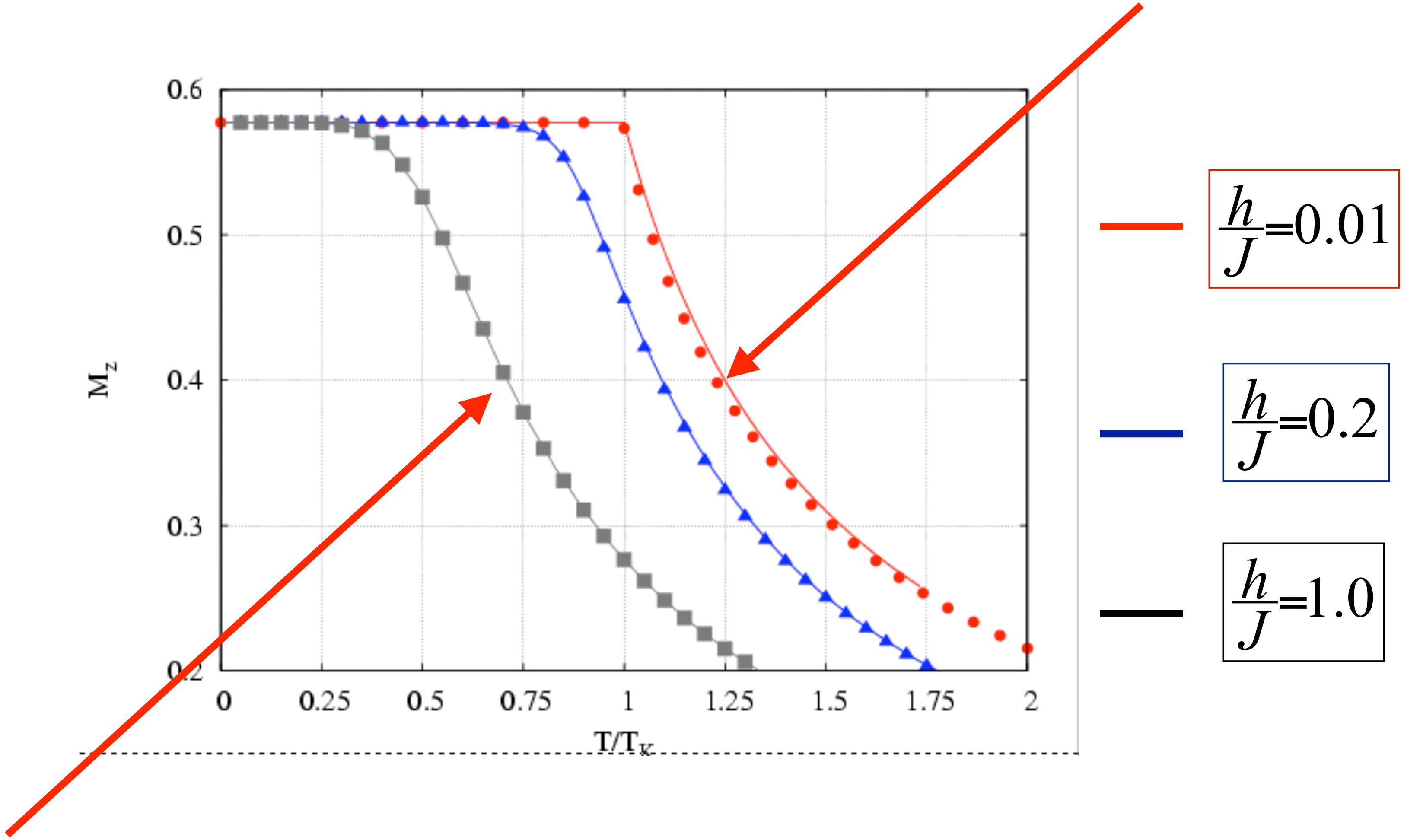
$$\boxed{Z(N,T) = \lim_{n\to\infty} Z_n([S_i])}$$

Kasteleyn transition due to similar line loops

$$\boxed{T_K = \frac{2h}{\log(2)\sqrt{3}}}$$

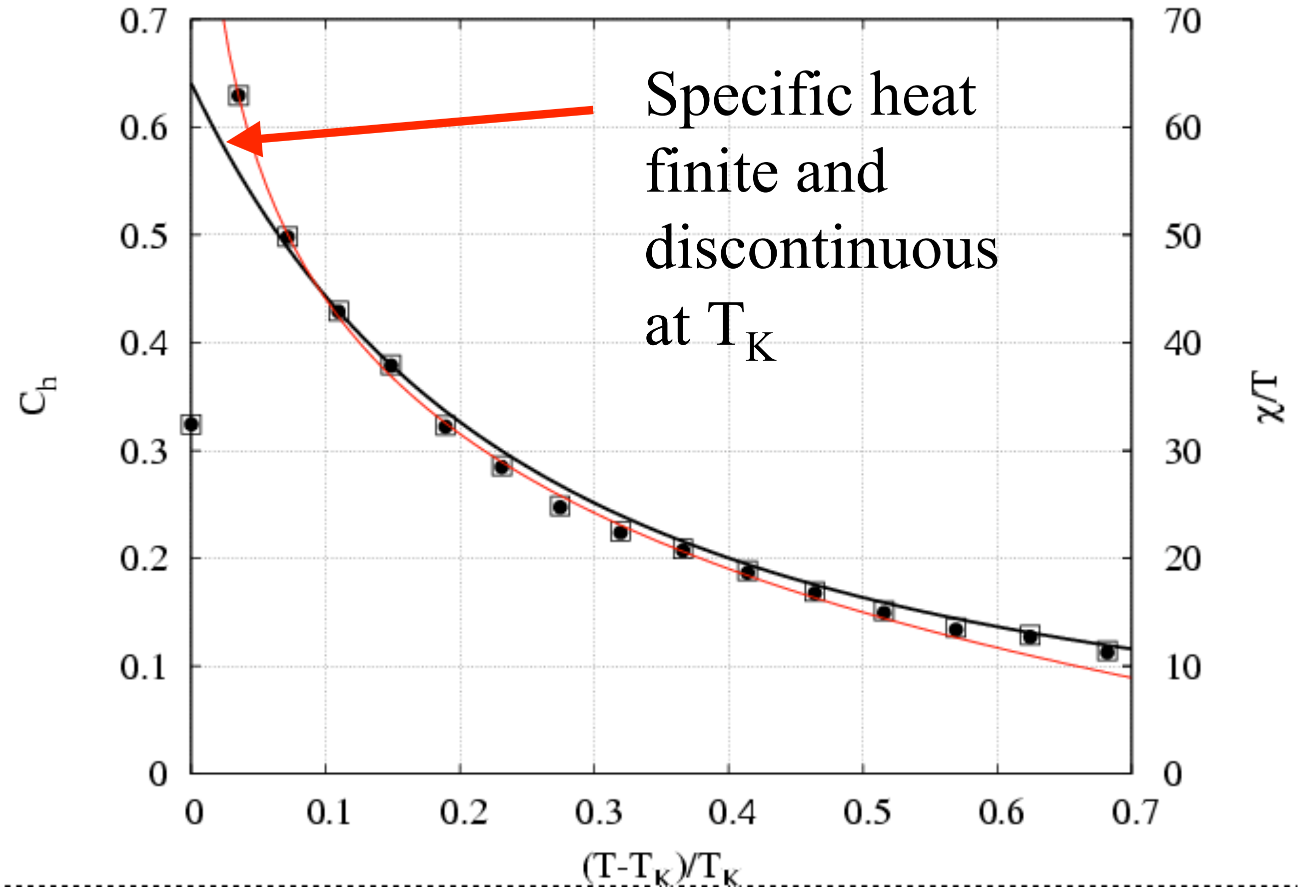
Kasteleyn transition on Cayley tree

small difference
for small h



Perfect agreement for rounded transition

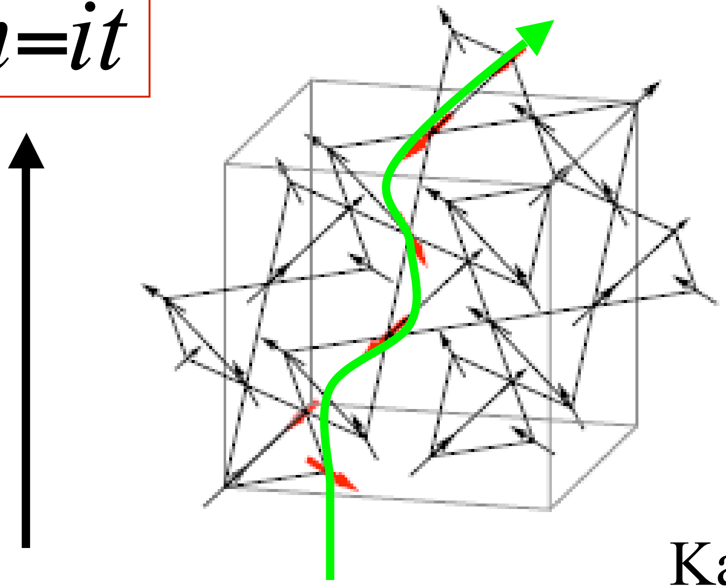
Kasteleyn transition on Cayley tree is mean field



Constraints and Boson world lines: $\vec{\nabla}.\vec{S}=0$

means that the magnetization on each plane is conserved

$h=it$



$\Rightarrow$2D quantum problem with time along z axis

Loop=world line for 2D Boson with weak repulsive interaction

Kasteleyn transition

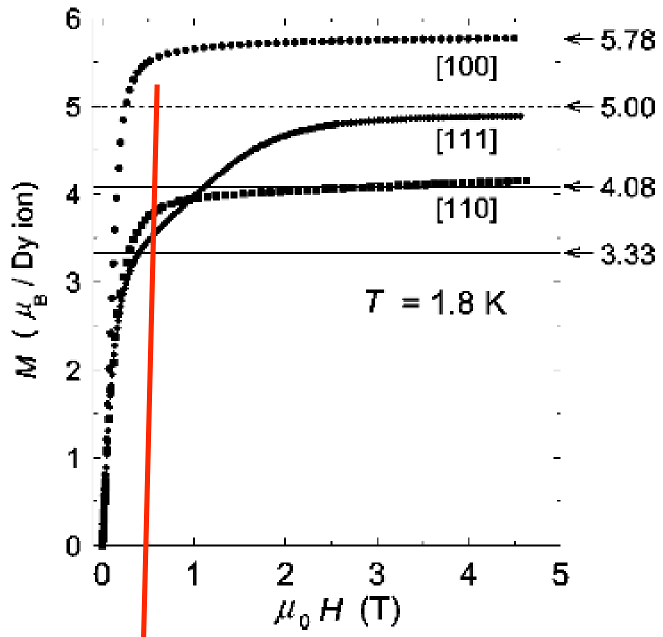
$\boxed{\equiv}$

Quantum (T=0) phase transition between vacuum state and Bose condensate (Fisher and Hohenberg, Phys. Rev. B, 37, 4936, (1988))

Jaubert et al, PRL., 100, 067207, 2008, Powell and Chalker, cond-mat/0803.4204 (2008)

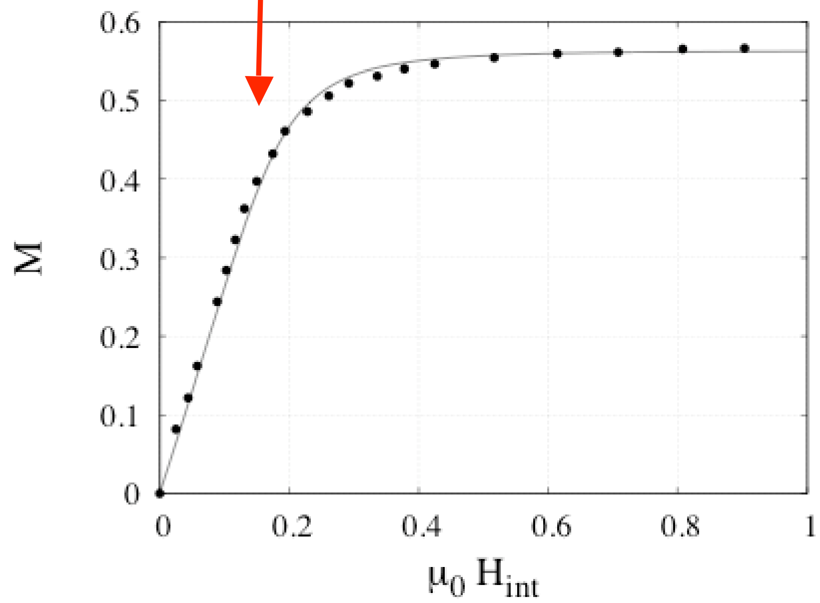
Dysprosium Titanate:

Fukazawa et al, Phys. Rev. B. 65, 054410, 2002



Data compared at T=1.8K
~ 1.6 times scale $J_{eff}S^2$

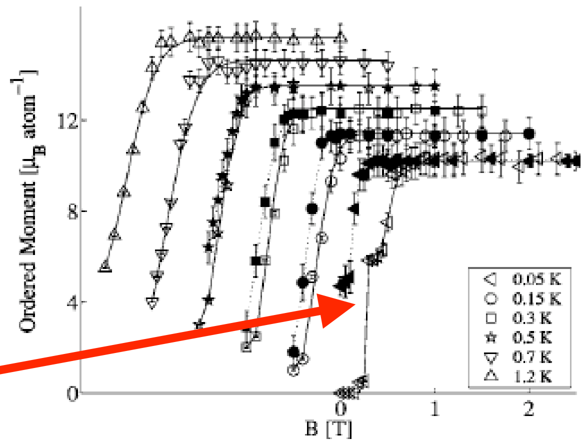
Our T=0.87 T_{exp}



Holmium Titanate:

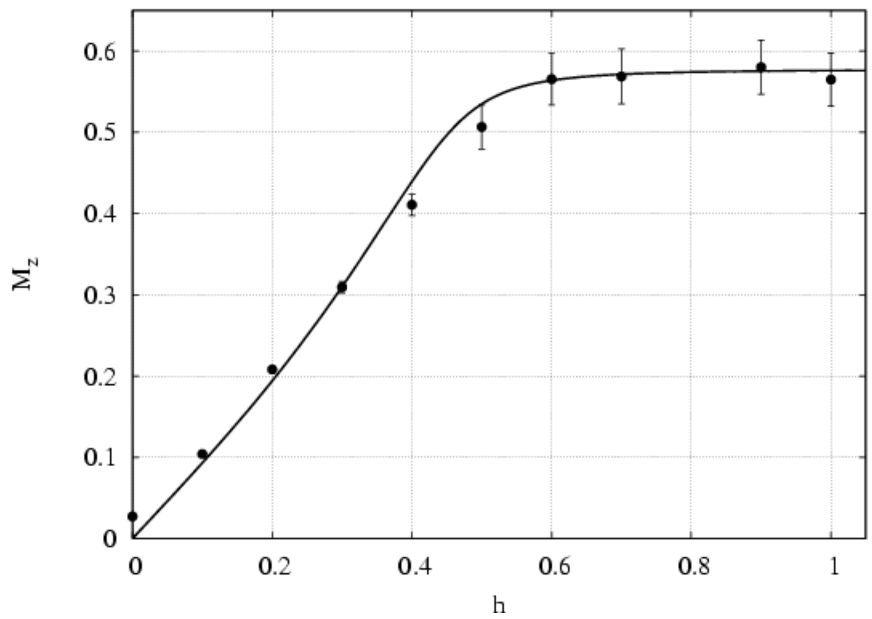
Fennell et al, PRB 72, 224411, 2005

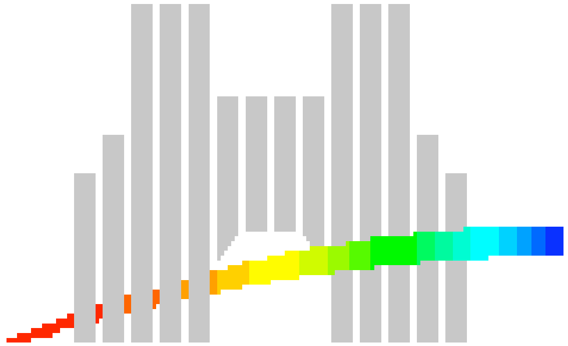
Out of equilibrium at low T



Data compared at T=1.2K ~ 2/3 of scale $J_{eff}S^2$

Our data at T/J~2/3.





Conclusions

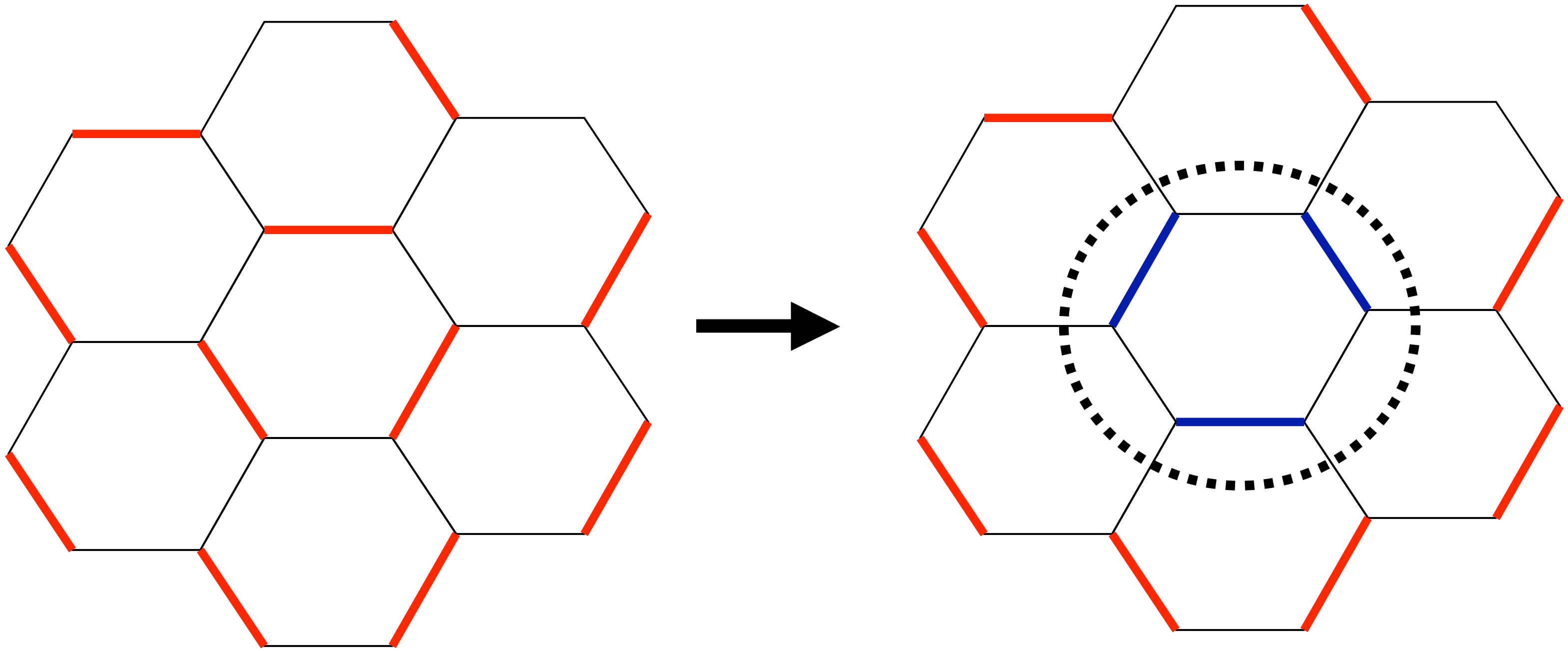
1. Topological constraints lead to rich and topical physics
2. Spin ice offers an experimental, numerical and analytical garden to study them.

Minneapolis
May 2008

I didn't talk about :
Kasteleyn's original model and mapping to [111] spin ice
Kasteleyn transition in Lipid bi-layers
Landau theory of Kasteleyn transition
Transitions in bond-distorted spin ice

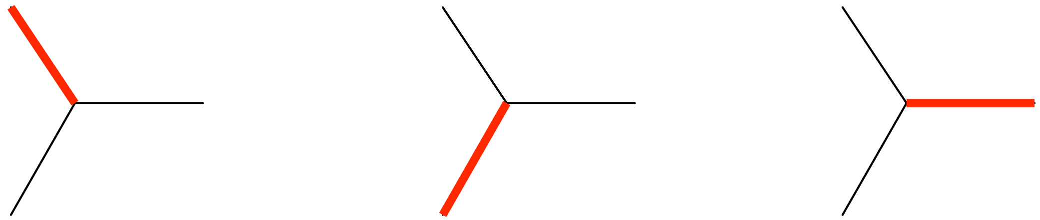
Dimers on a Honeycomb lattice

P.W. Kasteleyn, J.Math. Phys. 4, 287, 1963



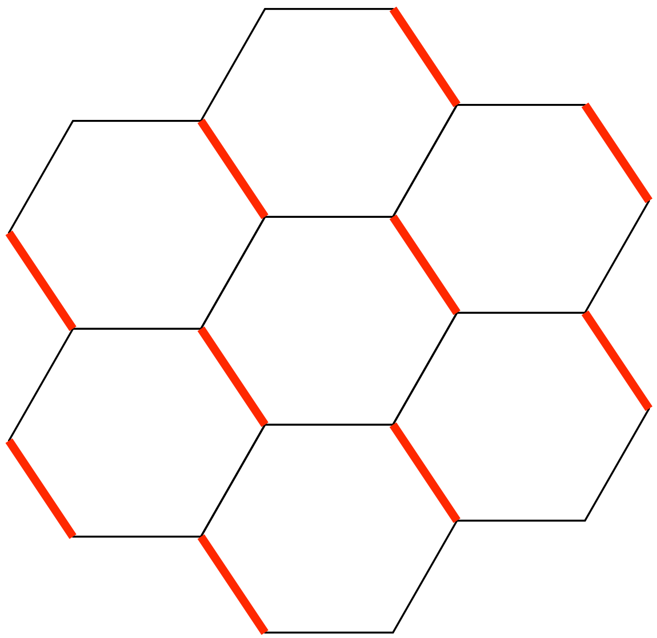
Localized excitation

$\Rightarrow \Omega \sim a^N, \quad S = Nk_B \log(a).$



μ_1 μ_2 μ_3

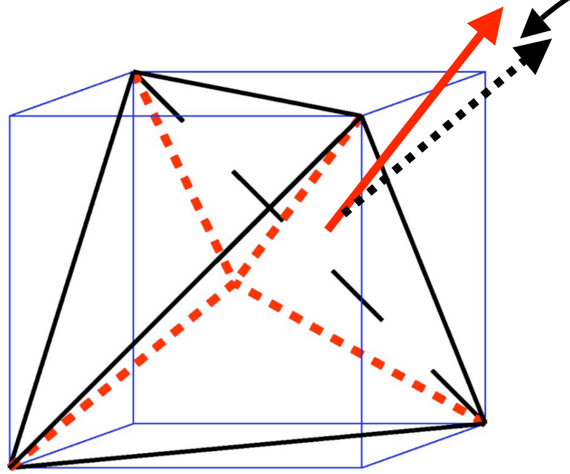
For critical value of μ_i

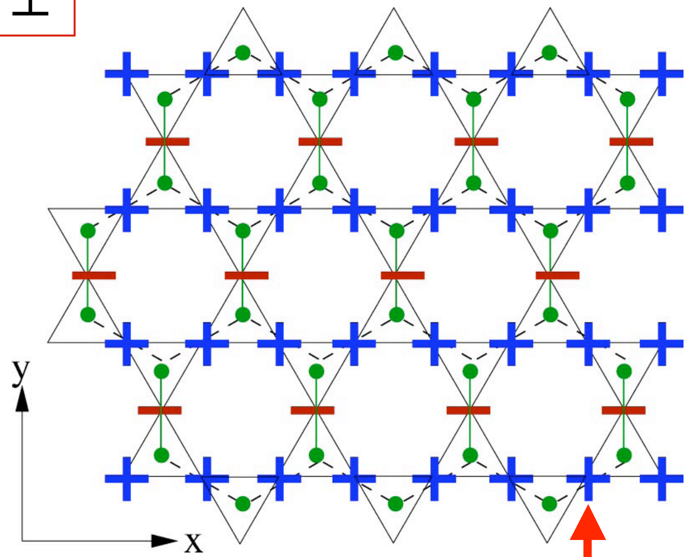


Long range order

Kasteleyn transition with field near the [111] direction:

$\vec{h}_\perp$

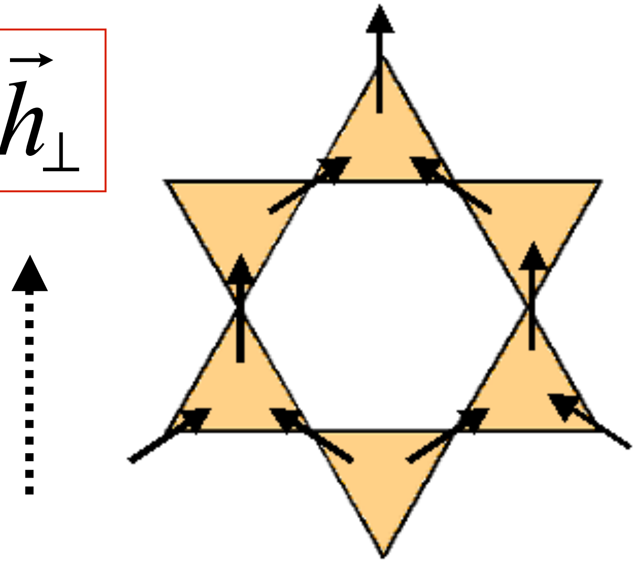




$\vec{h}_\perp = 0$ $\quad$ $S_0 \approx 0.08R$ $\quad$ $|\vec{h}_\perp| \geq h_K$ $\quad$ $S(h_K) = 0$

Moessner and Sondhi PRB 68, 064411, 2003

$\vec{h}_\perp$



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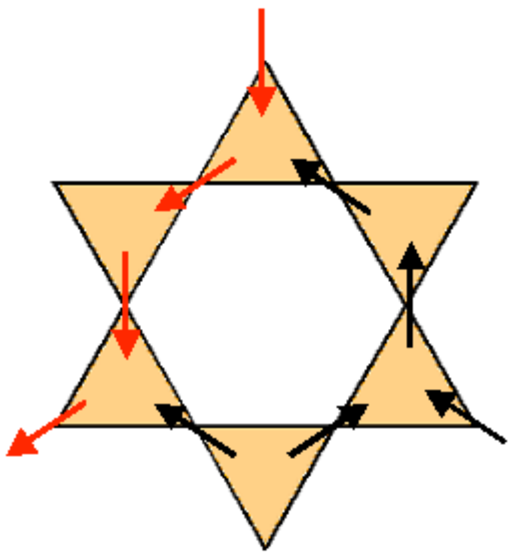


$\delta\varepsilon_{Zeeman}=3h_\perp S_\perp$

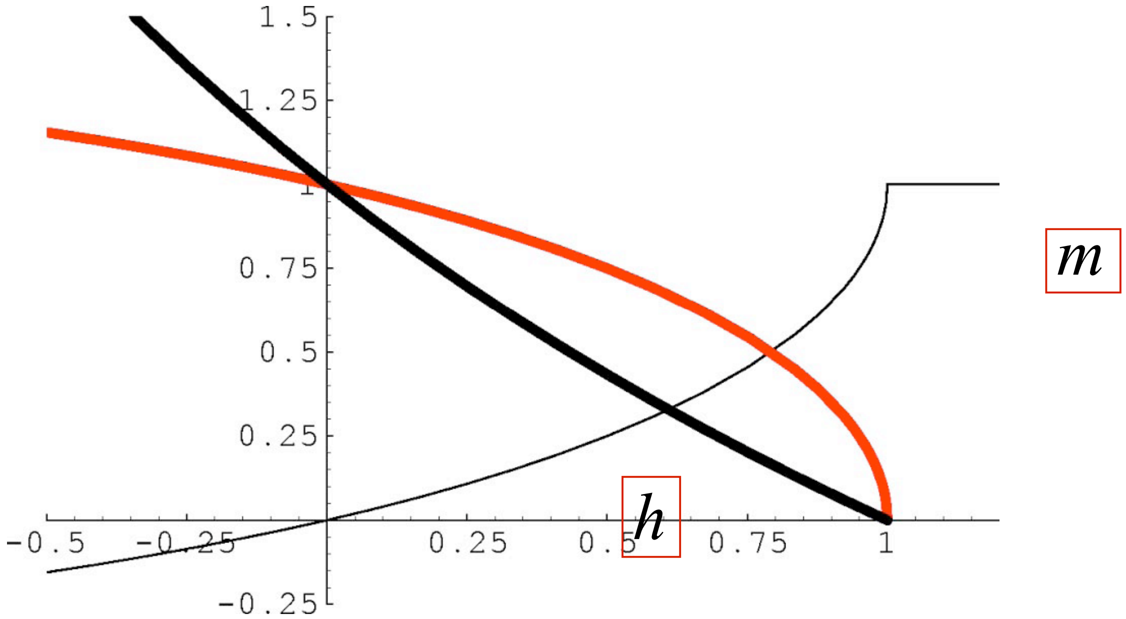
$\delta S = \log(2)$

$T_K=\frac{3h_\perp S_\perp}{\log(2)}$

$S_\perp=\frac{2\sqrt{2}}{3}$

=>

$T_K=\frac{2\sqrt{2}h_\perp}{\log(2)}$

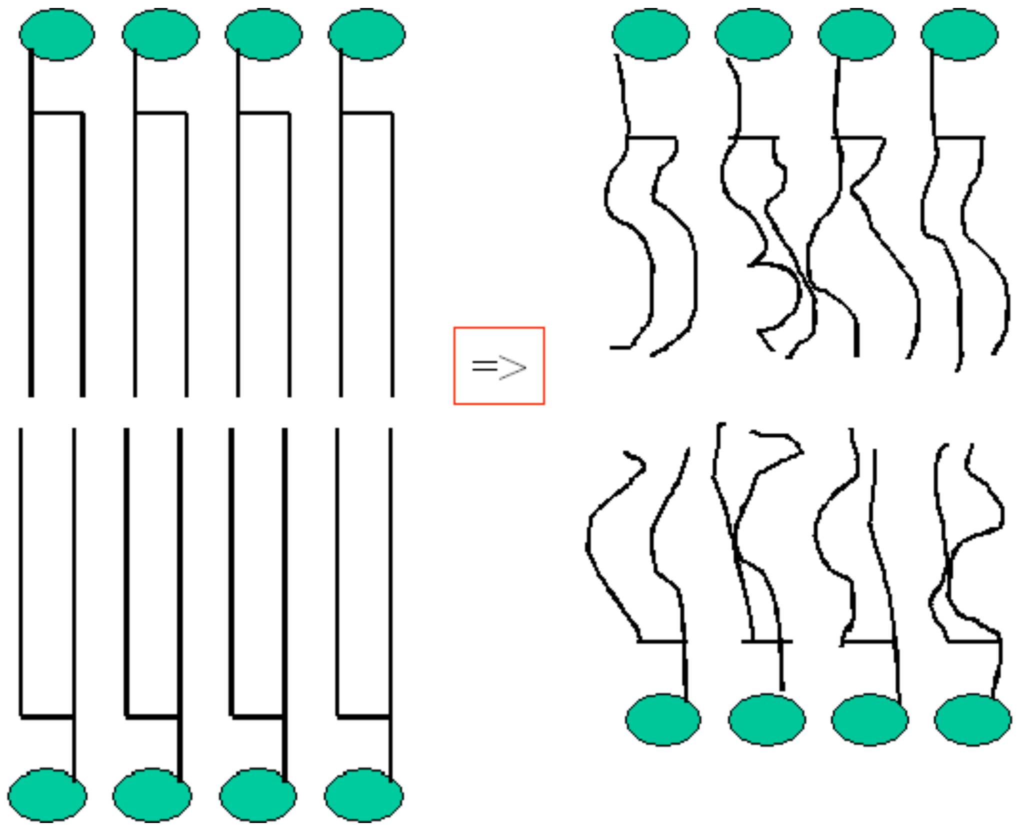


$$C_h \sim (h_K - h)^{-1/2} \sim \frac{\chi}{T}$$

Moessner and Sondhi PRB 68, 064411, 2003

K-transition in soft condensed matter:
Trans-gauche polymer transition in Lipid bylayer:

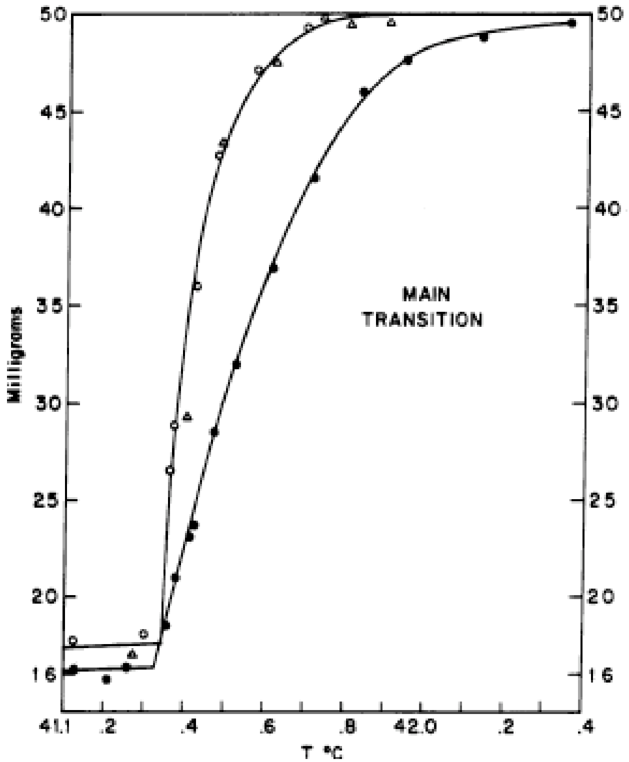
Nagle Proc. Nat. Acad. Sci. USA, 70, 3443, 1973.



Trans-gauche polymer transition in Lipid bylayer:

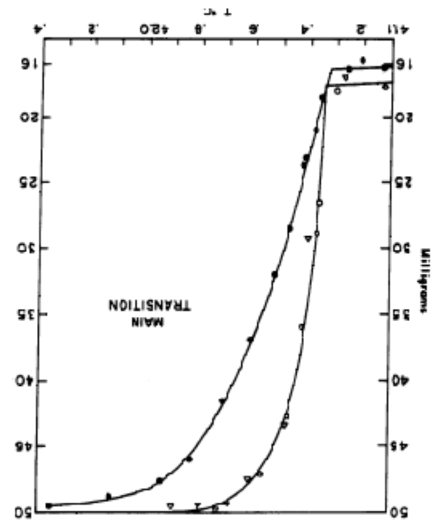
Nagle Proc. Nat. Acad. Sci. USA, 70, 3443, 1973.

Density

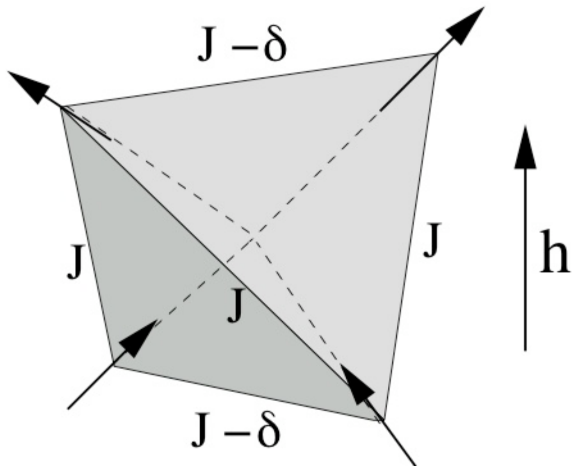


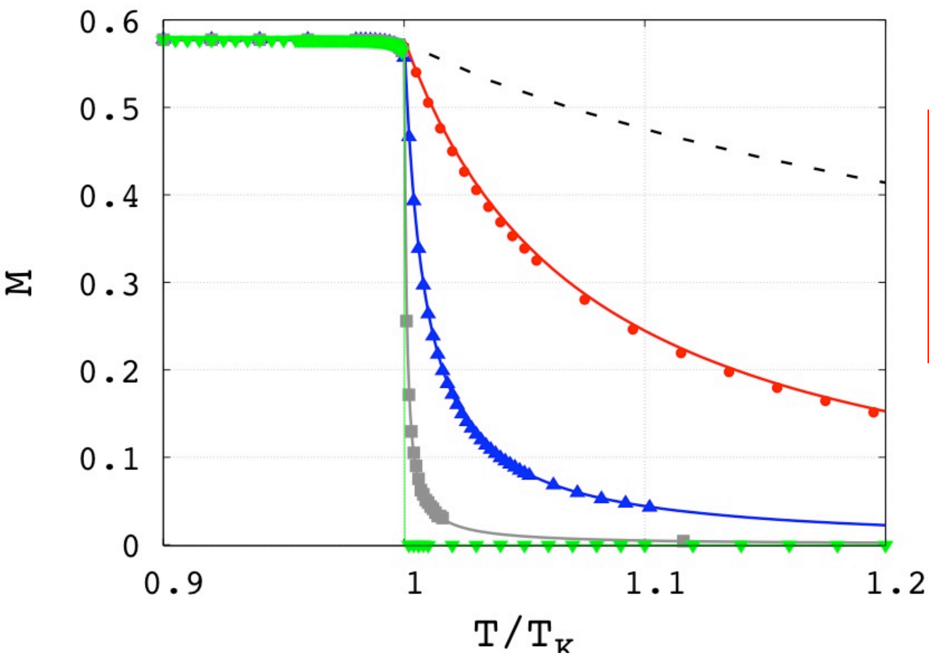
Temperature

Reversed image



Bond distorted spin ice





In zero field the transition breaks Z_2 symmetry but is not Ising like

Transition is multicritical with a perfectly flat free energy