Title: Spin fractionalization on a Pyrochlore Lattice

Date: May 28, 2013 03:30 PM

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Abstract: The decomposition of the magnetic moments in spin ice into freely moving magnetic monopoles has added a new dimension to the concept of fractionalization, showing that geometrical frustration, even in the absence of quantum fluctuations, can lead to the apparent reduction of fundamental objects into quasi particles of reduced dimension [1]. The resulting quasi-particles map onto a Coulomb gas in the grand canonical ensemble [2]. By varying the chemical potential one can drive the ground state from a vacuum to a monopole crystal with the Zinc blend structure [3].

The condensation of monopoles into the crystallized state leads to a new level of fractionalization:
the magnetic moments appear to collectively break into two distinct parts; the crystal of magnetic charge and a magnetic fluid showing correlations characteristic of an emergent Coulomb phase [4].

The ordered magnetic charge is synonymous with magnetic order, while the Coulomb phase space is equivalent to that of hard core dimers close packed onto a diamond lattice [5]. The relevance of these results to experimental systems will be discussed.

[1] C. Castelnovo, R. Moessner, and S. L. Sondhi, Nature 451, 42 (2008).
[2] L. D. C. Jaubert and P. C. W. Holdsworth, Nature Physics 5, 258 (2009).
[3] M. Brooks-Bartlett, A. Harman-Clarke, S. Banks, L. D. C. Jaubert and P. C. W. Holdsworth, In Preparation, (2013).
[4] C. L. Henley, Annual Review of Condensed Matter Physics 1, 179 (2010).
[5] D. A. Huse, W. Krauth, R. Moessner, and S. L. Sondhi, Phys. Rev. Lett. 91, 167004 (2003).

P.C.W. Holdsworth
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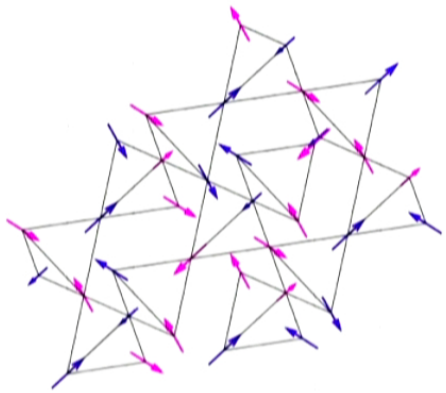
Magnetic moment fractionalization on the Pyrochlore lattice

1. Spin ice – a grand canonical Coulomb gas ?
2. Magnetization and lattice gauge fields.
3. Monopole crystalization
4. Confrontation with experiment ?

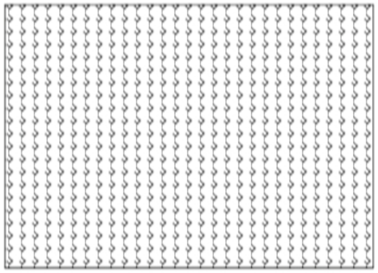
Ice rules in spin ice

Spin ice materials $Ho_2Ti_2O_7$, $Dy_2Ti_20_7$



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

Magnetic ice rules
two-in two-out



Pyrochlore lattice= corner sharing tetrehedra whose centres form a diamond lattice

Ice rules in spin ice

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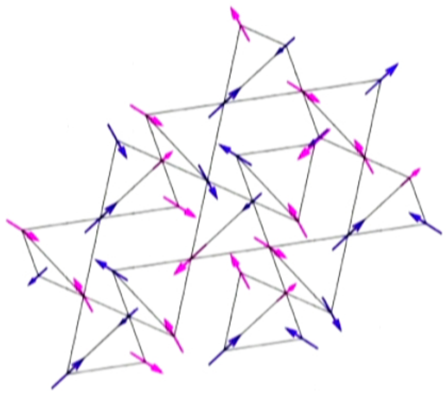

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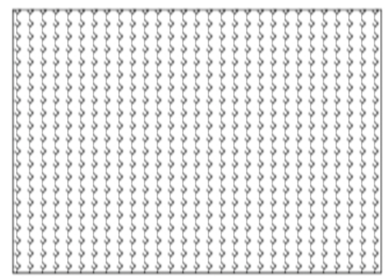

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Ice rules in spin ice

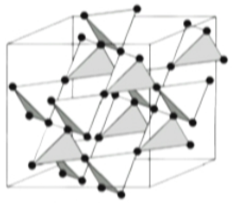
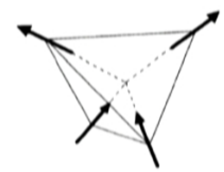


FIG. 1. The pyrochlore lattice

A good Hamiltonian for spin ice materials:
The dipolar spin ice model (DSI)

$$H = Jm^2 \sum_{ij} \vec{S}_i.\vec{S}_j + Dm^2 \sum_{ij} \left[\frac{\vec{S}_i.\vec{S}_j}{|\vec{r}_{ij}|^3} - \frac{3(\vec{S}_i.\vec{r}_{ij})(\vec{S}_j.\vec{r}_{ij})}{|\vec{r}_{ij}|^5} \right] - \Gamma m^2 \sum_i (\vec{S}_i.\vec{d}_i)^2$$

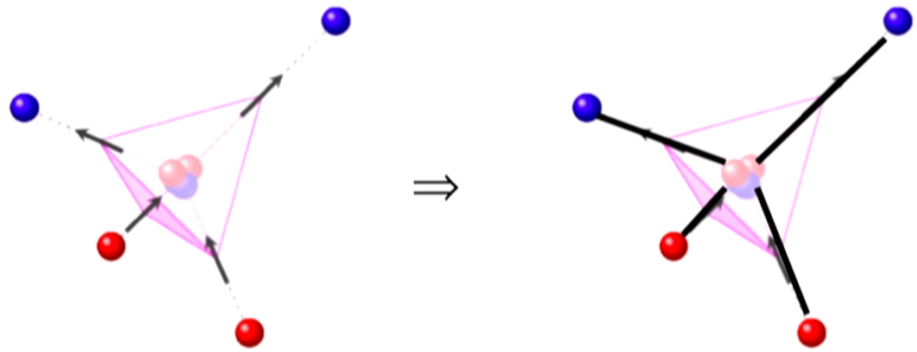
$|J| m^2$ and Dm^2 are O(1K), Γm^2 is O(100K)



0 - 10K => Ising like spins along <111> axes

In 2 in – 2 out states long range interactions are almost but not quite screened
den Hertog and Gingras, PRL.84, 3430 (2000), Isakov, Moessner and Sondhi, PRL 95, 217201, 2005

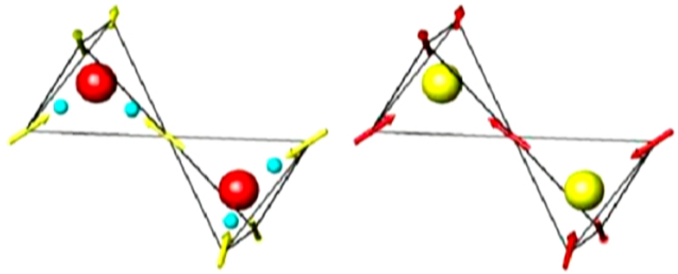
Extension of the point dipoles into magnetic needles/dumbbelles
Castelnovo, Moessner, Sondhi, Nature, 451, 42, 2008



Configurations of
magnetic charge
at tetrehedron centres

Dumbbell model ground state is macroscopically degenerate with the same phase space as Pauling's model of proton disorder in ice

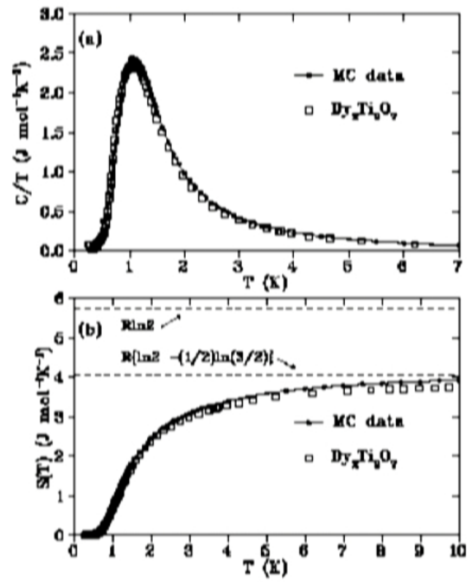
Magnetic ice rules =>
Pauling entropy.



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

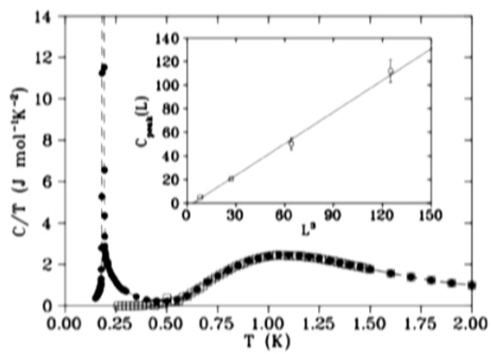
Magnetic
« Giauque and Stout »
experiment:

Ramirez et al, Nature 399,333, (1999)

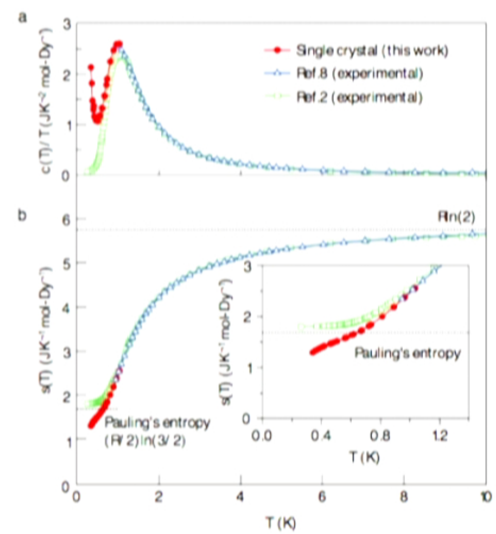


The dumbbell model is subject to corrections:

Long-Range Order at Low Temperatures in Dipolar Spin Ice
R. G. Melko, B. C. den Hertog, and M. J.P. Gingras
PRL, 87, 067203, 2001



Absence of Pauling's residual entropy in thermally equilibrated $Dy_2Ti_2O_7$
D. Pomaranski et al., Nat. Phys.
DOI: 10.1038/NPHYS2591, 2013

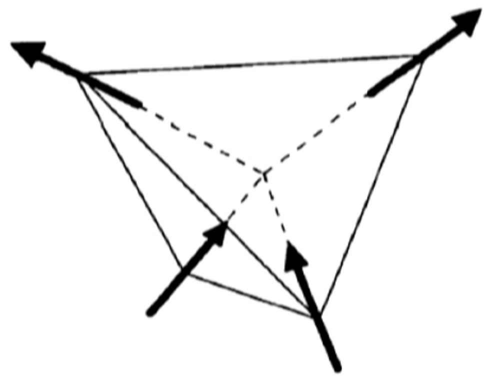


Ice rules, topological constraints

…… and divergence free condition:

The ice rules impose local constraints

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

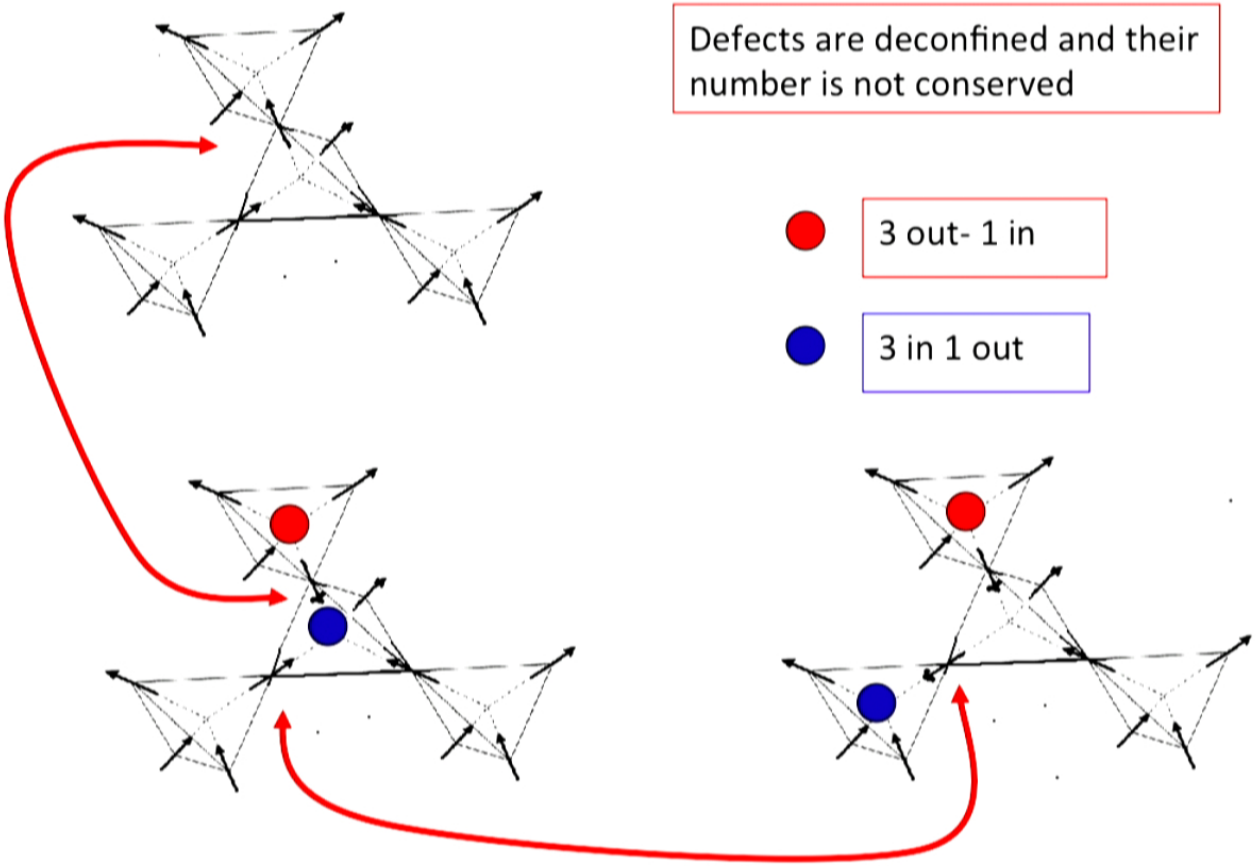


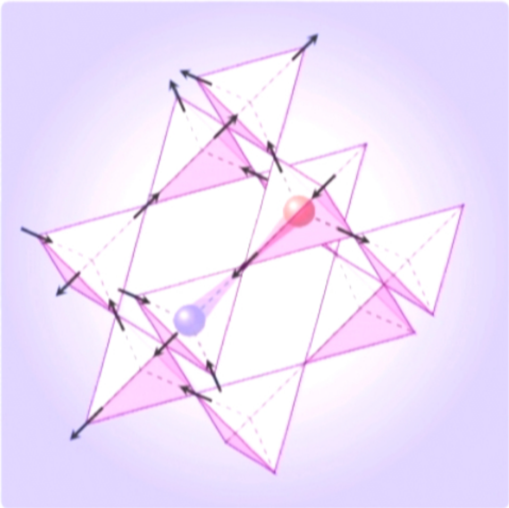
$$\vec{\nabla}.\vec{M} = 0$$

S. V. Isakov, K. Gregor, R. Moessner, and S. L. Sondhi PRL 93, 167204, 2004

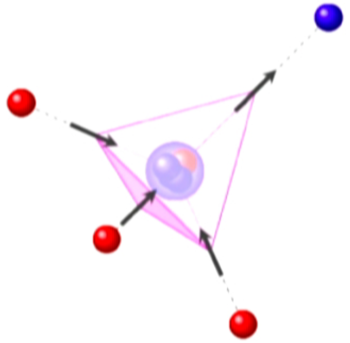
Excitations are topological defects that break the constraint.

Defects are deconfined and their number is not conserved



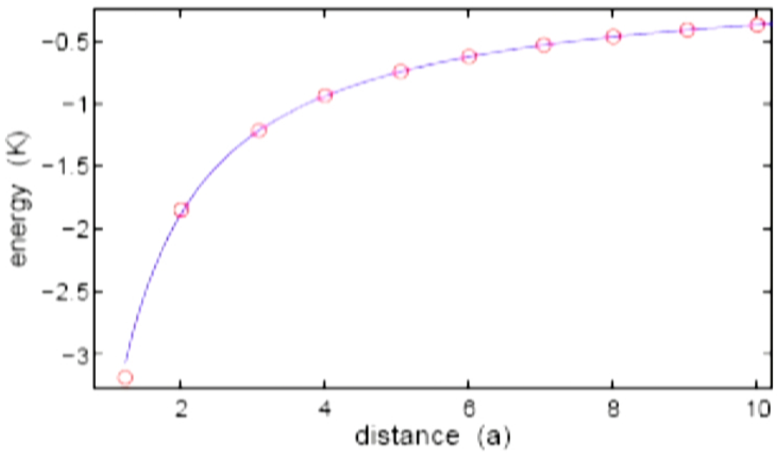


In dumbbell and DSI models topological defects also carry magnetic charge



$$V(a)=\frac{\mu_0}{4\pi}\ \frac{Q_i Q_j}{a};\ Q_i\ =\pm\frac{2\mu}{a_0}$$

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



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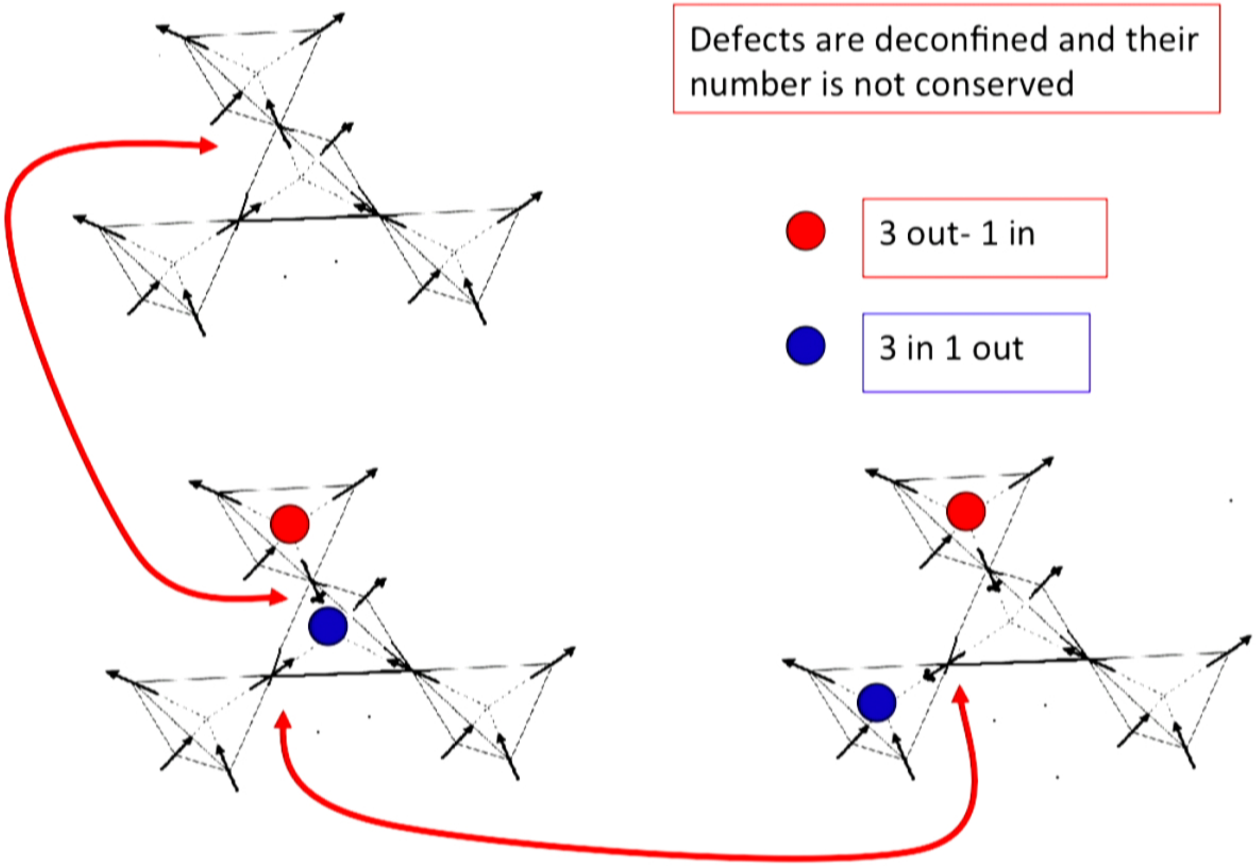

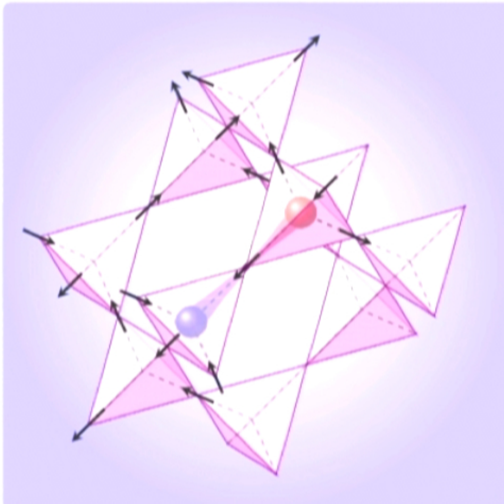

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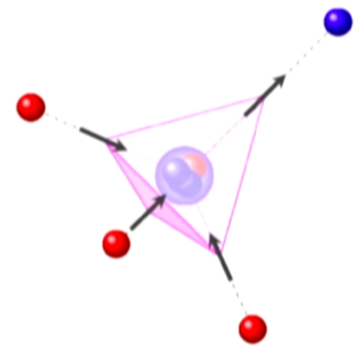
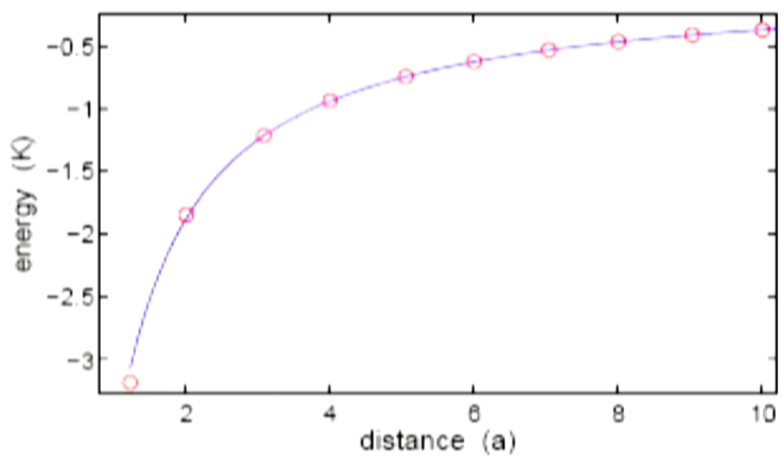


$$V(a) = \frac{\mu_0}{4\pi} \frac{Q_i Q_j}{a}; \; Q_i = \pm \frac{2\mu}{a_0}$$



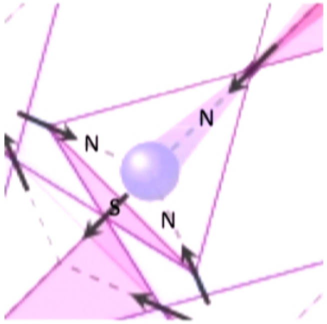
Castelnovo, Moessner, Sondhi, Nature, 451, 42, 2008

Magnetic monopole

=>

These particles do not require
a correction to Maxwell's equations

$$\vec{\nabla}.\vec{B} = 0 = \mu_0 \vec{\nabla}.(\vec{M} + \vec{H})$$



But they do have a Coulomb interaction

$$V(r) = \frac{\mu_0}{4\pi} \frac{Q_i Q_j}{r}; \; Q_i = \pm \frac{2\mu}{a_0}$$

Their number is not conserved

A grand canonical Coulomb gas of quasi particles.

Grand Canonical Ensemble

Independent variables are T and μ

Boltzmann weight

$$P(\tilde{U}_r) = \frac{\exp(-\beta \tilde{U}_r)}{\Psi}$$

$$\tilde{U}_r = U_r - \mu N_r$$

U_r=Coulomb energy of microstate 'r'

Valid for all microstates, including low density ones for which U_r=0

Energy required to place a pair of particles separated by infinity

$$\tilde{U}_2 = -2\mu$$

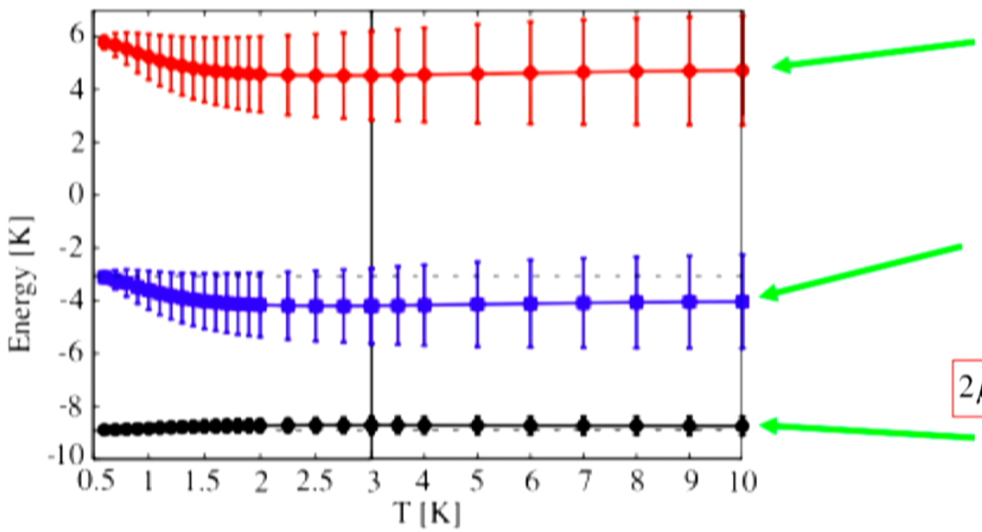
Example: Estimate for DTO from a DSI driving a "slave" Coulomb gas

Jaubert and Holdsworth, J. Phys. Cond Matt. 23, 164222, (2011)

$$\mu \approx -4.46K$$

Energy required to create a NN pair is

$$\delta U_{def} = \delta U_{Coul} - 2\mu$$



$$2\mu = \delta U_{Coul} - \delta U_{def} \approx -8.92K$$

Magnetic moments and charge: Lattice Gauge Field

Coulomb fluid satisfies magnetic Gauss' law:

$$\vec{\nabla}.\vec{M} \Rightarrow \oint \vec{M}.d\vec{S}_i = -Q_i$$

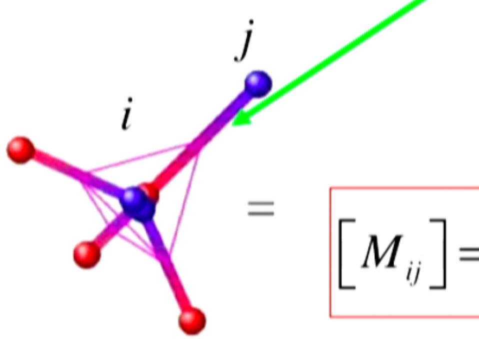
$$\left(\vec{\nabla}.\vec{H} = -\vec{\nabla}.\vec{M} = \rho\right)$$

Lattice gauge field

$$M_{ij} = \vec{M}.d\vec{S} = -M_{ji} = \pm\frac{m}{a}$$

$$\Rightarrow \sum_j M_{ij} = -Q_i$$

Three in one out defect



$$= \quad \left[M_{ij}\right] = \frac{m}{a}[-1,-1,-1,1]$$

$$Q_i = \frac{2m}{a}$$

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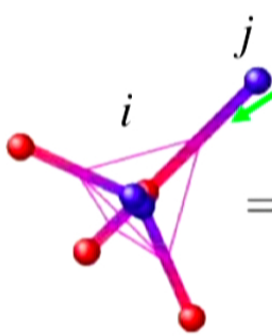
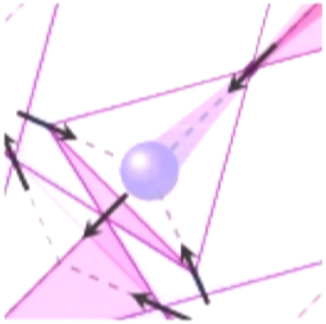
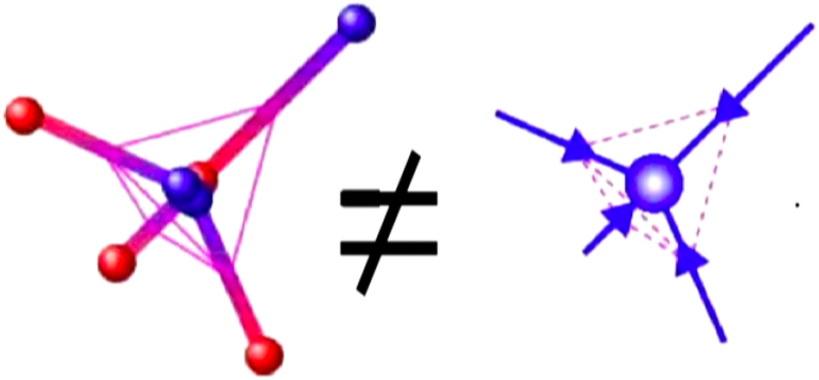


$$= \quad \left[M_{ij}\right] = \frac{m}{a}[-1,-1,-1,1]$$

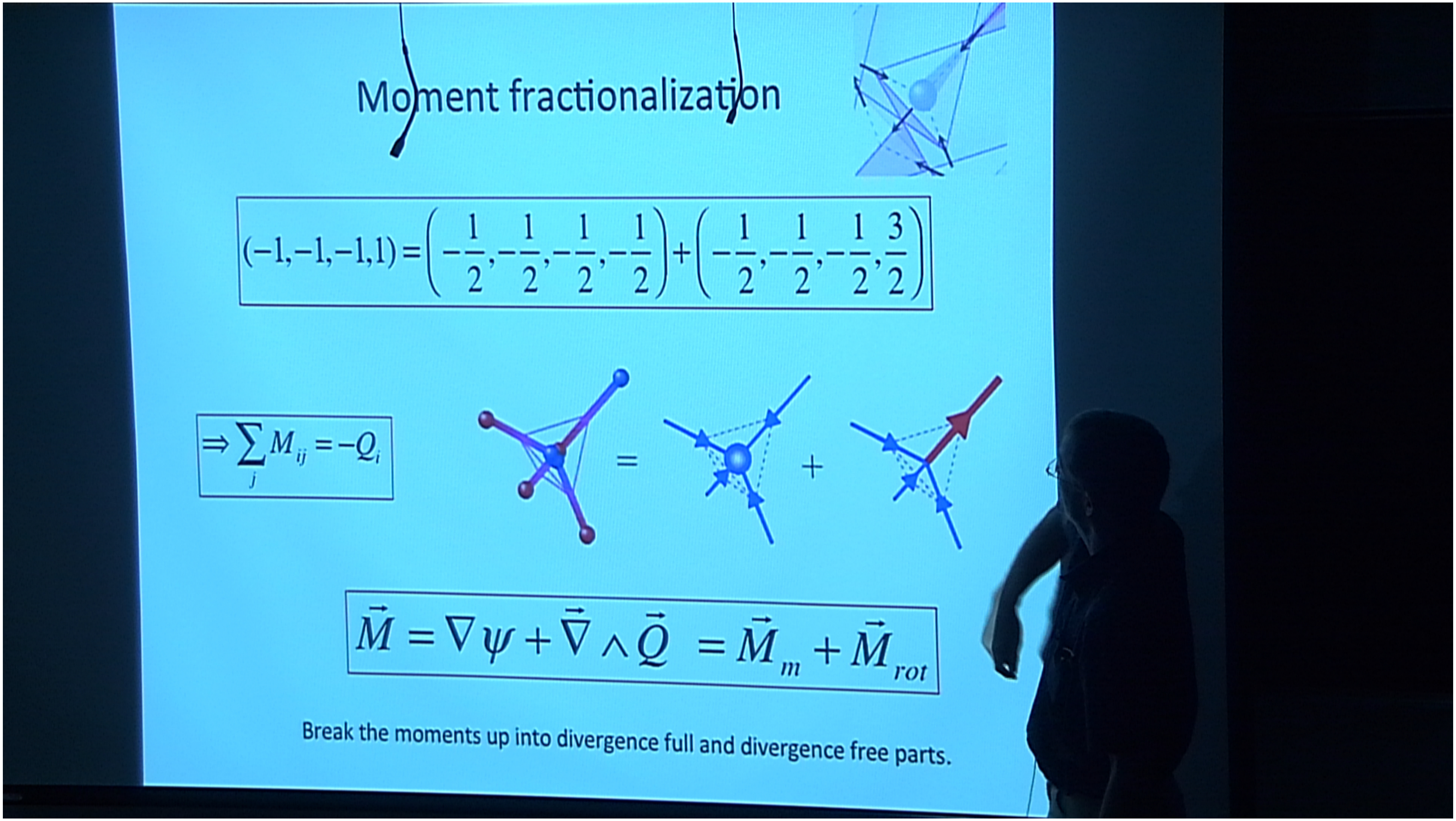
$$Q_i = \frac{2m}{a}$$

Field lines from an isolated magnetic charge Are not symmetrically distributed:





Need to break the field in two parts


Moment fractionalization
$(-1,-1,-1,1)=\left(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right)+\left(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},\frac{3}{2}\right)$
$\Rightarrow \sum_j M_{ij}=-Q_i$
=
+
$\vec{M}=\nabla\psi+\vec{\nabla}\wedge\vec{Q}\ =\vec{M}_m+\vec{M}_{rot}$
Break the moments up into divergence full and divergence free parts.

Electrostatics

Maggs and Rossetto, PRL, 88, 196402, 2002

S. T. Bramwell, Phil. Trans. R. Soc. A 370, 5738 (2012).

Gauss' law $\vec{\nabla}.\vec{E} = \frac{\rho}{\varepsilon_0}$ => Laplace $\vec{E} = -\vec{\nabla}\phi$

This is only one solution from an infinity of possible gauges:

$$\vec{E} = -\vec{\nabla}\phi + \vec{\nabla} \wedge \vec{Q} = \vec{E}_c + \vec{E}_{rot}$$

$$U = \frac{\varepsilon_0}{2}\int (\vec{E}_c^2 + E_{rot}^2)\, d\vec{r}$$

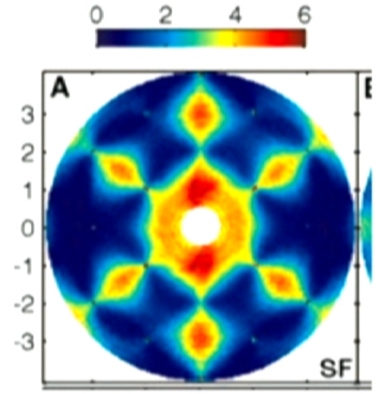
Electrostatics - minimum energy => $\vec{E}_{rot} = 0$

Electrodynamics - Coulomb gauge => $\vec{E}_{rot} = -\frac{\partial \vec{A}}{\partial t}$

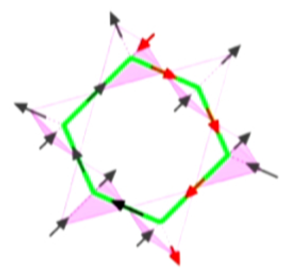
Monopole vacuum has divergence free gauge fields only
« Coulomb phase » Physics.

Pinch Points:

T. Fennell *et. al*., Magnetic Coulomb Phase in the Spin Ice $Ho_7O_2Ti_2$ *Science*, 326, 415, 2009.



Strong internal fields
Dunsinger et al Phys. Rev. Lett. 107, 207207, (2011)
Sala et al cond-mat/1112.3363



Single charges distort but do not kill the divergence free gauge field

The Coulomb fluid has a divergence full and divergence free field living in parallel up to high temperature

Pinch points live to high temperature (A. Sen, R. Moessner, and S. L. Sondhi, Phys. Rev. Lett. 110, 107202 (2013).)

Monopole Crystalization

For the parameters of DTO/HTO the ground state is a monopole vacuum.
This could change by changing the chemical potential:

Crystal of N :S charges in ZnS (Zinc Blend) structure of the diamond lattice if

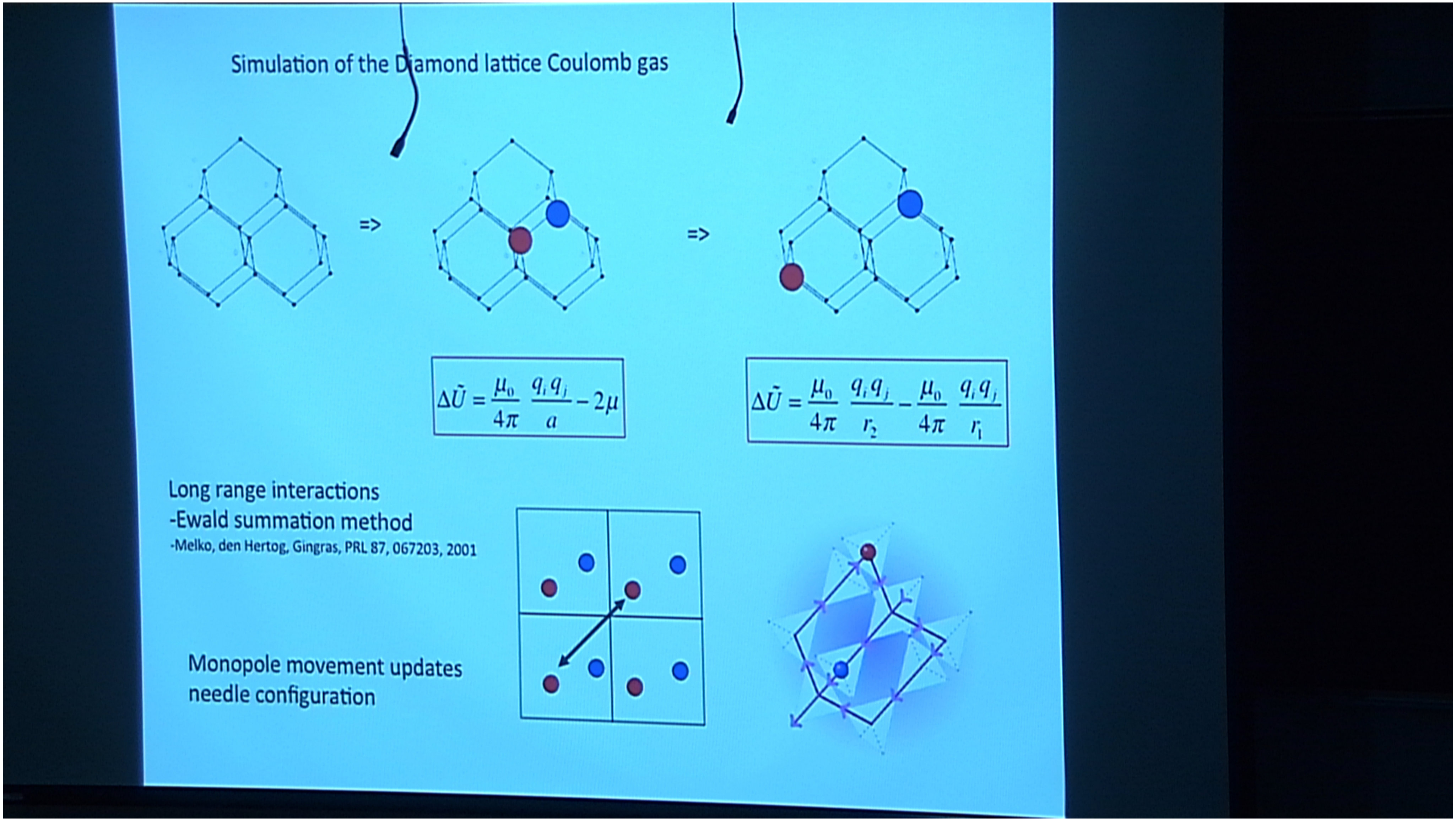
$$\tilde{U} = U_C - \mu N_0 < 0$$

$$U_C = N_0 \alpha \left(\frac{u(a)}{2} \right)$$

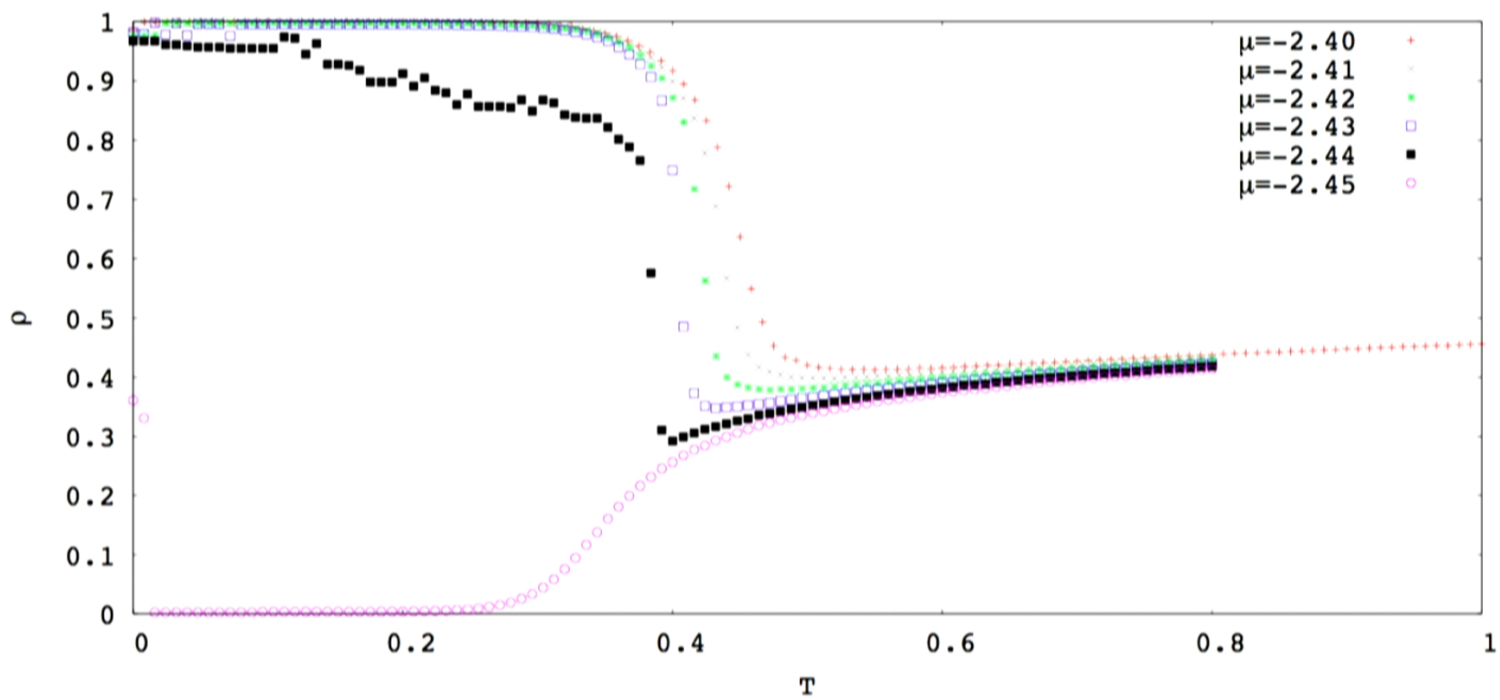
$$\alpha = 1.638$$ Madalung constant for diamond lattice

$$\mu > -2.49K$$ For parameters of DTO

Breaking of a Z_2 symmetry


Simulation of the Diamond lattice Coulomb gas
=>
=>
$\Delta\tilde{U} = \frac{\mu_0}{4\pi}\frac{q_i q_j}{a} - 2\mu$
$\Delta\tilde{U} = \frac{\mu_0}{4\pi}\frac{q_i q_j}{r_2} - \frac{\mu_0}{4\pi}\frac{q_i q_j}{r_1}$
Long range interactions
-Ewald summation method
-Melko, den Hertog, Gingras, PRL 87, 067203, 2001
Monopole movement updates
needle configuration

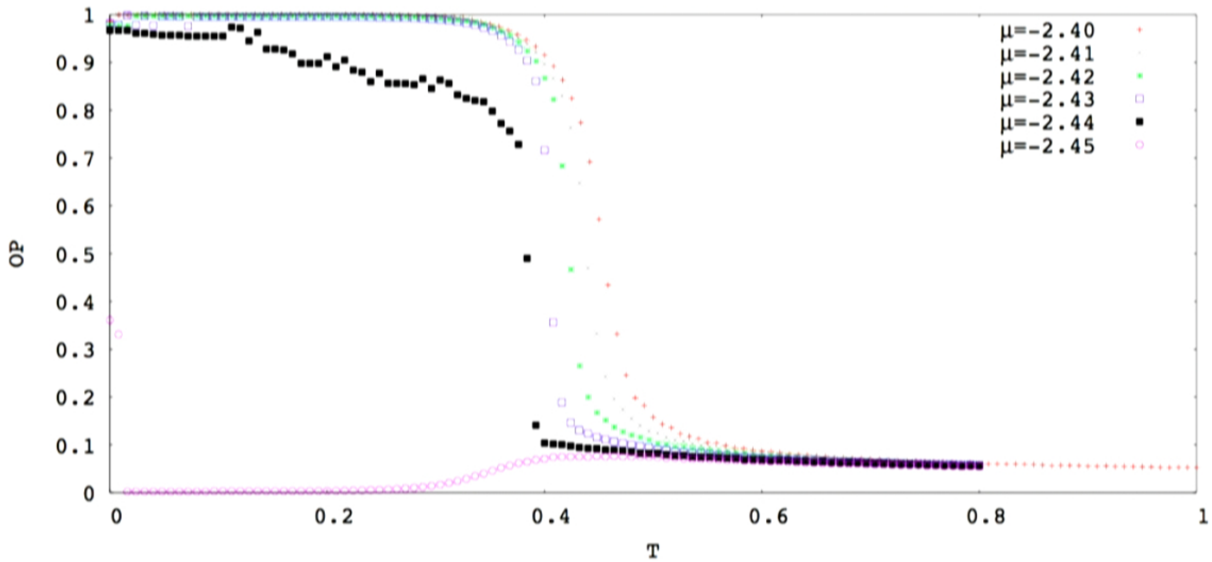
Monopole density: $\rho = \frac{<N>}{N_0}$



Crystlization (Z_2) order parameter

$$OP = \frac{1}{N_0} \sum_i q_i \Delta_i$$

$$q_i = 0, 1, -1, \ \Delta_i = \pm 1$$

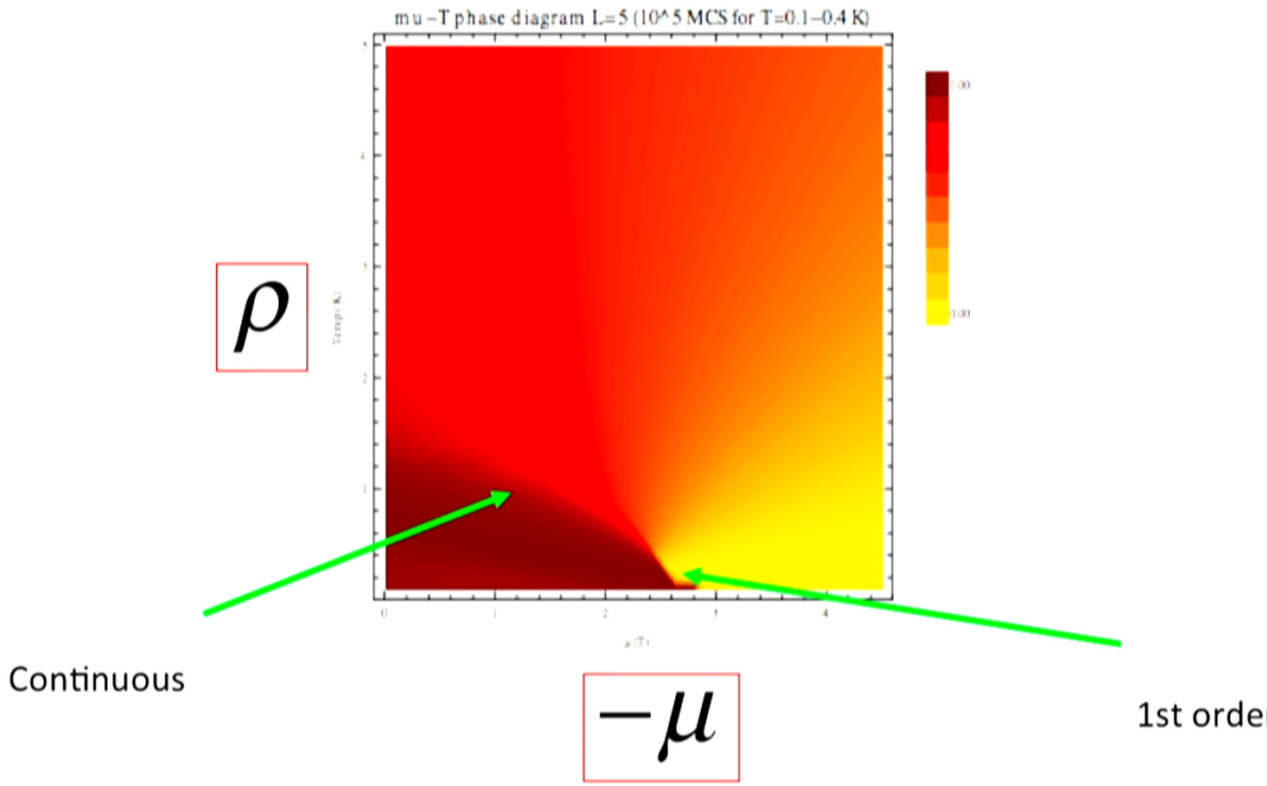


Second order transition becoming first order near phase boundary limit

Phase diagram similar to that of Blume Capel model

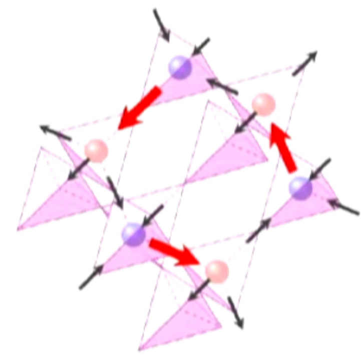
V. Kobelev, B. Kolomeisky, and M. E. Fisher, J. Chem. Phys. 116, 7589 (1992).

R. Dickman and G. Stell, AIP Conf. Proc. 492, 225 (1999).



Magnetic degrees of freedom are partially ordered: all in on A sites all out on B sites

$$(-1,-1,-1,1)=\left(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right)+\left(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},\frac{3}{2}\right)$$

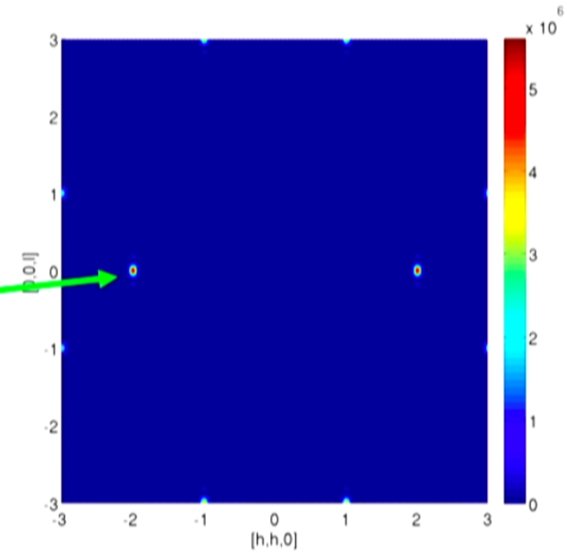


Partial all in all out order

Partial lattice gauge field

Simulated S(Q) off the needles of the dumbbell model in Monopole crystal phase

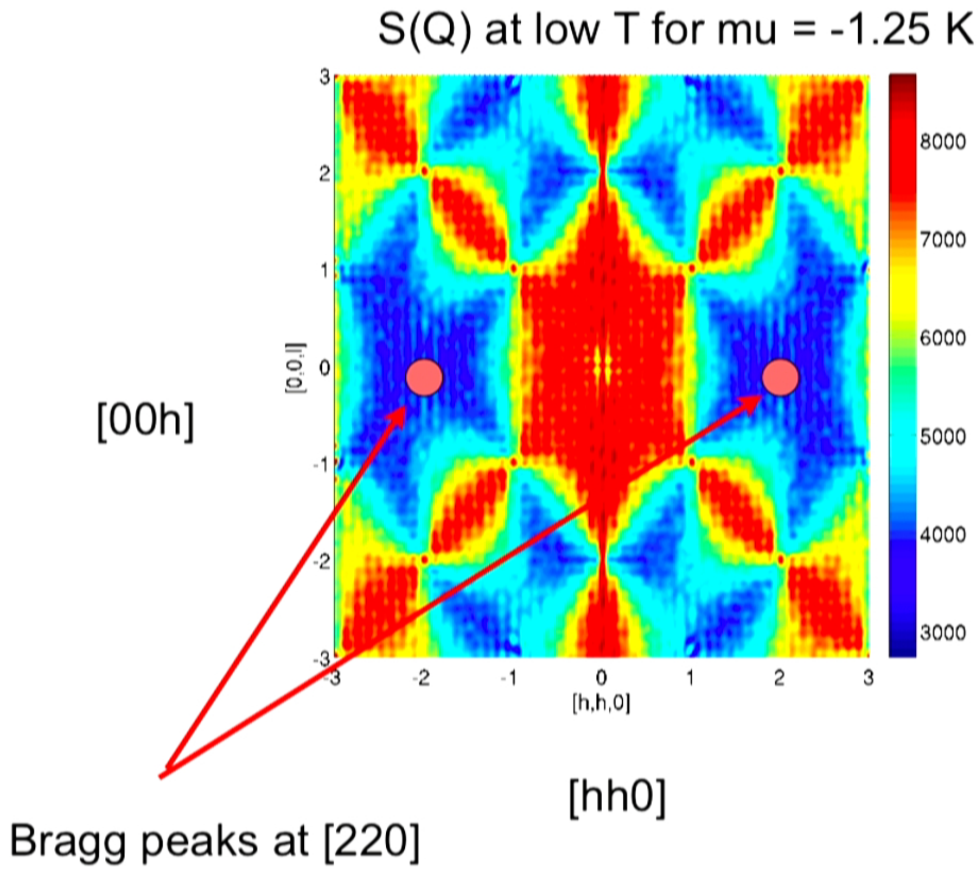
(220) Peaks characteristic of partial all in all out order

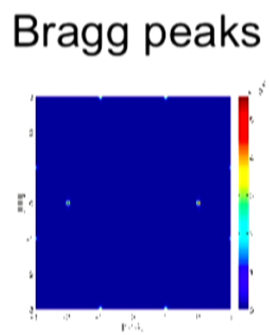


Intensity

$$I=\frac{I_0}{4}$$

When coherent scattering is subtracted a Coulomb phase of diffuse scattering is revealed





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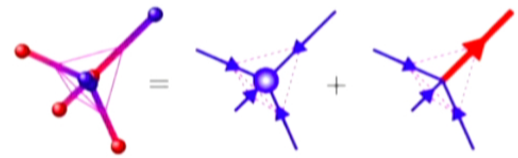
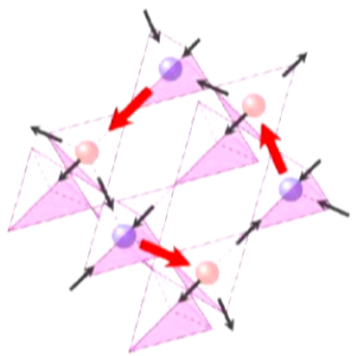
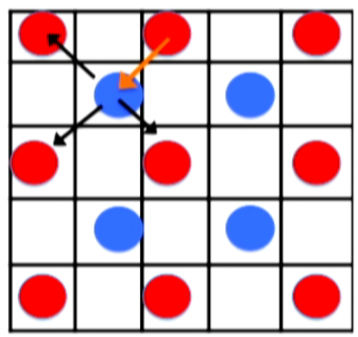
Crystal order allows sharing of the strong gauge field links

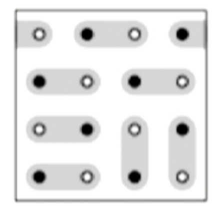
$$(-1,-1,-1,1)=\left(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right)+\left(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},\frac{3}{2}\right)$$



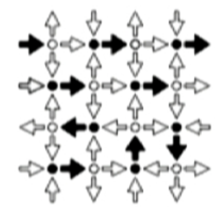


The red spins map onto dimers on a diamond lattice



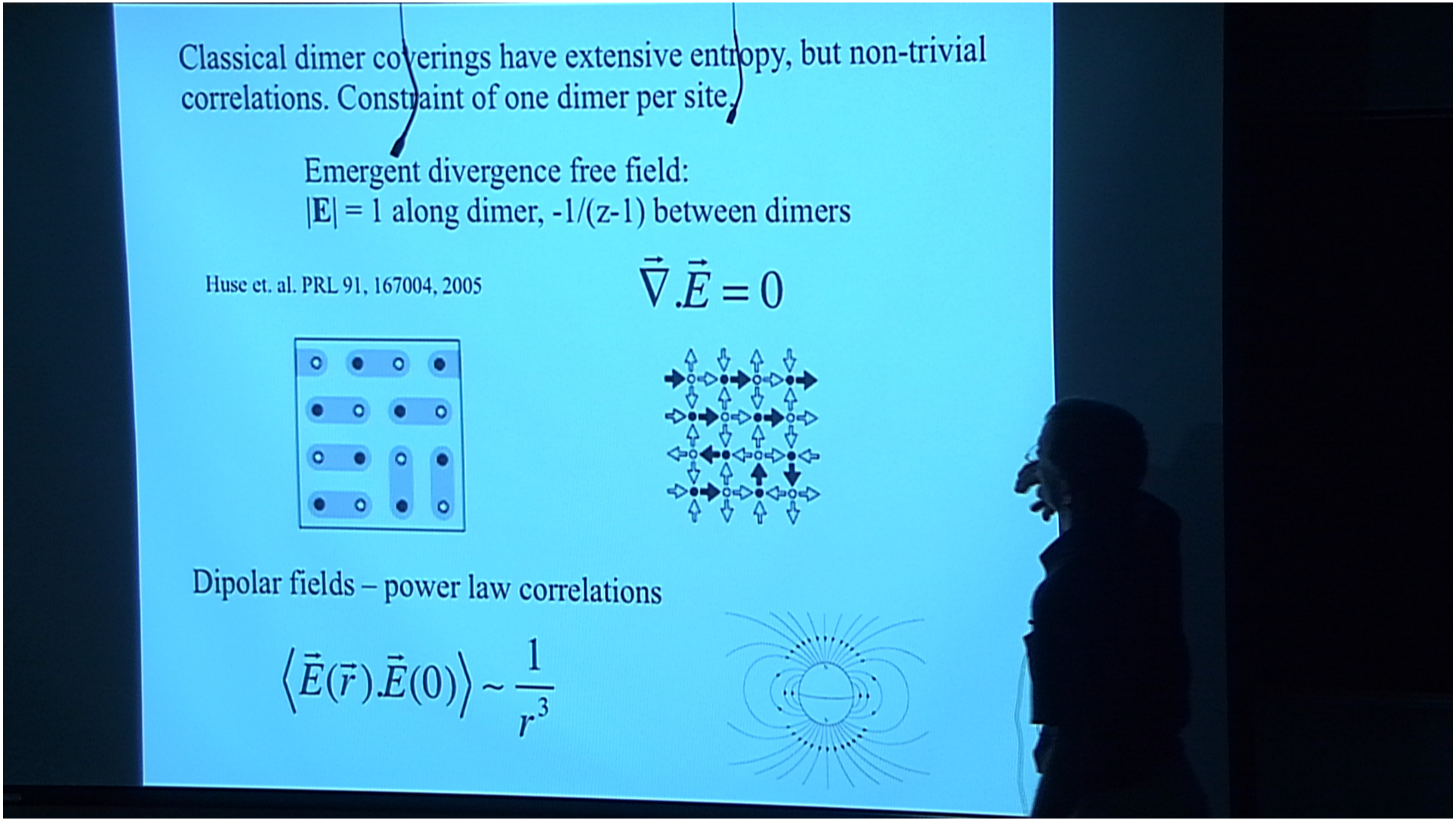


Divergence free part maps onto the emergent gauge field from the dimers

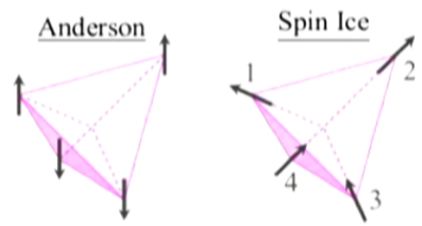


Huse et. al. PRL 91, 167004, 2005

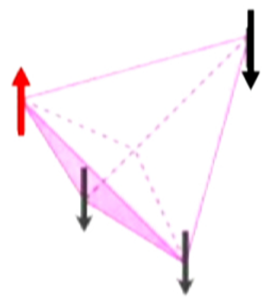
7


Classical dimer coverings have extensive entropy, but non-trivial correlations. Constraint of one dimer per site.
Emergent divergence free field:
|E| = 1 along dimer, -1/(z-1) between dimers
Huse et. al. PRL 91, 167004, 2005
$\vec{\nabla}.\vec{E} = 0$
Dipolar fields – power law correlations
$\left\langle \vec{E}(\vec{r}).\vec{E}(0) \right\rangle \sim \frac{1}{r^3}$

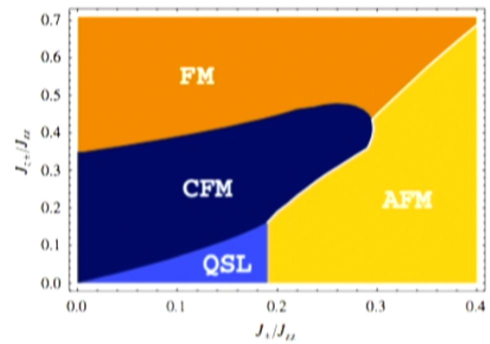
Mapping between Ising antiferromagnet and spin ice



Monopole crystal maps onto the 1 up 3 down sector of the IAF: red becomes the dimer



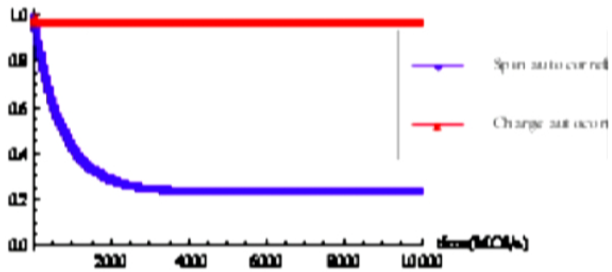
Classical example of the ferromagnetic Coulomb phase (L. Savary and L. Balents, PRL 108, 37202 (2012)

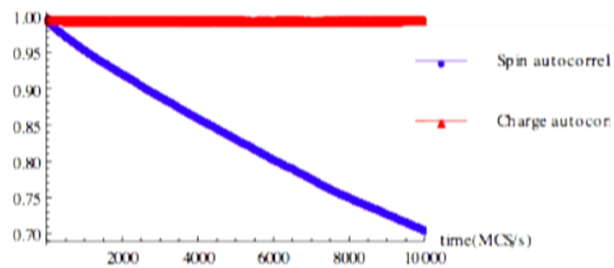


The Coulomb phase is ergodic and fluctuates below the transition, even with local dynamics

$$C_c(t) = \left\langle \frac{n}{N_0} \sum_{i=1}^{N_0} q_i(0)\, q_i(t) \right\rangle, \quad C_s(t) = \left\langle \frac{1}{2N_0} \sum_{j=1}^{2N_0} \vec{S}_j(0).\, \vec{S}_j(t) \right\rangle.$$

C

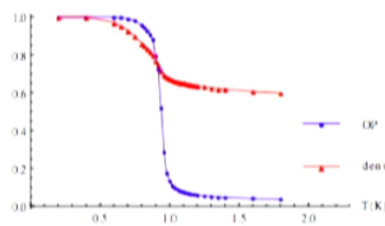


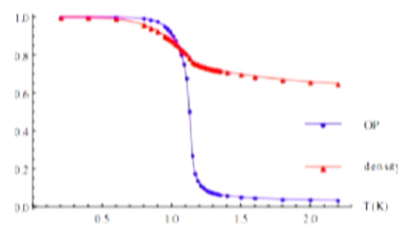


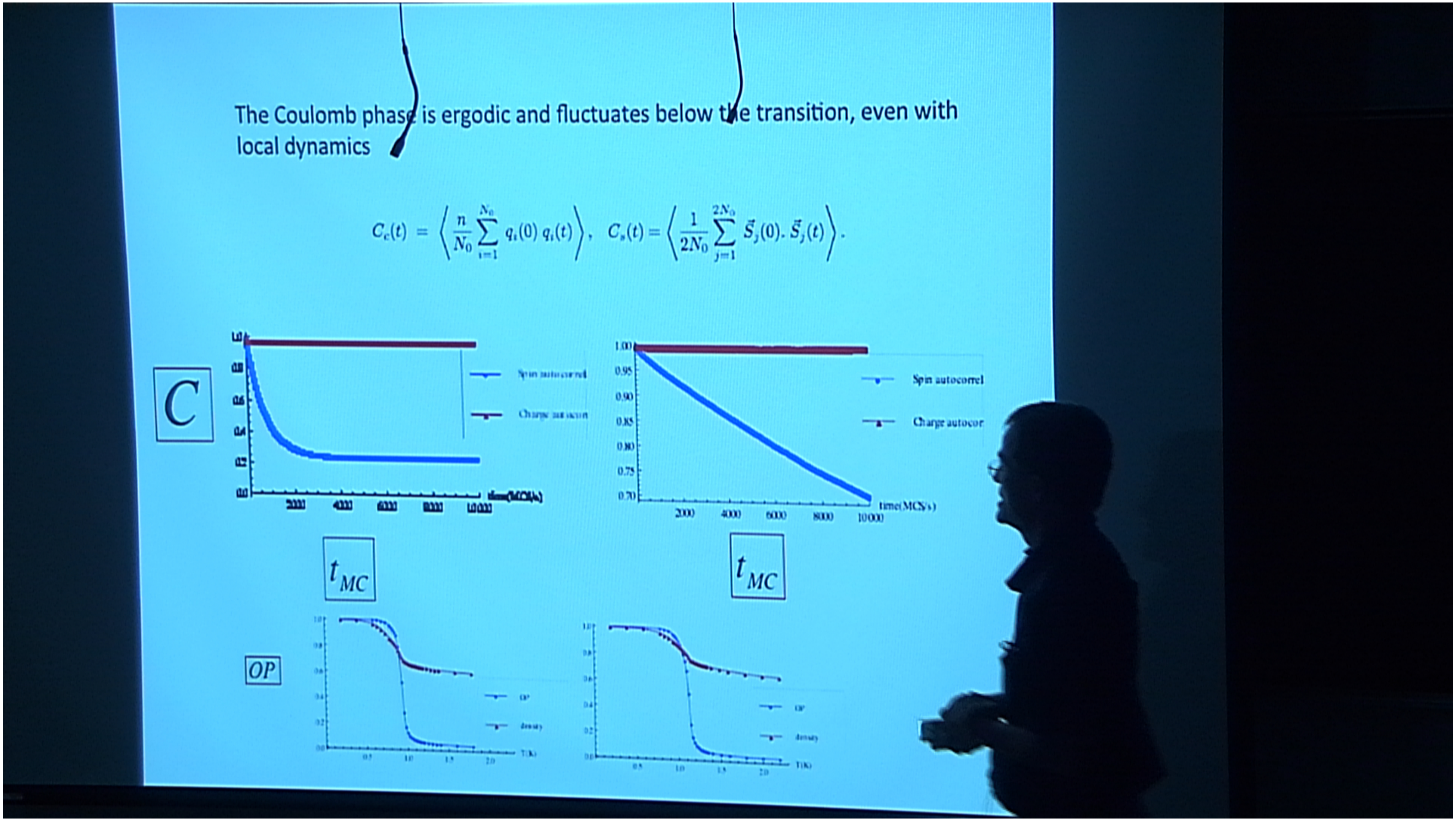
t_{MC}

t_{MC}

OP



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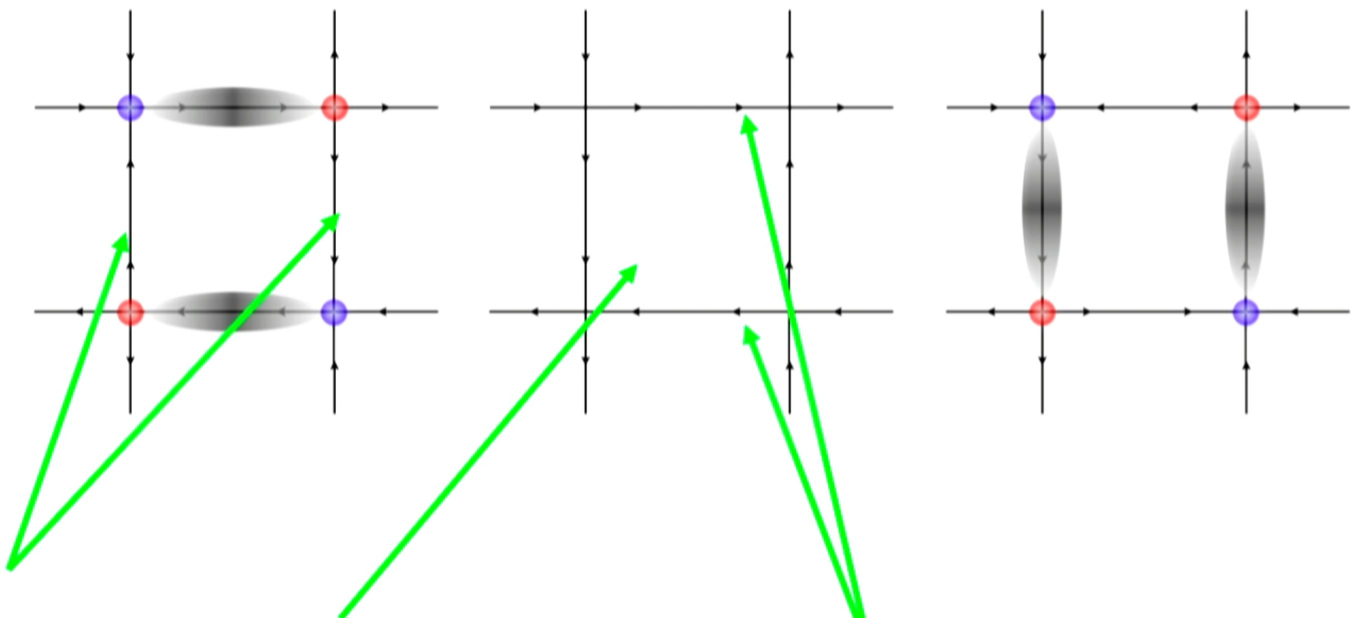
C
Spin autocorrel
Charge autocor
time(MCS/s)
t_{MC}
t_{MC}
OP
OP
density
T(K)

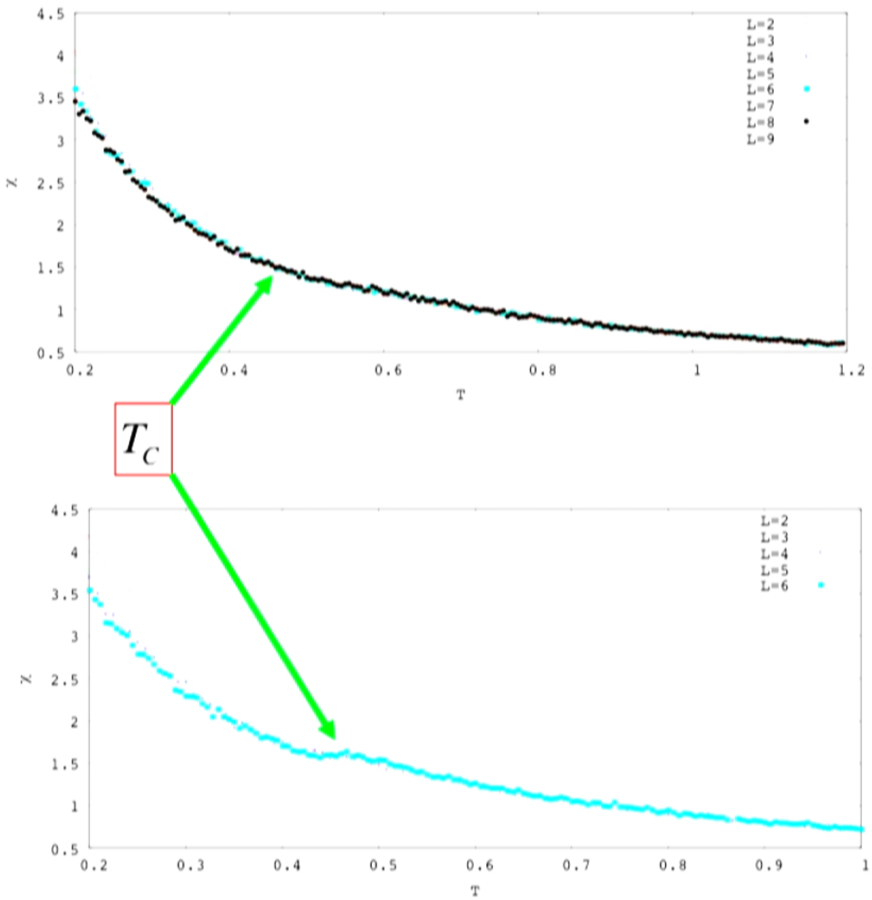
Dynamics simmulates dimer plaquette flips



Flipping these needles
Re-establishes the ice rules

Flipping these two re-establishes
the monopole crystal with
displaced dimers

What other magnetic signal is there of this transition ? Virtually none!
(This is an Ising antiferromagnet but there is no cusp)

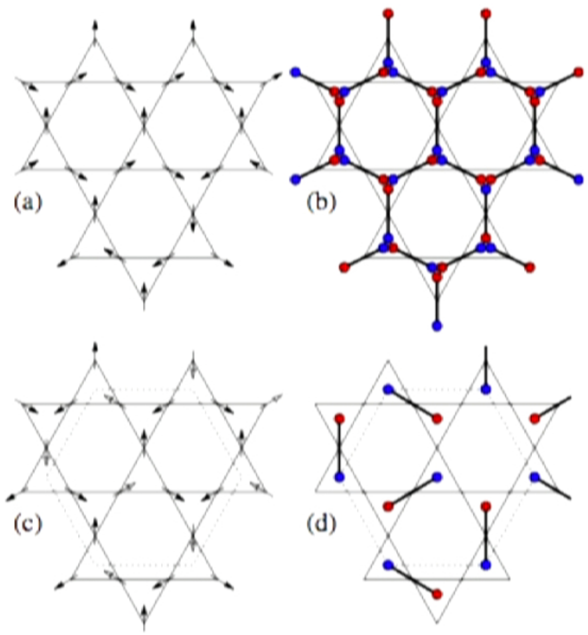


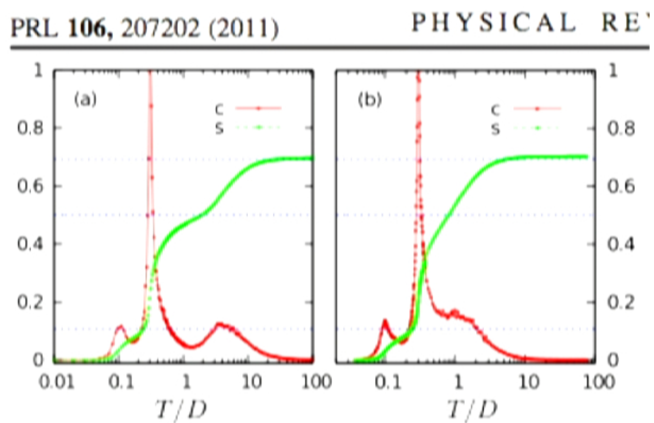
Mu=-2.1
2nd order

Mu=-2.45
1st order

A word about charge orderig in kagomé ice

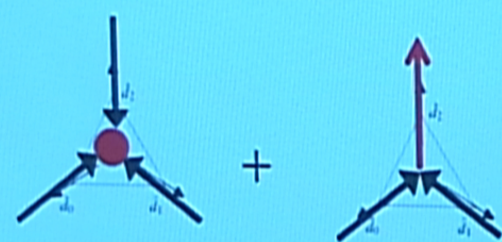
G.-W. Chern, P. Mellado, and O. Tchernyshyov, Phys. Rev. Lett. 106, 207202 (2011).





Moment fractionalization (kagomé)

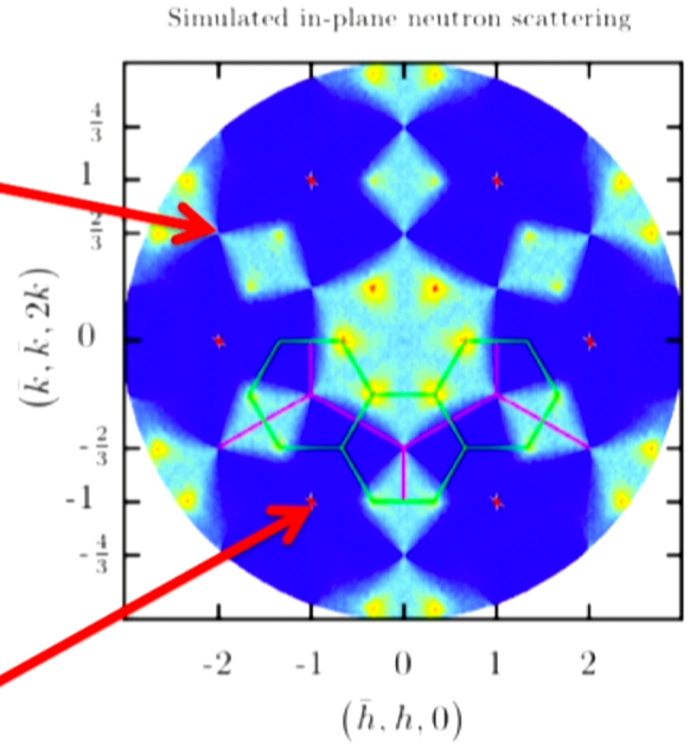
$$(-1,-1,1)=\left(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3}\right)+\left(-\frac{2}{3},-\frac{2}{3},\frac{4}{3}\right)$$



$$\vec{M}=\nabla\psi+\vec{\nabla}\wedge\vec{Q}\ =\vec{M}_m+\vec{M}_{rot}$$

S(Q) for kagomé KII ice

Scattering from $\mathbf{M}_{rot}$



Bragg peaks from $\mathbf{M}_{m}$

Bragg peak intensity is 1/9 of that for full all in all out order

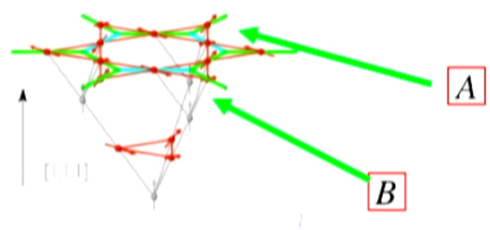
$$(-1,-1,1)=\left(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3}\right)+\left(-\frac{2}{3},-\frac{2}{3},\frac{4}{3}\right)$$

Encounter with experiment ??

Already done in a certain sense – spin ice in a <111> field:

T. Sakakibara, T. Tayama, Z. Hiroi, K. Matsuhira, and S. Takagi, Phys. Rev. Lett. 90, 207205 (2003)

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



Field provides a staggered chemical potential on the A and B sites

But also couples to the gauge field providing ferromagnetic order

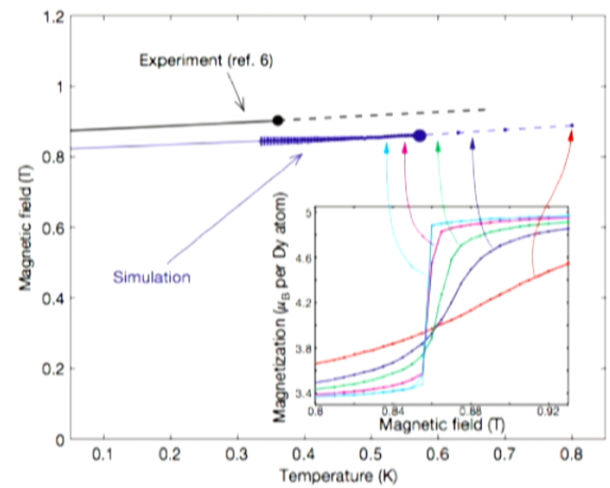
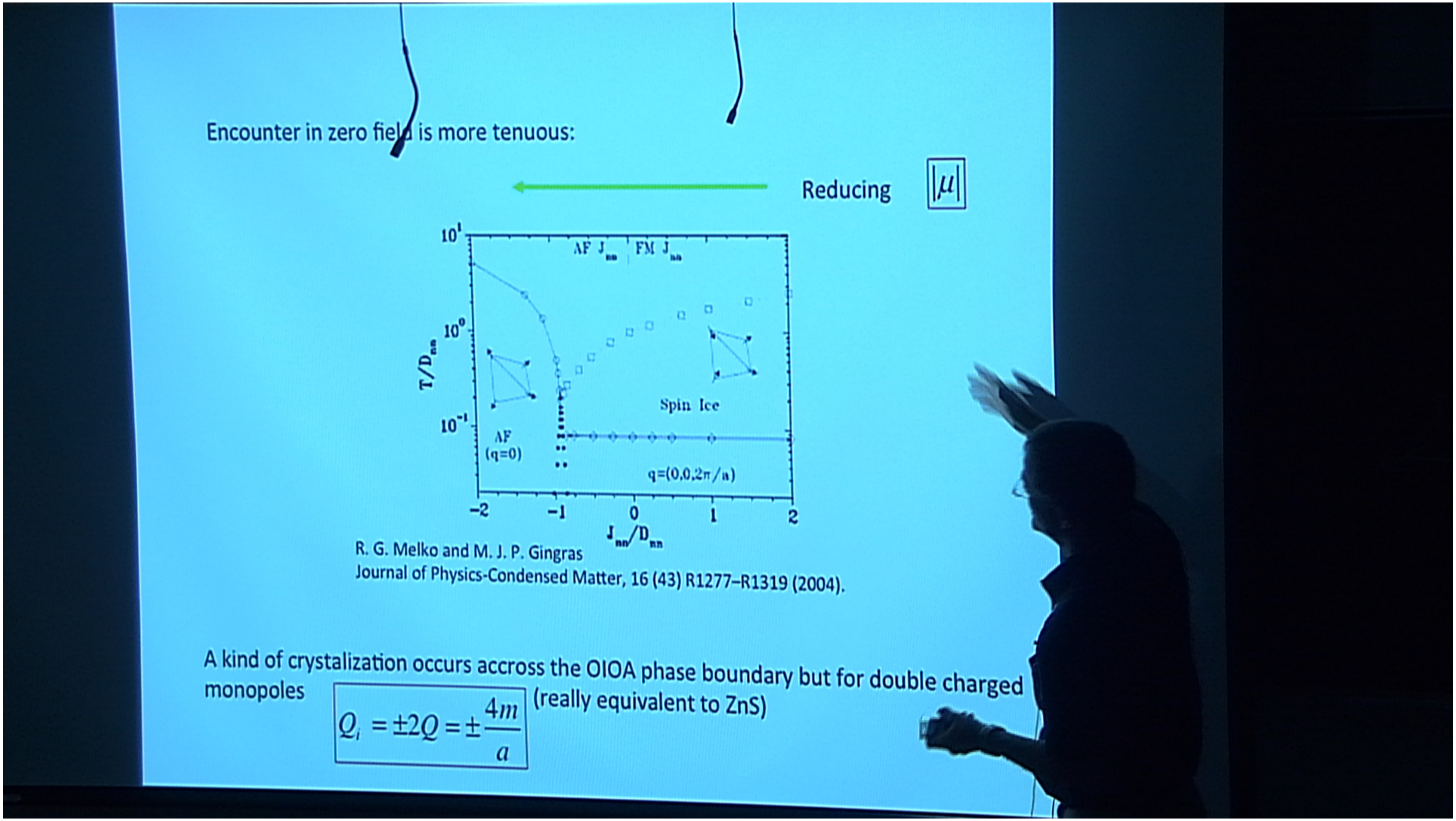


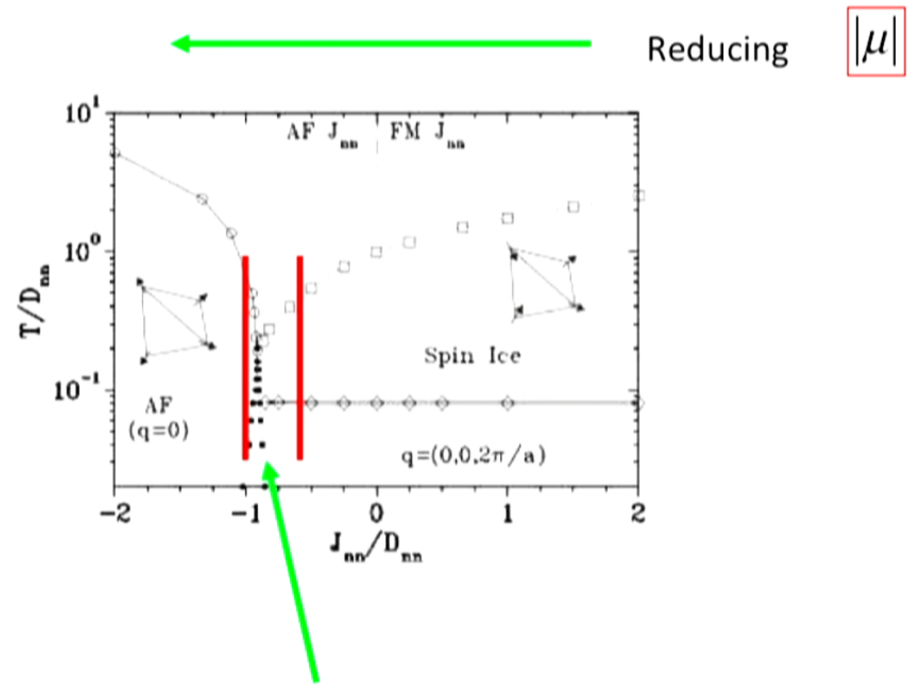
Figure 4 | Phase diagram of spin ice in a [111] field. The location of the

Observed phase transition and critical end point is monopole crystalization



Encounter in zero field is more tenuous:
Reducing $|\mu|$
AF J_{nn} | FM J_{nn}
T/D_{nn}
10^1
10^0
10^{-1}
Spin Ice
AF
(q=0)
q=(0,0,2π/a)
−2
−1
0
1
2
J_{nn}/D_{nn}
R. G. Melko and M. J. P. Gingras
Journal of Physics-Condensed Matter, 16 (43) R1277–R1319 (2004).
A kind of crystalization occurs accross the OIOA phase boundary but for double charged monopoles
$Q_i = \pm 2Q = \pm \frac{4m}{a}$
(really equivalent to ZnS)

Encounter in zero field is more tenuous:



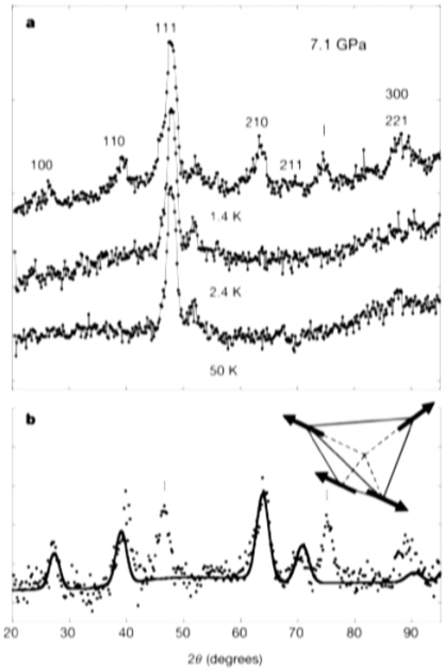
One would need quantum fluctuations (for example) to suppress double defects near the phase boundary

But QF means transverse fluctuations and relaxation off spin ice axes........

However, one such material is $Tb_2Ti_2O_7$

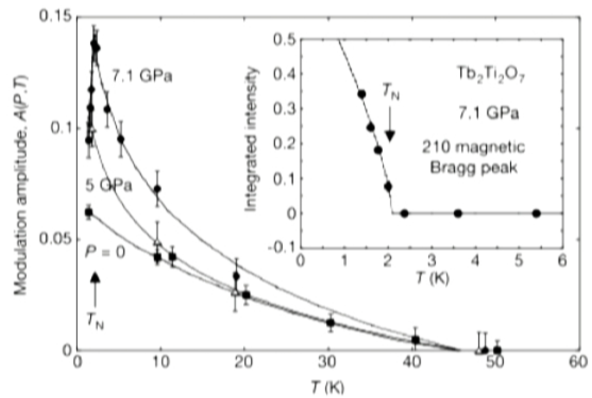
Molavian, Gingras, Canals, Phys Rev Lett 98, 157204, (2007)

No order is observed down to zero temperature at ambiant pressure, but Partial ordering is observed under pressure.



Pressure-induced crystallization of a spin liquid

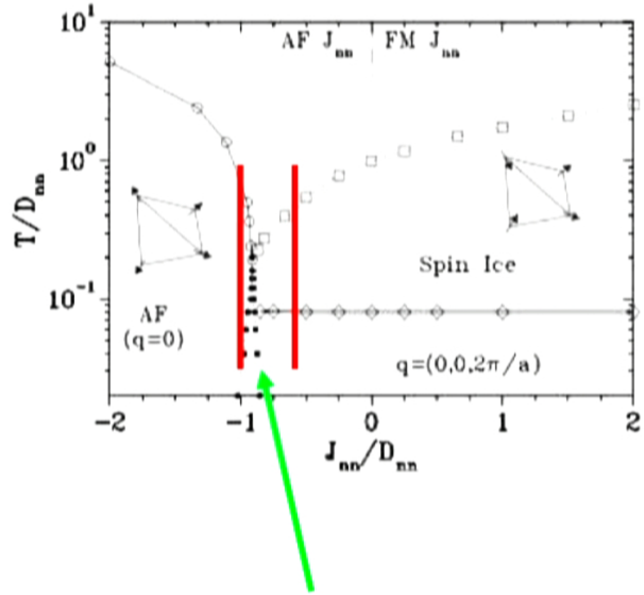
I. Mirebeau, I. N. Goncharenko, P. Cadavez-Peres , S. T. Bramwell, M. J. P. Gingras, J. S. Gardner, Nature 420, 54, (2002).



Ordering does have a (kind of) 3-1 structure and an A-B arrangement of tetrehedra in a fluctuating background

Encounter in zero field is more tenuous:

Reducing $|\mu|$



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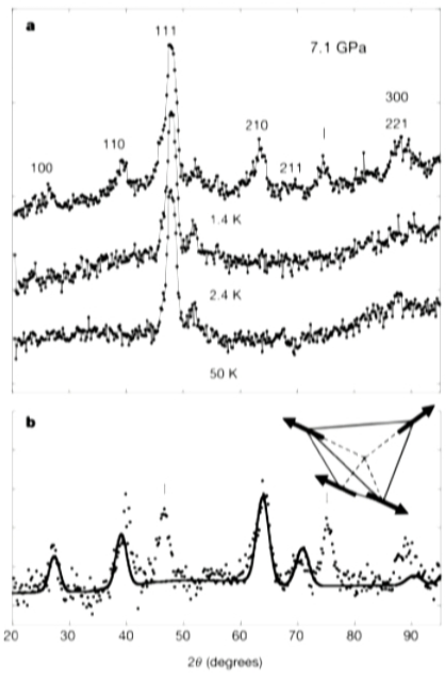

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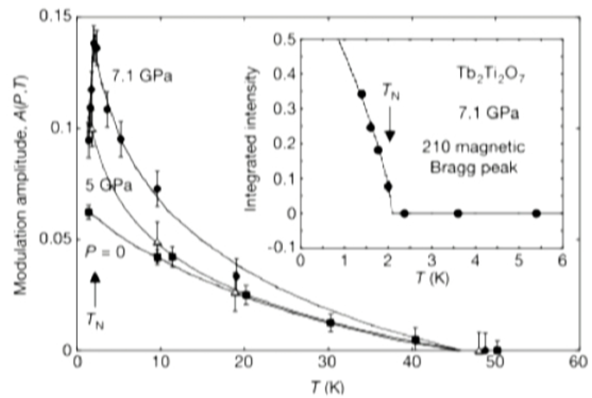

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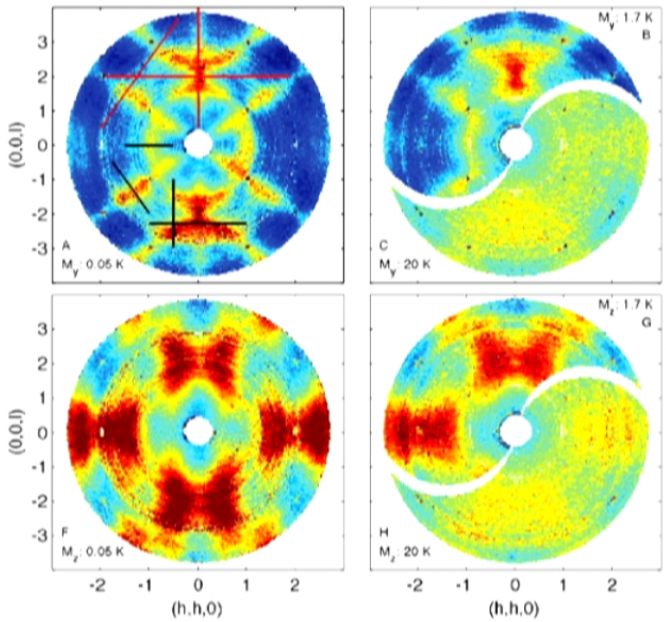
…. there are pinch points!

Power-Law Spin Correlations in the Pyrochlore Antiferromagnet $Tb_2Ti_2O_7$

T. Fennell, M. Kenzelmann, B. Roessli, M.K. Haas and R.J. Cava

PRL **109,** 017201 (2012) PHYSICAL REVIEW



And there are reports of « incipient » all in all out order on adding a small <111> field

S. Legl et al , Phys. Rev. Lett. 109, 047201 (2012).

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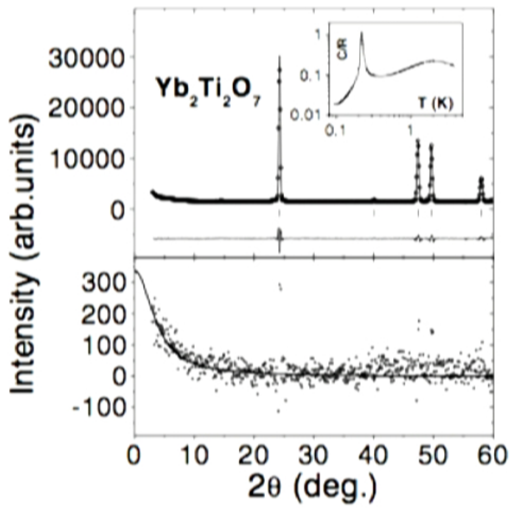
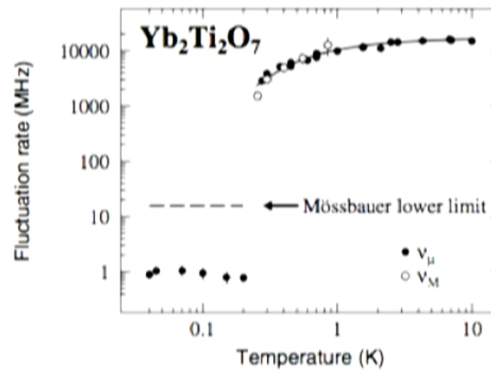
First-Order Transition in the Spin Dynamics of Geometrically Frustrated $Yb_2Ti_2O_7$

J. A. Hodges, et al Phys. Rev. Lett. **88**, 077204, 2002





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But also of quantum spin ice behaviour (L. Savary and L. Balents, PRL 108, 37202 (2012).
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And of a quantum spin liquid – classical spin gas transition (L. Savary and L. Balents, PRB 2013)

Could our model provide a further alternative........

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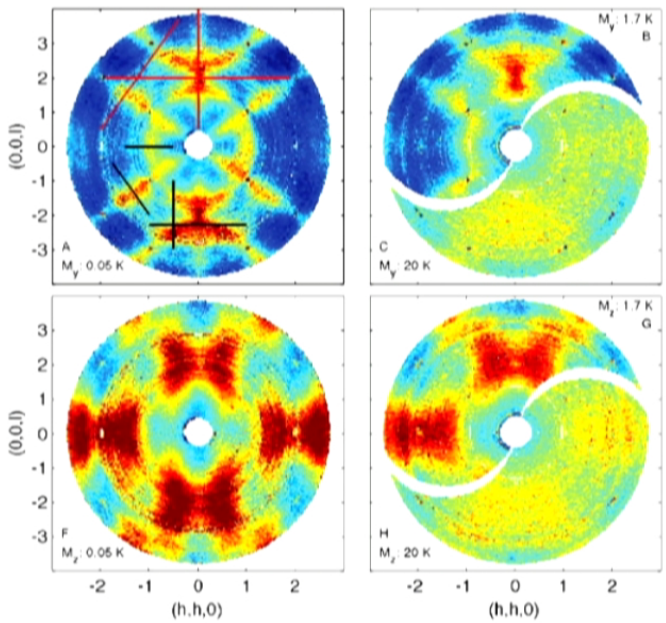

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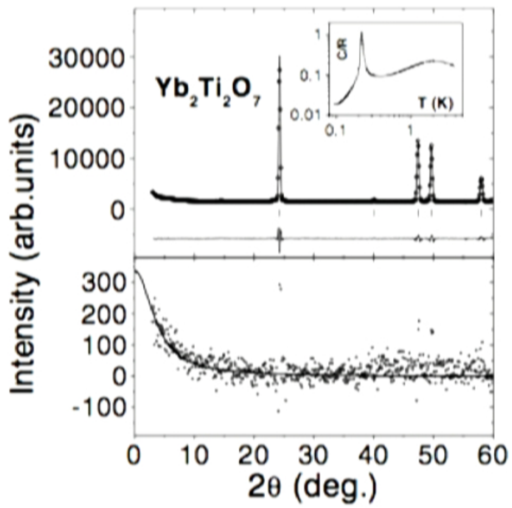

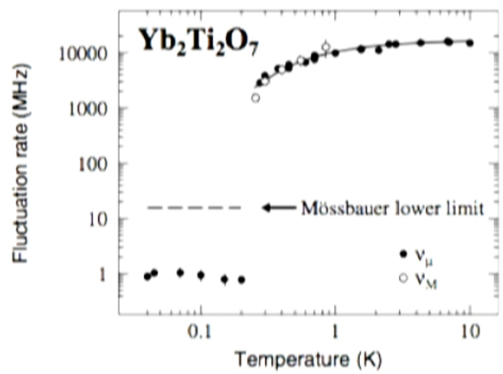

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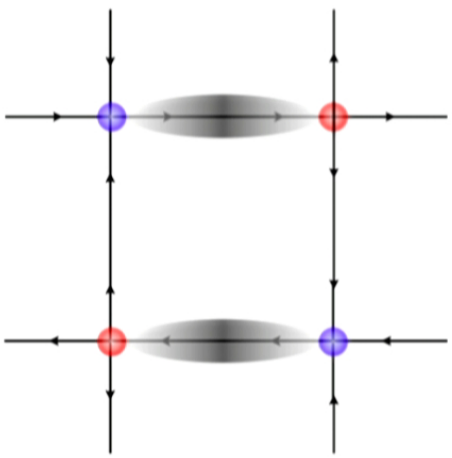
ENS DE LYON

Conclusion

.......or maybe not, but our monopole crystalization does show that the phase space exists in these frustrated magnetic systems for both phase transtions and highly fructuating background – an omnipresent phenomenon in frustrated magnetism.



PI May 2013