Magnetic Order in the FCC Kagome Lattice:

Hard drives and basket weaving

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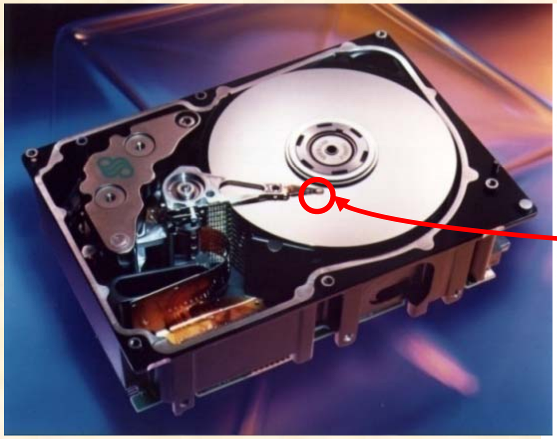
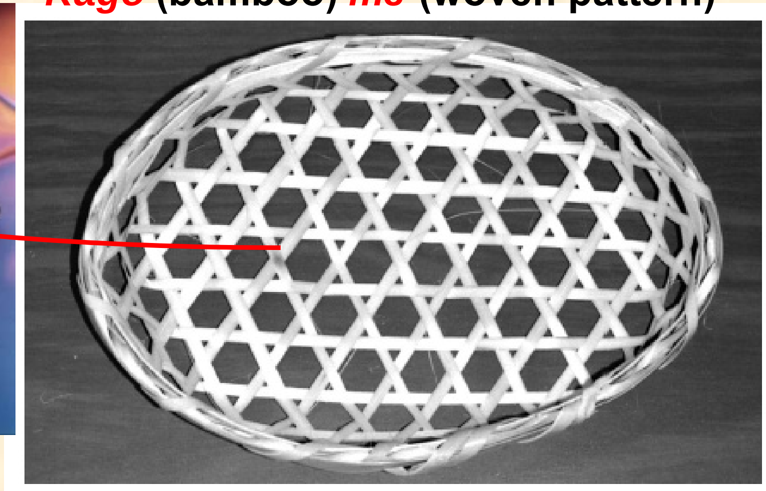


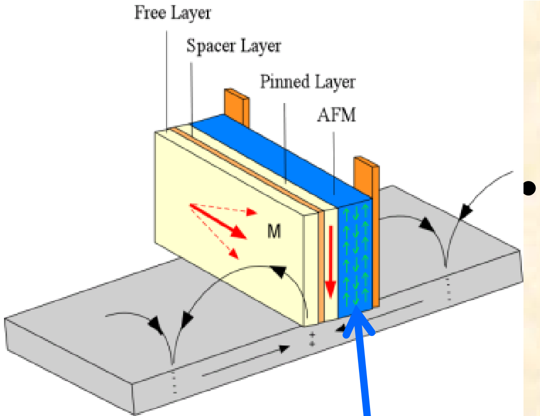
Kago **(bamboo)** ***me*** **(woven pattern)**

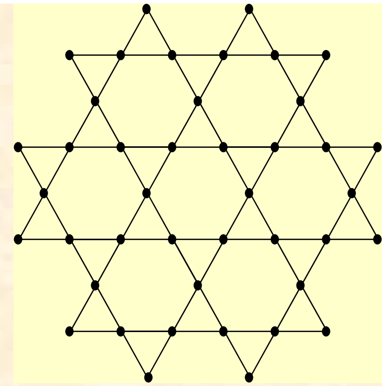


Kagome: The Story of the Basketweave Lattice. M. Mekata, Physics Today Feb. 2003.

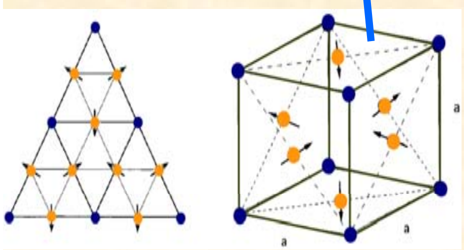
First study of magnetic properties: I. Syozi, Prog. Theor. Phys. (1951).

Outline

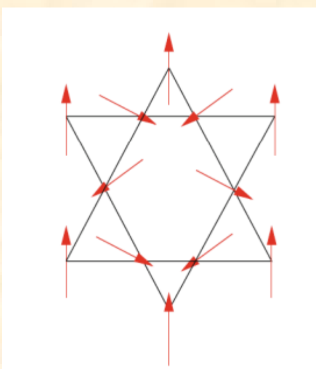




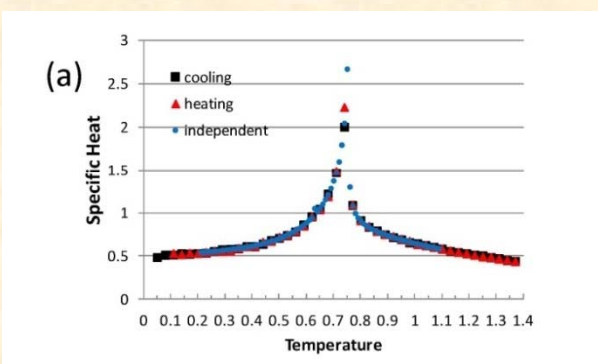
- *Motivation*: Spin valves and exchange pinning.



- *$IrMn_3$*: *ABC* stacked kagome layers (FCC).

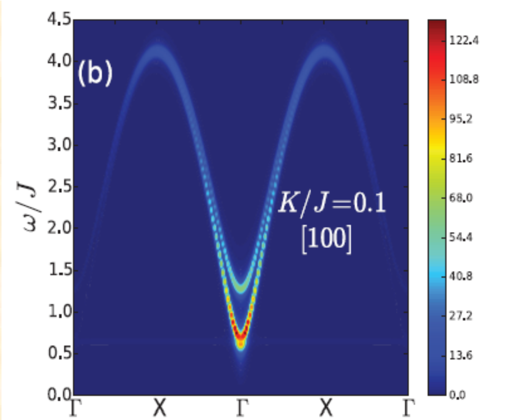


- *Degeneracy* of the spin structure for the 2D kagome lattice with exchange only (review).

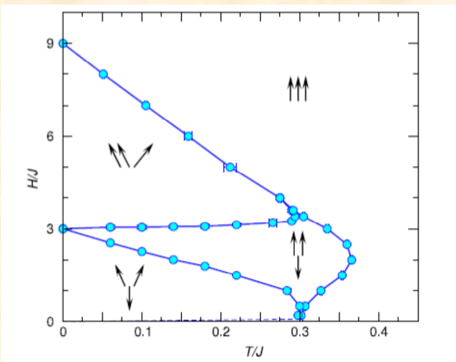


- *Monte Carlo 3D FCC*
  - degeneracy in 3D: first order phase transition.
  - anisotropy (cubic): continuous phase transition.

More Outline

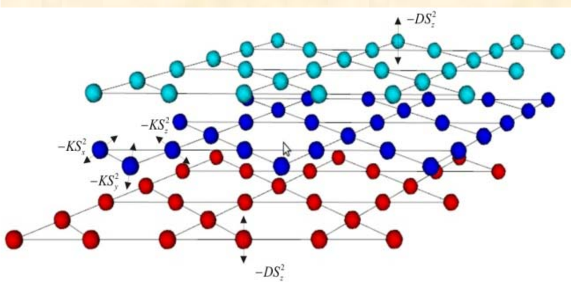


• *Spin waves* **and inelastic scattering: impact of cubic anisotropy.**



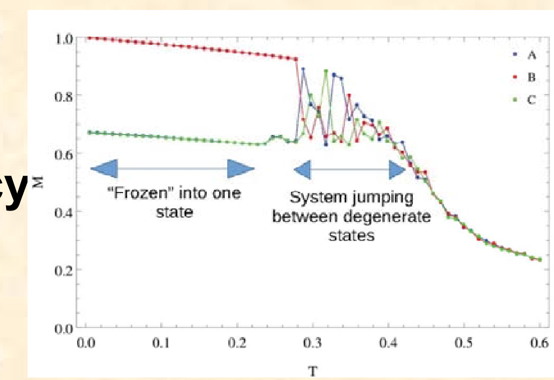
• ***Preliminary Monte Carlo results***

-*H-T phase diagram*: 3D FCC Kagome looks like 2D triangular.



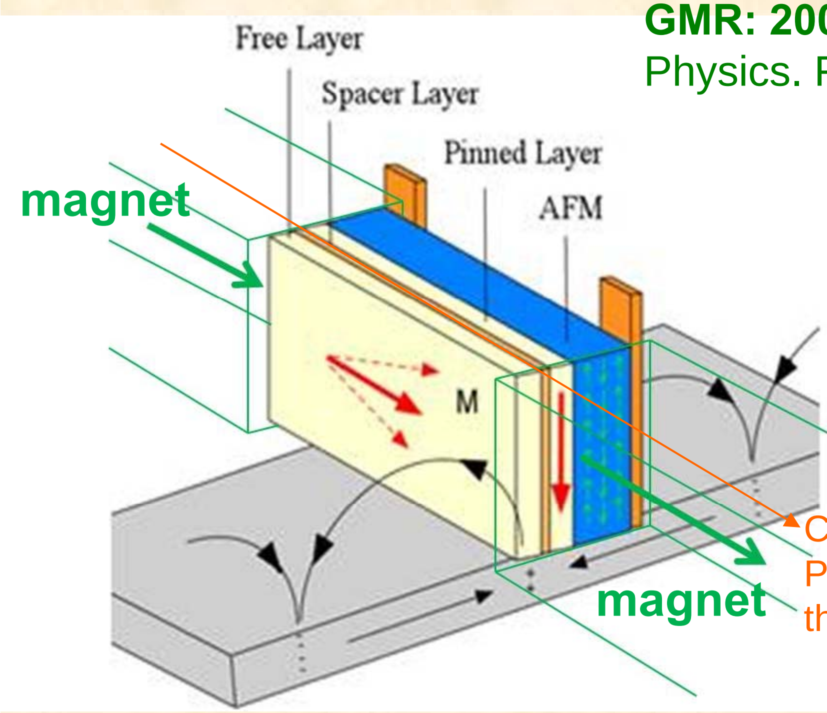
-*Thin films*: surface anisotropy (axial).

- *2D dipole interactions only:* competition between degeneracy and thermal fluctuations.

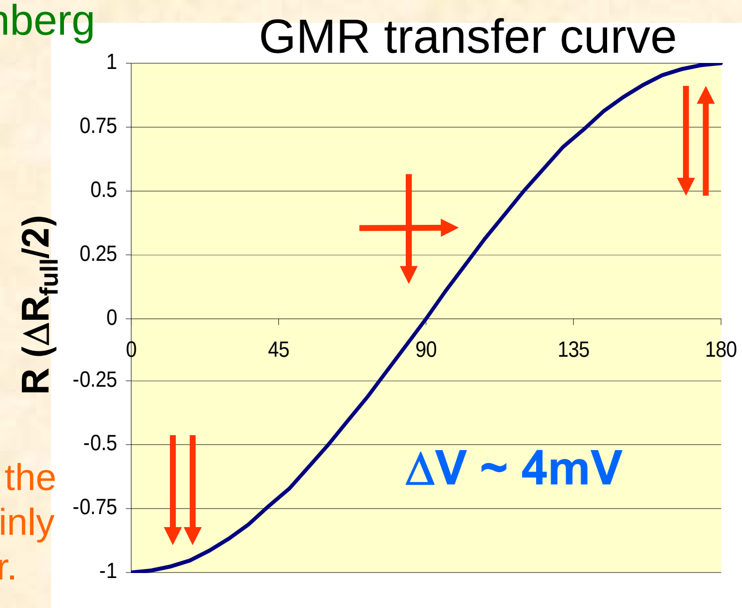


Spin Valve: Detection of media magnetization reversal.

GMR: 2007 Nobel Prize in Physics. Fert and Grünberg



Current flows In the Plane (**CIP**), mainly through Cu layer.

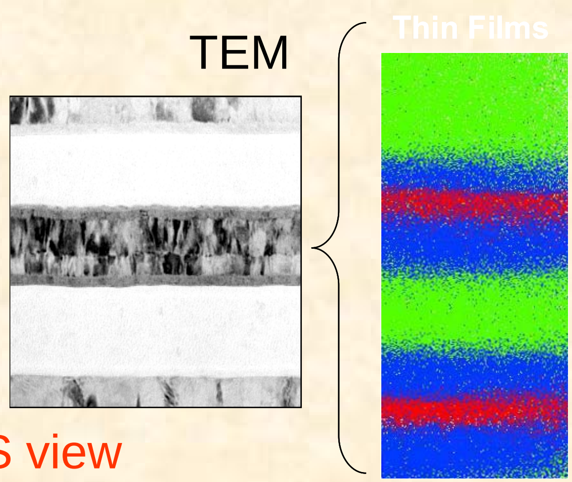


AFM = Ir-Mn (High T_N). 200 Å

PL = CoFe (big moment). 25 Å

FL = $Ni_{80}Fe_{20}$ Permalloy 25 Å

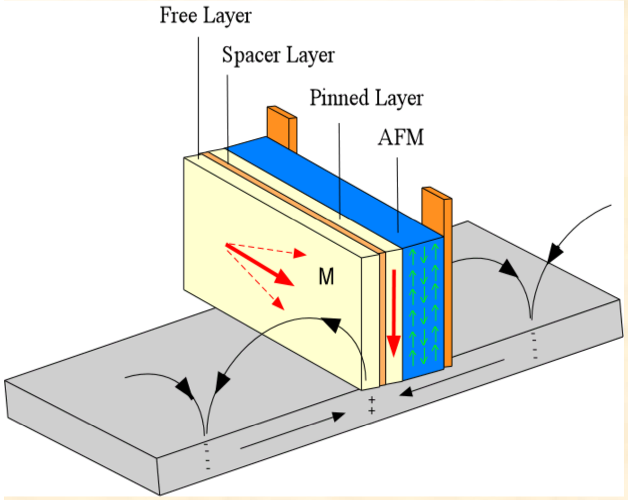
TEM



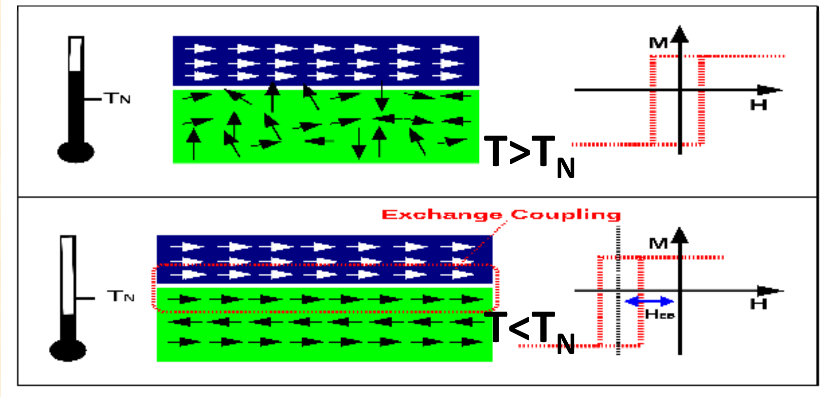
ABS view

GMR effect involves surface and bulk scattering of spin polarized electrons between the Free Layer and Pinned Layer.

Exchange Pinning in Spin Valves



- Pins the Pinned Layer so it does not respond to media bit transition fields.
- Requires T_N >> drive operating temperatures~ 350 K.

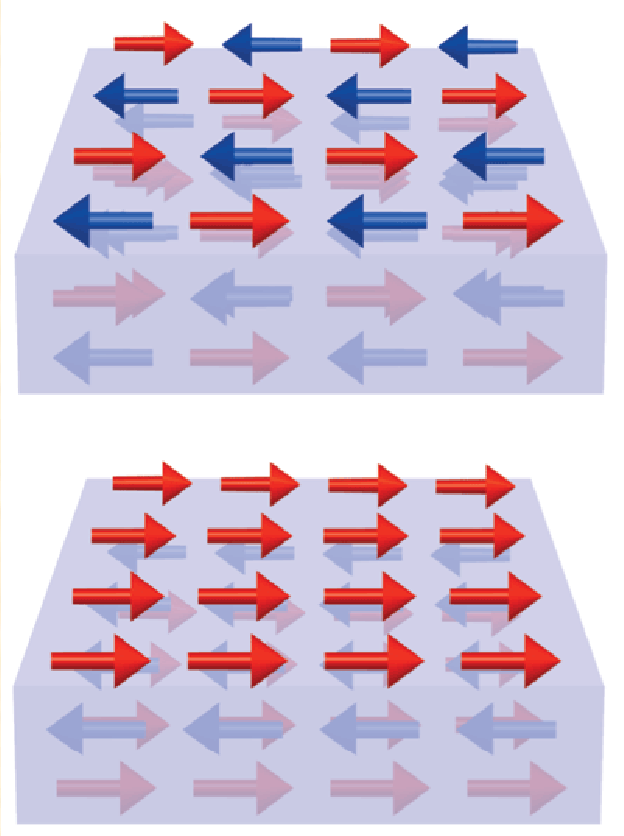


Field cooling to obtain exchange bias.

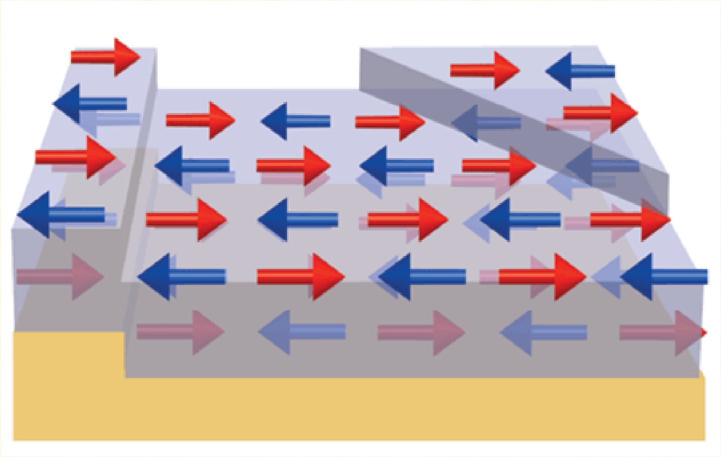
- Surface spin structure in AF results in a small ferromagentic moment.
- Induces a *uni-directional* field on the PL.
- "After more than 50 years there is still no definitive theory that can account for the observed effects.." K. O'Grady et al., JMMM 322, 883 (2010).

A model...

No obvious mechanism for exchange pinning from compensated surface (M=0).



The atomic-scale *Roughness* can create uncompensated spins (red)



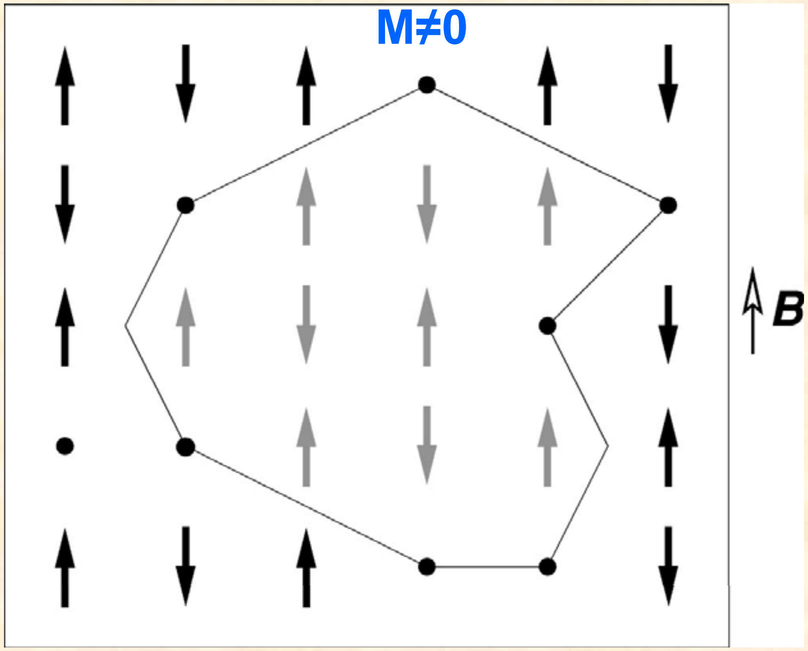
M. Blamire and B. Hickey, Nature Mater. 5, 87 (2006).

J. Spray and U. Nowak, J. Phys. D 39, 4536 (2006).

Another model (Irmy-Ma)...

Domains **involving non-magnetic surface sites.**

Thin films are sputtered: they are *not* uniform single crystals.



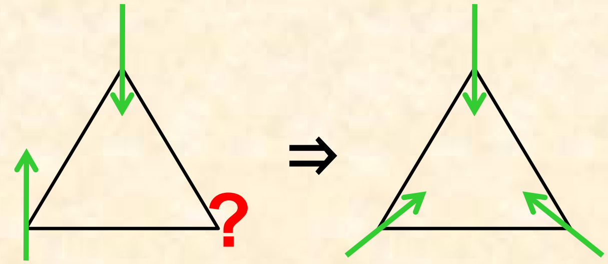
U. Nowak et al PRB 66, 014430 (2002).

M. R. Fitzsimmons et al, PRB 77, 224406 (2008).

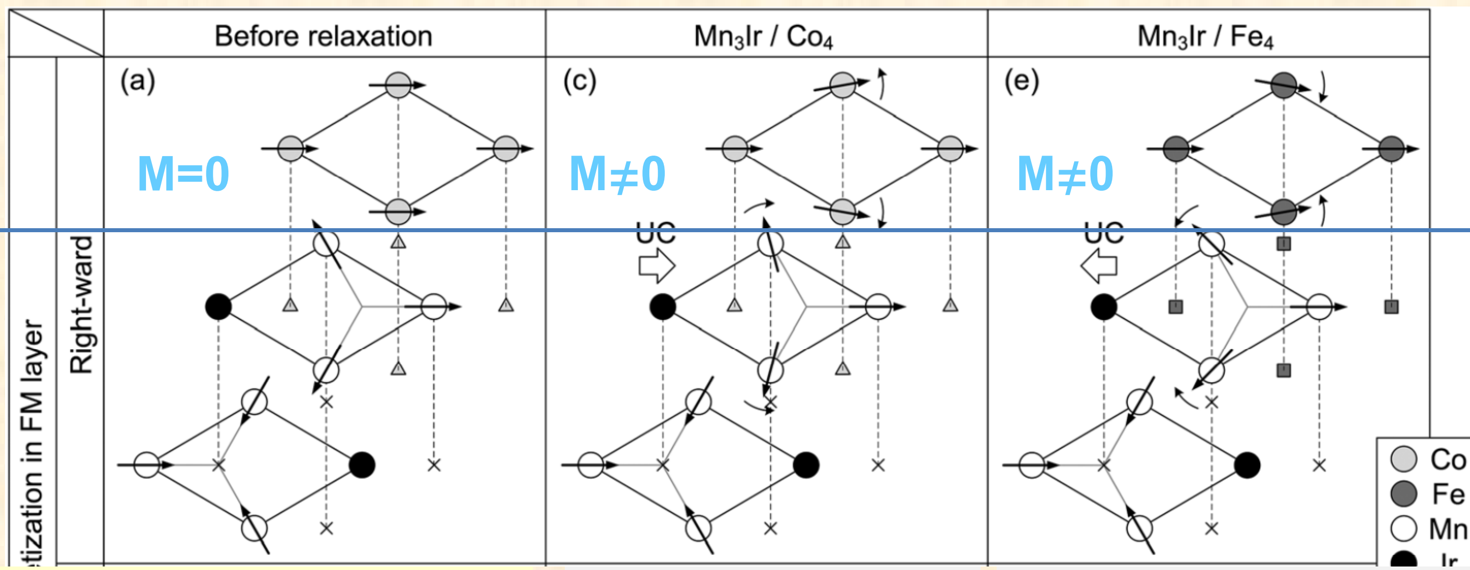
$IrMn_3$: Interaction with a Ferromagnet + Frustration ⇒ M≠0?

XRD, and DFT calculations of $IrMn_3/CO_4$ and $IrMn_3/Fe_4$ interface spin structures.
H. Takahashi et al, J. Appl. Phys. 110, 123920 (2011)

Geometrical frustration is believed to be important.



Interface



Interaction with ferromagnetic layer induces a net moment in surface Mn spins.

Mn moments rotate toward Co-moments

Mn moments rotate away from Fe-moments

Relation to exchange pinning?

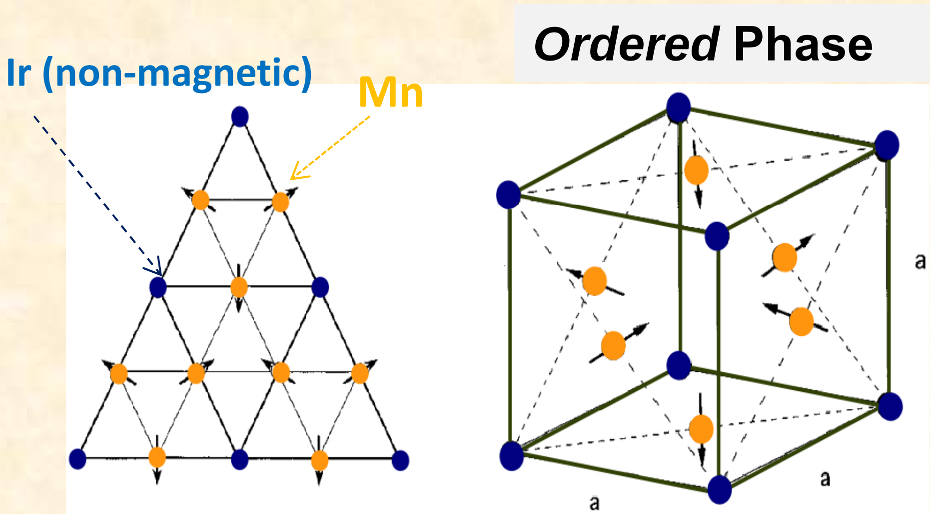
A closer look at $IrMn_3$.

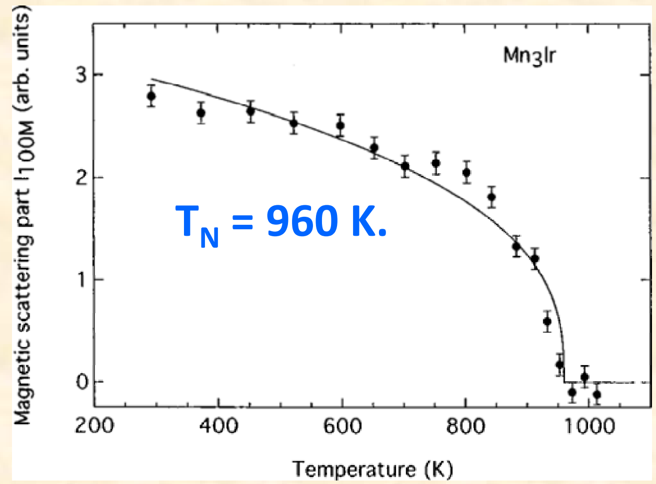
Ir-Mn ($IrMn_3$) most popular AF material in spin valves.

$IrMn_3$ = FCC $AuCu_3$ crystal structure. Also: $RhMn_3$ and $PtMn_3$

I. Tomeno et al J. Appl. Phys. 86, 3853 (1999).

Neutron diffraction on bulk single crystals.



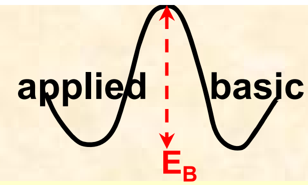


'T1' ⇒ planar spin structure

Very large T_N.

FCC lattice = *ABC* stacked triangular layers ⊥ <111>

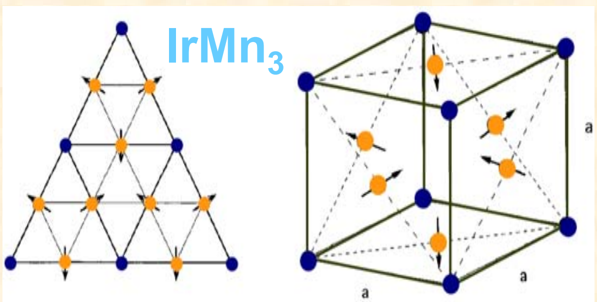
A tale of two physics



***Applied Physics*: 'T1' spin structure (*no* mention of Kagomé) ~ 50 years**

E. Krén et al, Phys. Lets. 20, 331 (1966).
I. Tomeno et al J. Appl. Phys. 86, 3853 (1999).

Ordered $IrMn_3$ ⟹



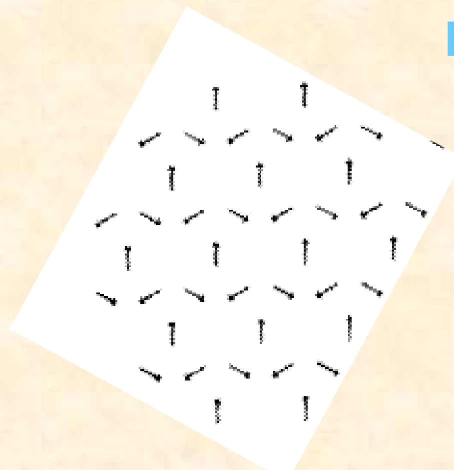
Thin films of $IrMn_3$ form <111> planes.

***Basic Physics*: 'q=0' spin structure (*no* mention of 'T1') ~ 60 years.**

I. Syozi, Prog. Theor. Phys. (1951).
A.B. Harris et al, PRB 45, 2899 (1992).

FCC Kagomé lattice = *ABC* stacked Kagomé layers ⊥ <111>

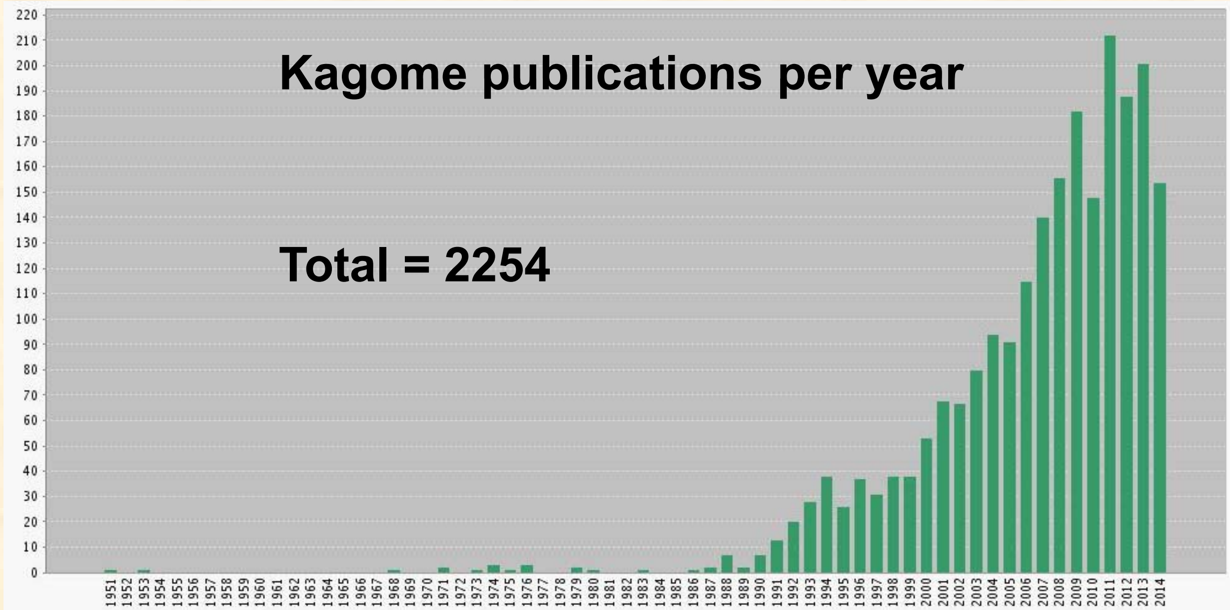
2D Kagomé: Highly Frustrated AF



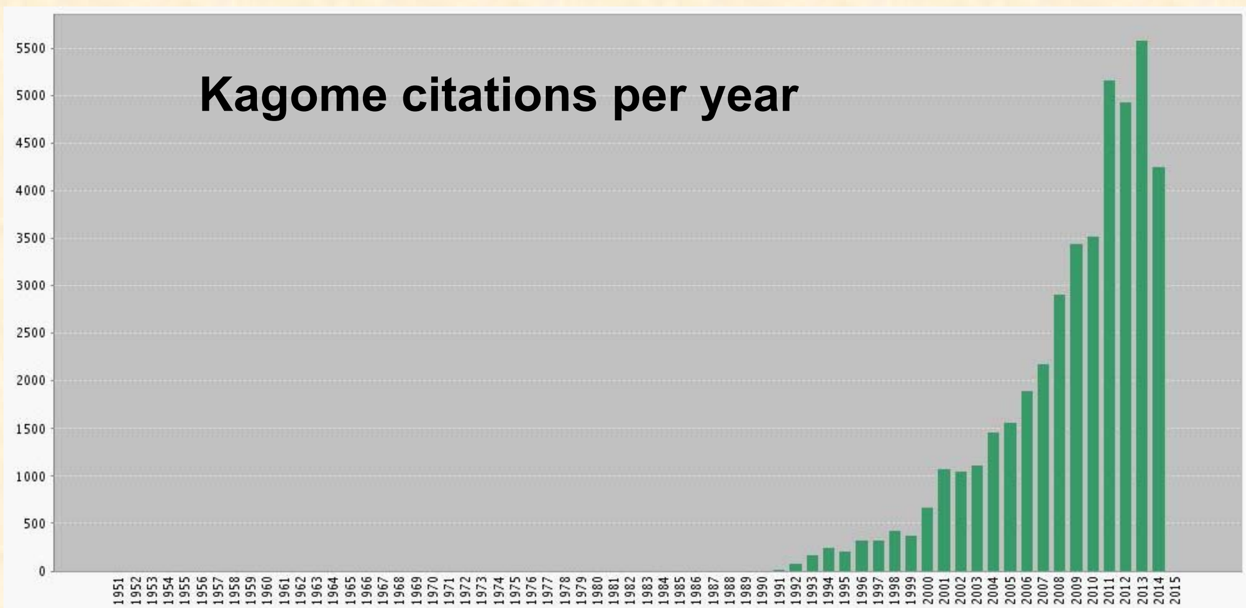
Each triangle forms 120^0 spin structure

Evidently, there is interest

210



5500



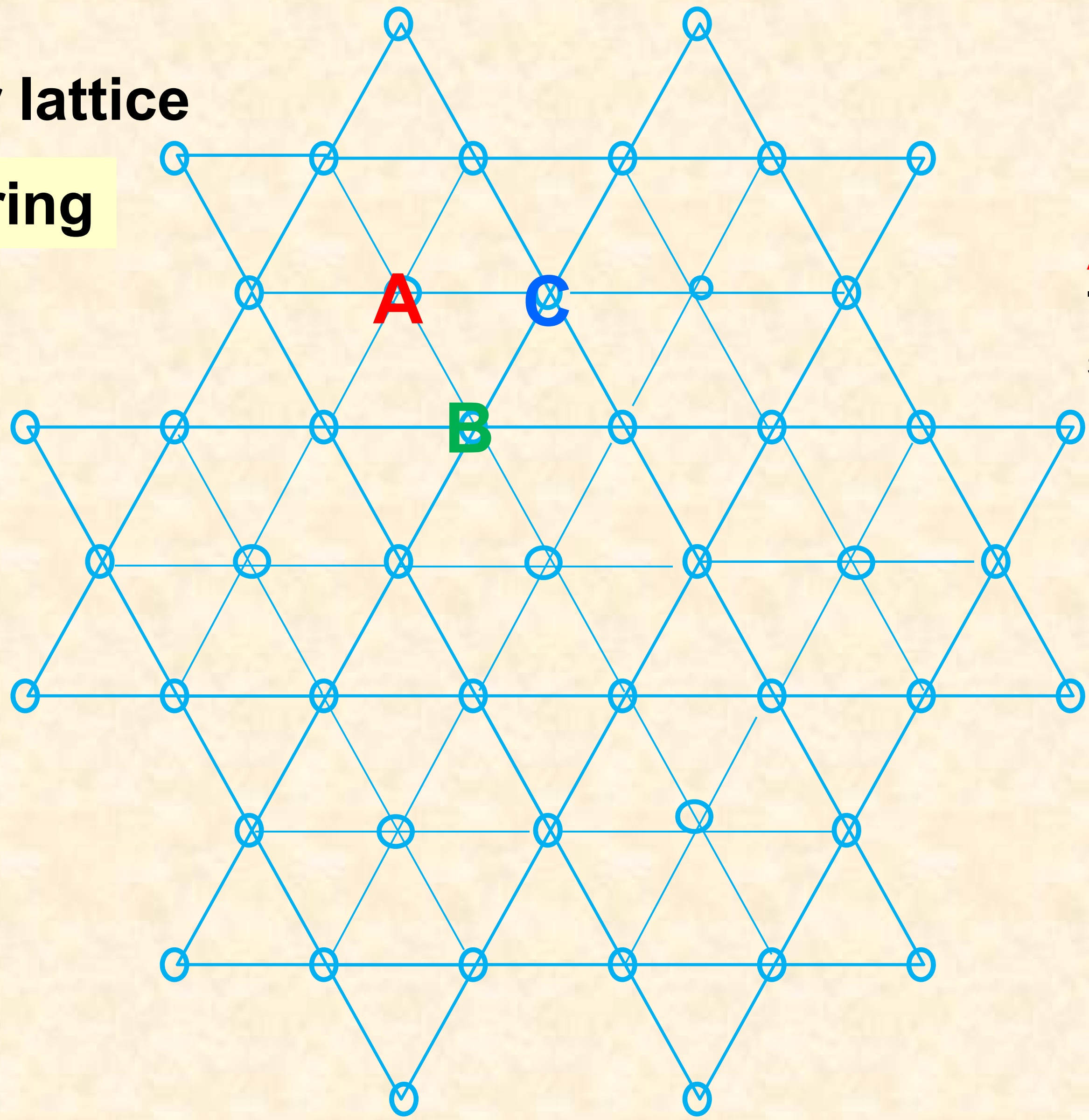
1951 2014

Topic = kagome

What is so interesting about the Kagome?

Triangular lattice

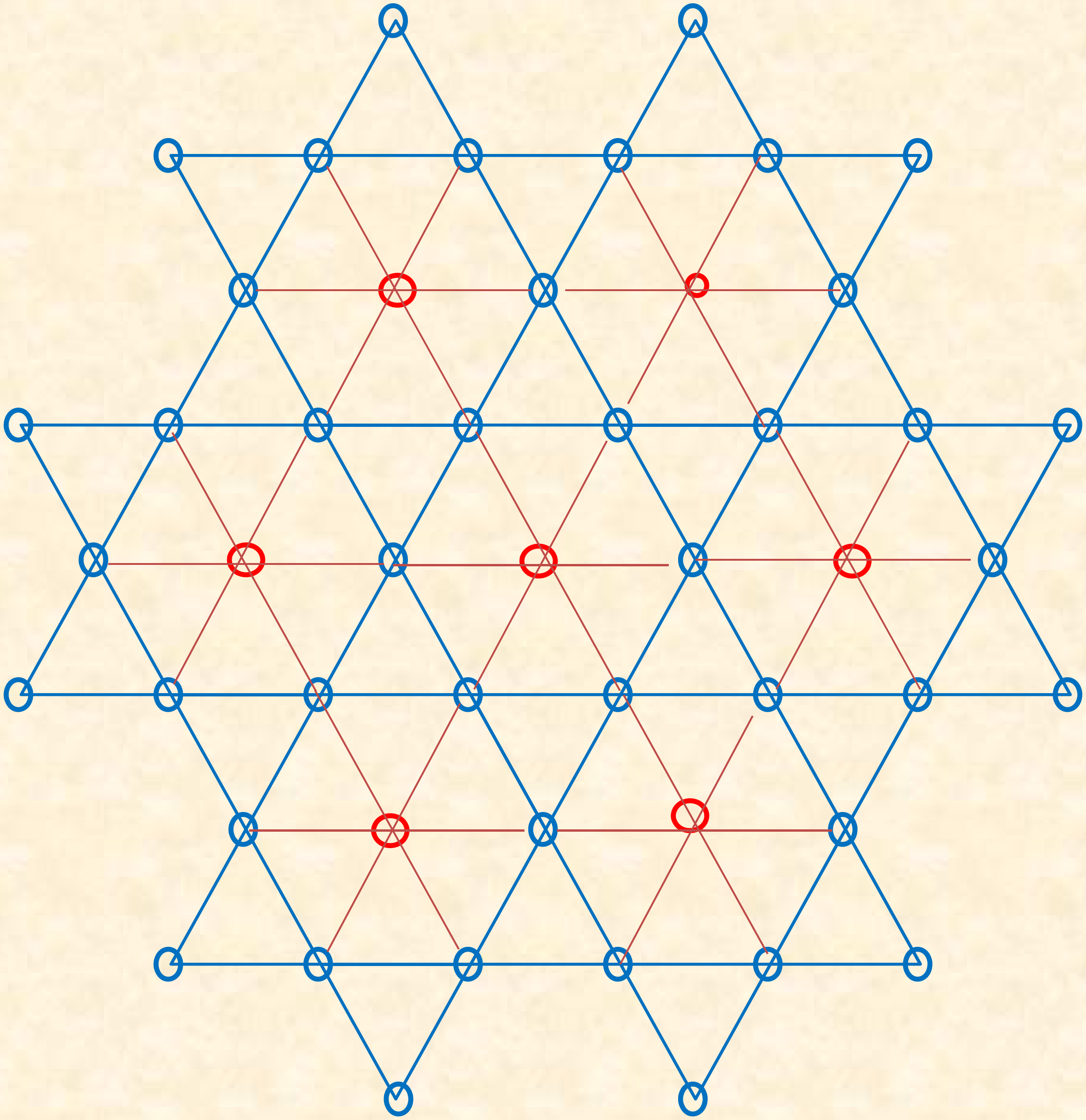
Edge-sharing



A B C
Three sublattice spin structure

from Byron Southern

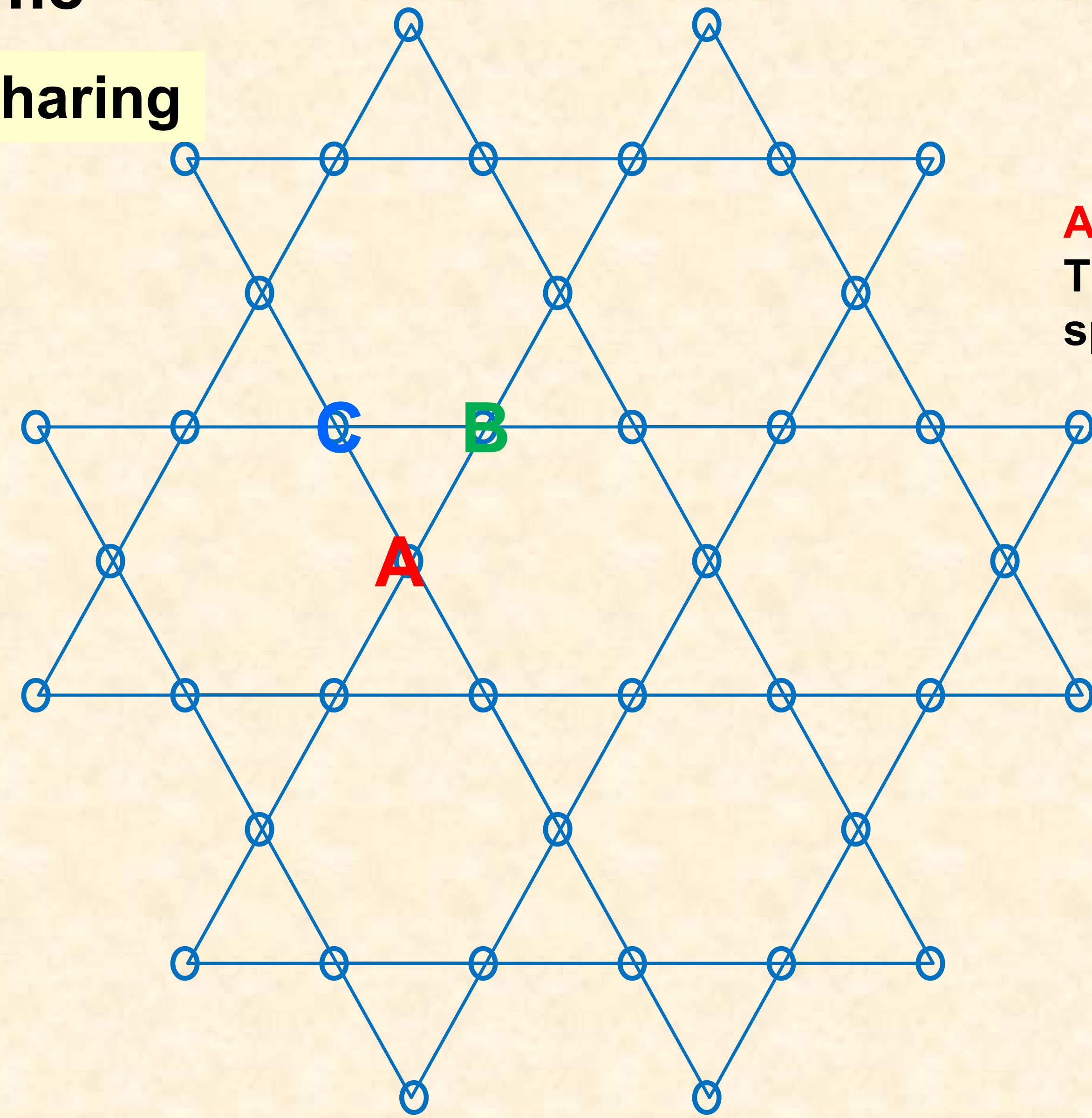
Remove ¼ of the sites



from Byron Southern

Kagome

Corner-sharing

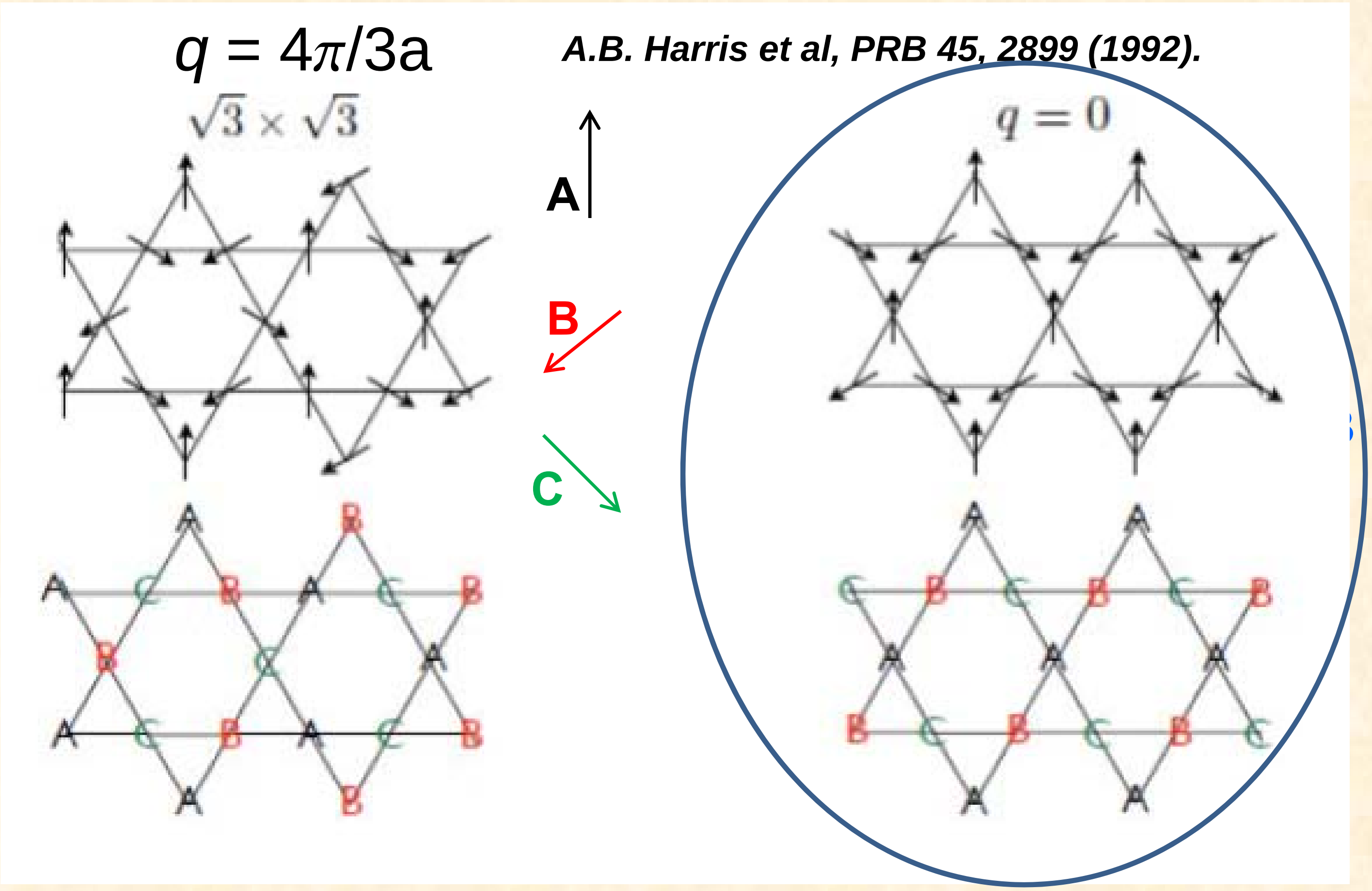


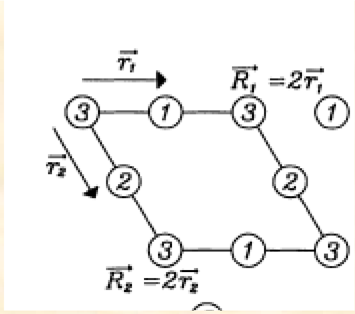
A B C
Three sublattice spin structure

from Byron Southern

Among all the possible ground states are two simple 120^0 arrangements

NN exchange only





Unit cell

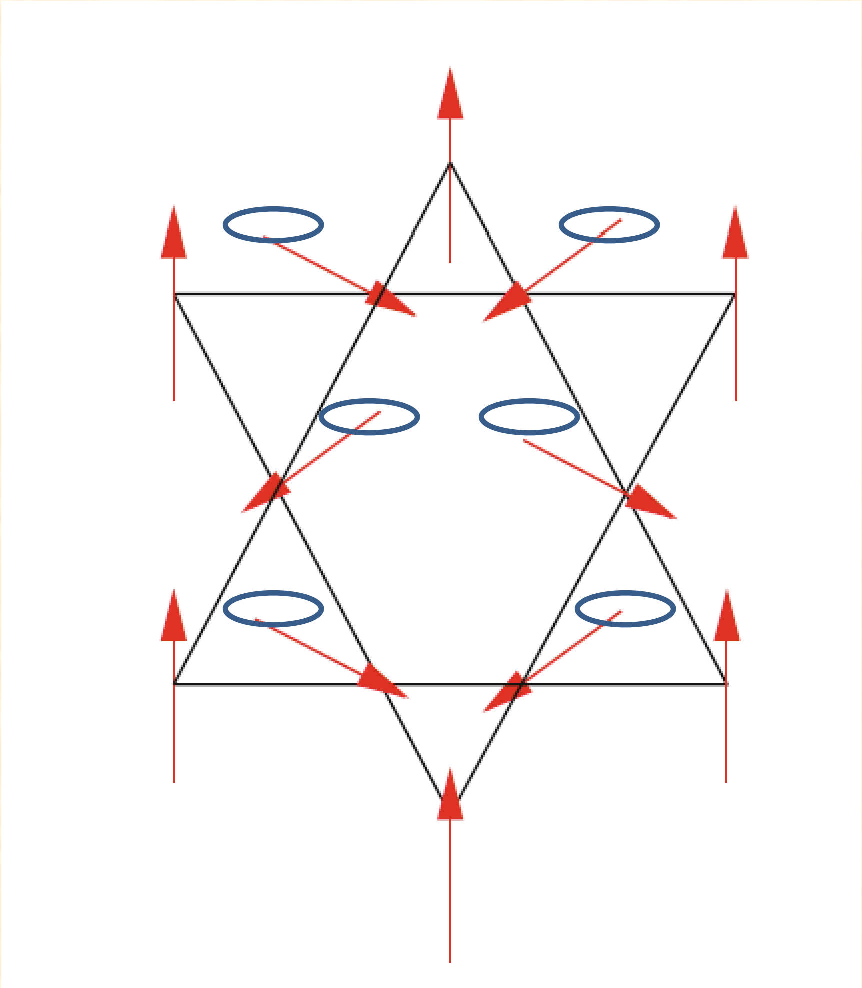
Spin structures are *coplanar*

Period-3 (*ABC* repeated in all 3 directions).
Also describes the ground state of the *Triangular* lattice.

No modulation cell to cell (*AC, AB, BC* repeated)

Macroscopic Degeneracy

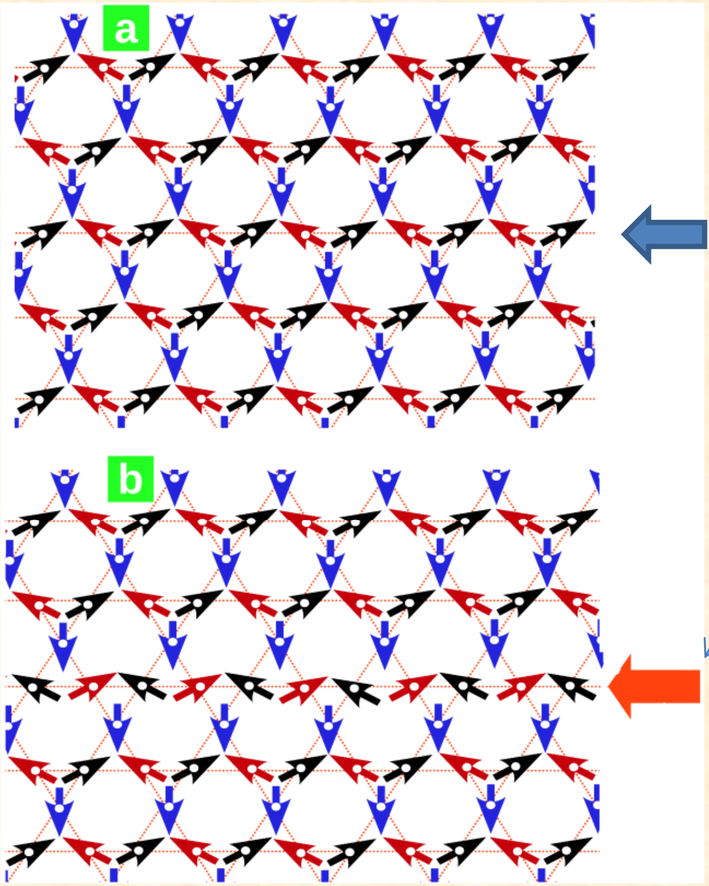
- **Rotate inner spins about the outer vertical spins with no cost in energy.**
- **Need only maintain the 120^0 spin structure *around each triangle***



from Byron Southern

More on Spin Degeneracies of the q=0 structure.

120^0 = 3 ferromagnetic sub-lattice magnetization vectors: black, blue red.



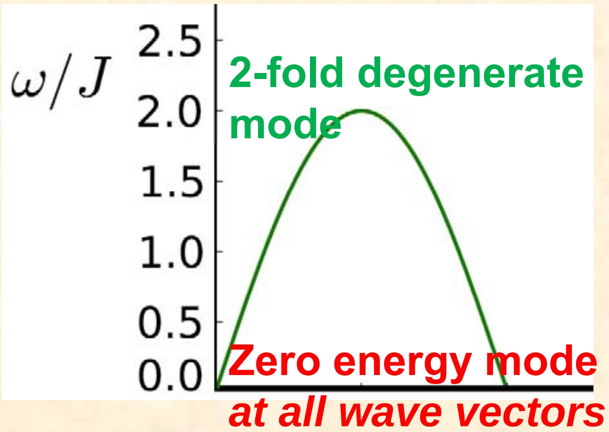
'q=0' magnetic structure ⇒ 3 spins around each triangle at 120^0

In 2D, can interchange two of the sub-lattice vectors in a row (e.g., **black** ⟷ **red**) with no change in energy.

In 3D, can switch direction of two of the sub-lattices vectors in a plane with no change in energy

2D spin waves

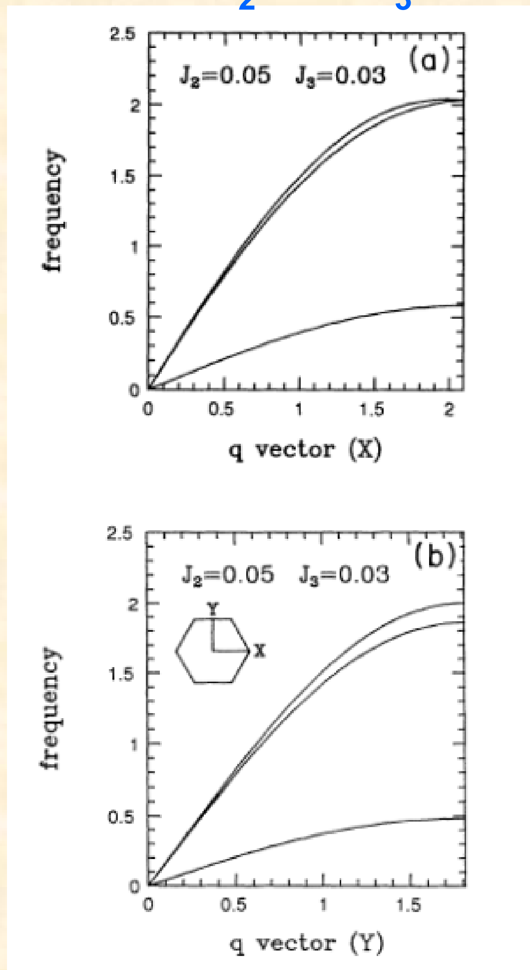
NN exchange only J_1



Associated with spin rotations of independent corner-sharing triangles.

Does not occur for edge-sharing triangles (triangular lattice)

Add J_2 and J_3



A.B. Harris et al, PRB 45, 2889 (1992).

- **2D Heisenberg model exhibits coplanar spin structure.**
- **Macroscopic spin degeneracy at T=0**

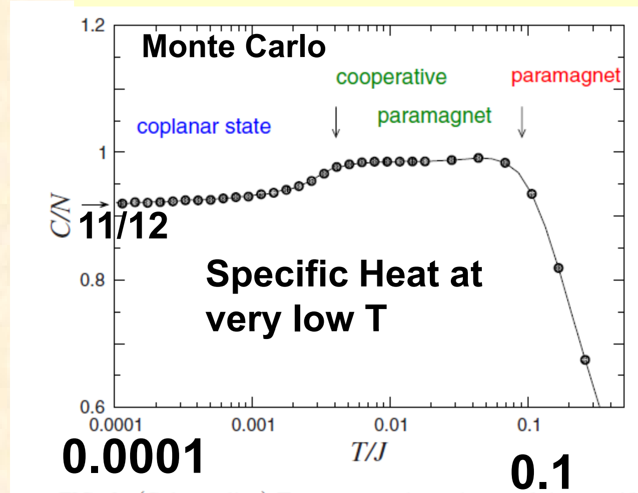


FIG. 3. (Color online) Temperature dependence of the specific heat for a kagome lattice cluster with $L=36$. The horizontal arrow denotes the value $C/N=\frac{11}{12}$. The two vertical arrows indicate boundaries between three different regimes.

M. Zhitomirsky, PRB 78, 094423 (2008).

Monte Carlo simulations of the (3D) FCC Kagomé lattice.

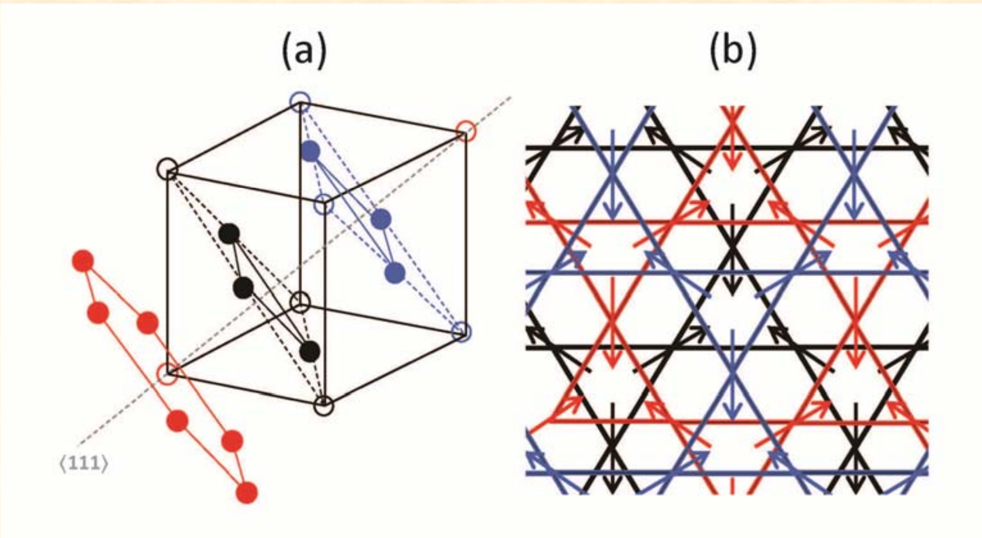
Heisenberg and XY Models with NN Exchange J Only.

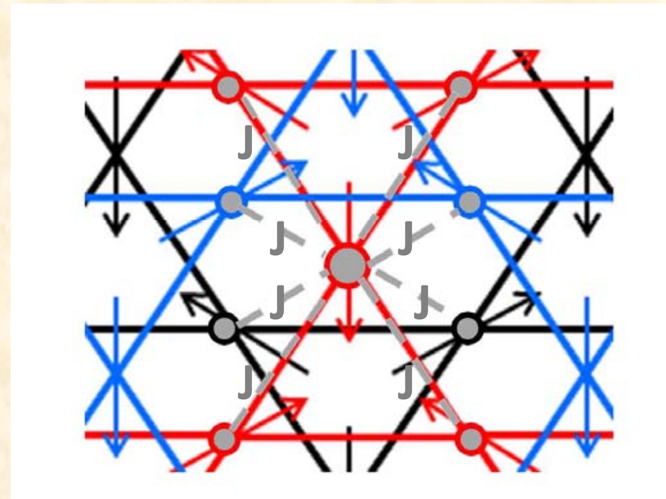
V. Hemmati, M.L. Plumer, J.P. Whitehead, and B.W. Southern, PRB 86, 104419 (2012).

J ⇒ 4 NN in-plane
+ 2 NN above + 2 NN below

ABC stacked

View along <111>





Ground State from simulations:
- Each layer has ‘q=0 spin’ structure.
- 120^0 between all 8 NNs.

- Recall fcc = ABC stacked triangular layers with 12 NN^s.
- Regular fcc AF with NN Heisenberg exchange shows first order transition to a collinear state.

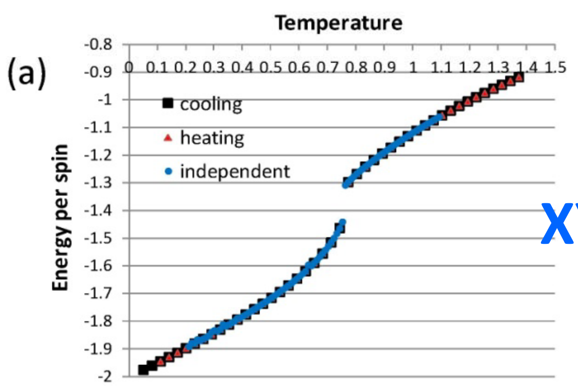
Monte Carlo simulations of the FCC Kagomé lattice.

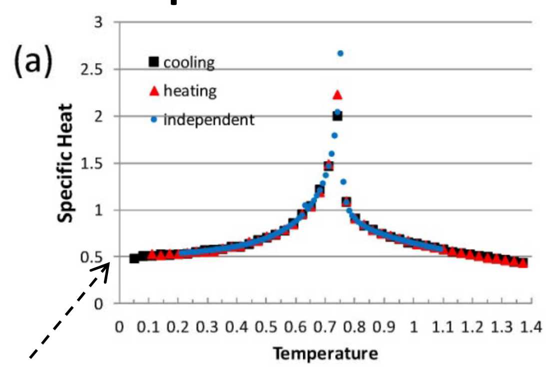
Energy and Specific Heat.

- *Standard Metropolis MC.*
- *LxL* layers of ABC stacked *L* Kagomé planes with PBC.
- *L* = 12, 18, 24, 30, 36, 60 with MCS = $10^6 - 10^7$
- *Cooling*, *Heating and Independent* temperature runs.

Energy **L=24** **Specific Heat**

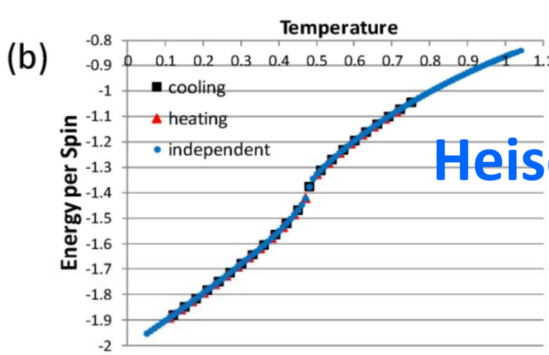
XY

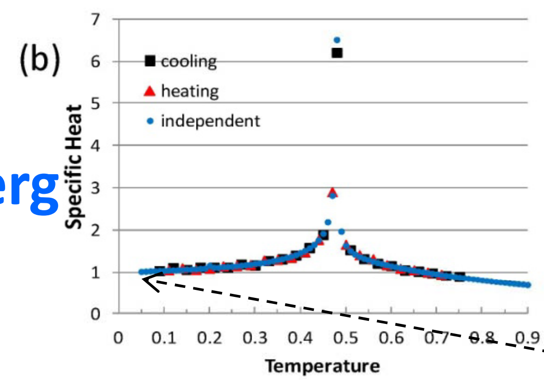




C(T=0) = 5/12 k_B.

Heisenberg





C(T=0) = 11/12 k_B?

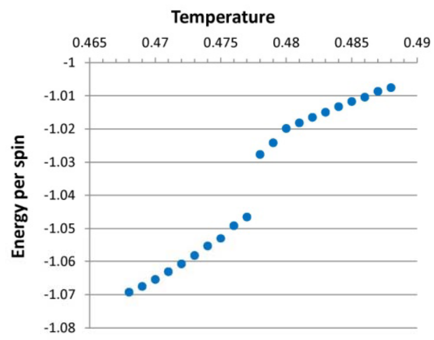
- **All three types of simulations yield equivalent results: same Energy.**
- **For XY model, T_N = 0.760 and appears to be strongly first order.**
- **For Heisenberg model, T_N = 0.476 and could be first order.**

Monte Carlo simulations of the FCC Kagomé lattice.

Order of the Transitions (*First order).*

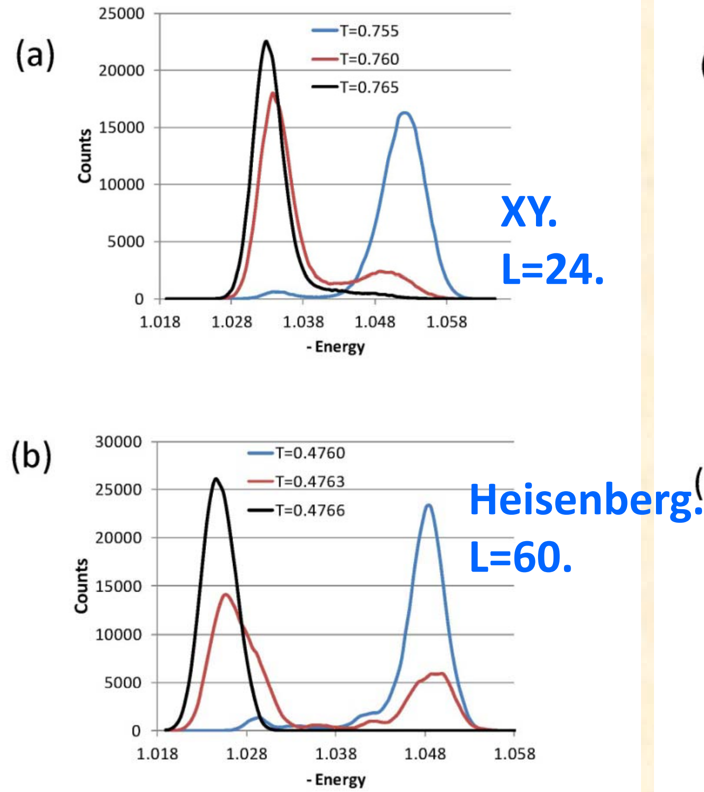
Heisenberg Energy.

L=36.



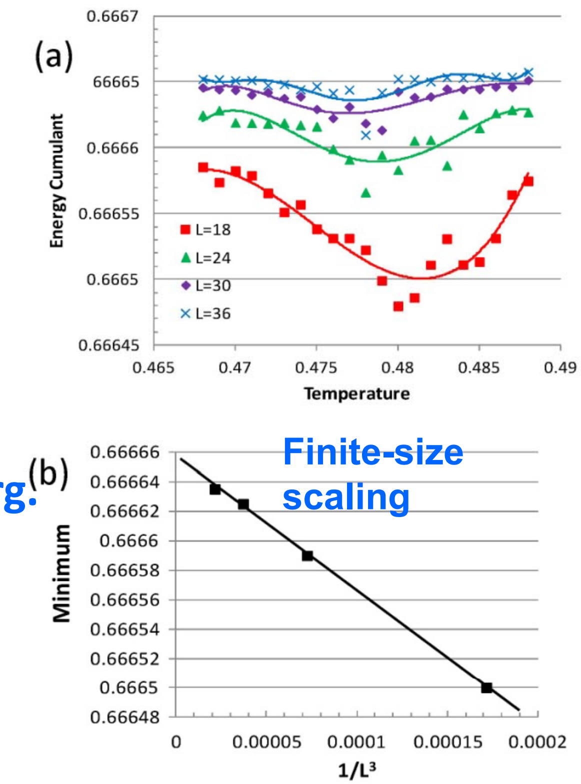
Discontinuity in Heisenberg energy clearer at L=36.

Energy Histograms near T_N



Indicate energy gap between disordered and ordered phases for *both* models.

Binder *Heisenberg* Energy Cumulant near T_N.

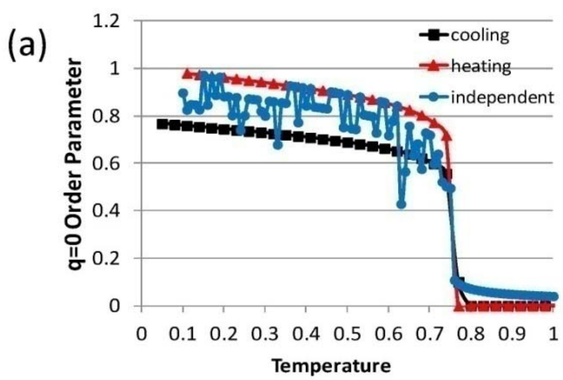


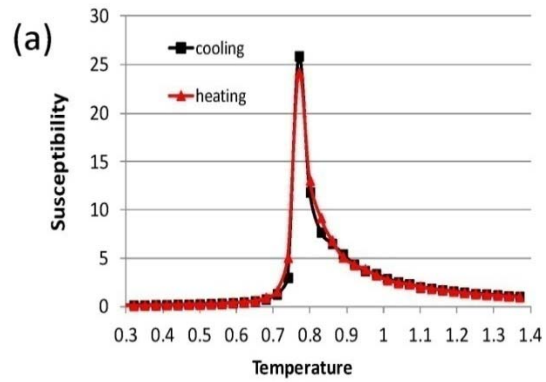
Inconclusive: Could be 2/3, or just close.

Monte Carlo simulations of the FCC Kagomé lattice.

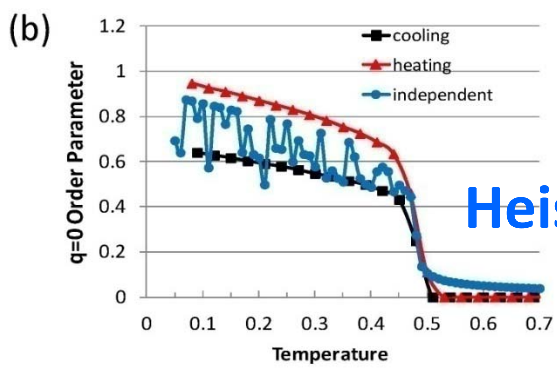
Degeneracy: q=0 Order Parameter and Susceptibility.

Order Parameter **L=24** **Susceptibility**

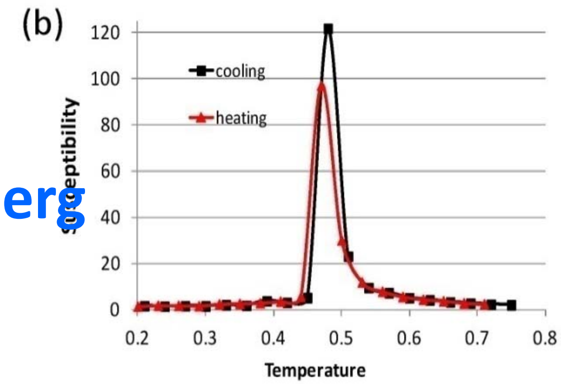




XY



Heisenberg



- **Heating runs start at T=0 from fully order q=0 state.**
- **Cooling runs start at high T with random config.**
- **Independent T runs start with a random config at each T.**

- **Order Parameter and Susceptibility show strong dependence on simulation mode (heating, cooling or independent temperature) and order parameter fluctuates between values for indep. T runs, *in contrast with energy and specific heat.***
- **This feature is due to Kagomé-lattice spin degeneracies**

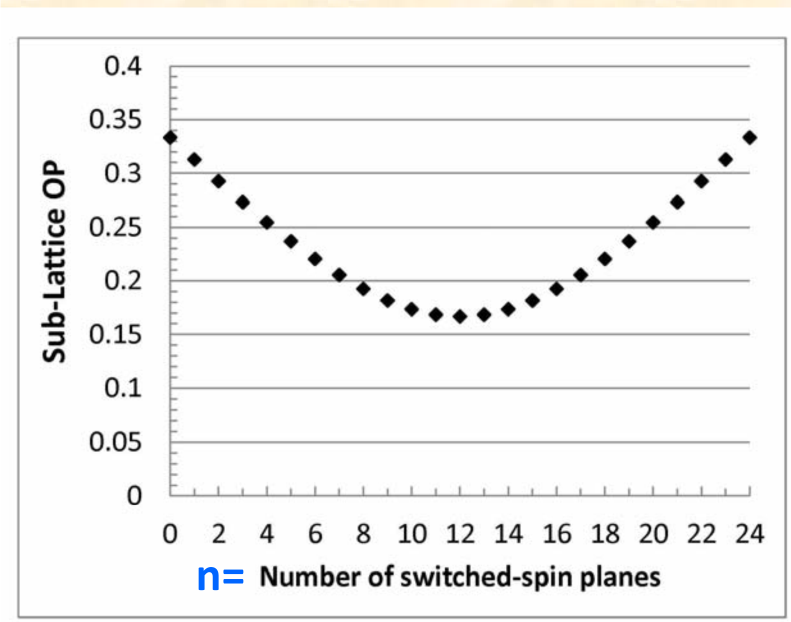
Monte Carlo simulations of the FCC Kagomé lattice.

Spin Degeneracies.

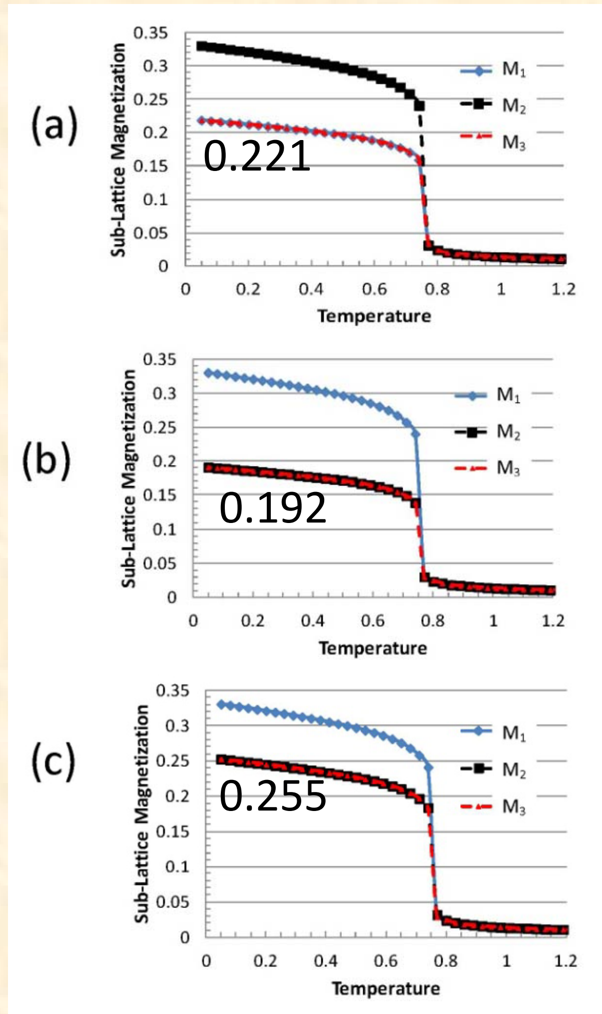
Enumerate all possible switches for L=24 and determine size of ground-state sub-lattice moment:

$$M_\eta = \frac{\sqrt{\left(\frac{1}{4}\,L^3 - \frac{3}{2}\,n\right)^2 + \left(\frac{\sqrt{3}}{2}\,n\right)^2}}{\frac{3}{4}\,L^3}$$

$L^3/8 \leq n \leq L/2$



Three different MC *cooling* runs (different random initial configuration).



- **One sub-lattice is always fully saturated.**
- **The other two randomly approach (T=0) predicted values.**

Summary of Monte Carlo simulations of the (3D) FCC Kagomé lattice.

Heisenberg and XY Models with NN Exchange J Only.

1. Degeneracies persist in 3D.

2. Transitions appear to be first order.

- Mean field theory predicts continuous.

3. Items one and two above are related?

Monte Carlo simulations of the fcc Kagomé lattice. Add cubic anisotropy

Martin Leblanc. PhD student

M.D. Leblanc, M.L. Plumer, J.P. Whitehead, and B.W. Southern, PRB 89, 094406 (2013).

L. Szunyogh et al PRB 79, 020403 (2009)

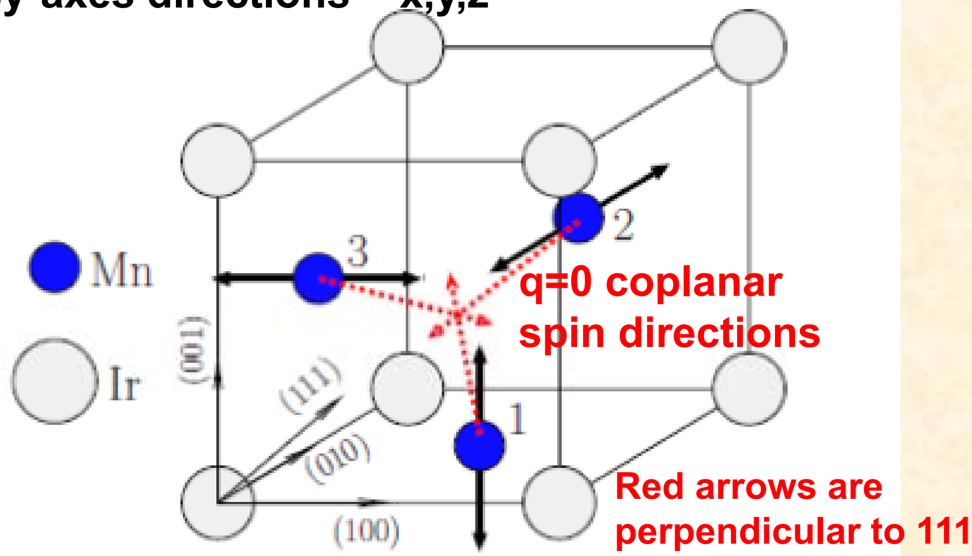
$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij}\vec{S}_i\vec{S}_j - \frac{K_{\text{eff}}}{2}\sum_i (\vec{S}_i\cdot\vec{n}_i)^2,$$

$$\vec{n} = \hat{x}, \hat{y}, \hat{z}$$

Effective local anisotropy axes (similar to spin-ice pyrochlore tetrahedrons).

In case of Hamiltonian with only exchange interactions and K-term there are 8 degenerate ground states.

Easy-axes directions = x,y,z



Mn moments are *not* aligned in the easy-axes directions for the coplanar q=0 spin structure.

Impact of cubic anisotropy

- Distortion of the 120^0 spin structure
- Induced uniform magnetization M_f along 111

T=0

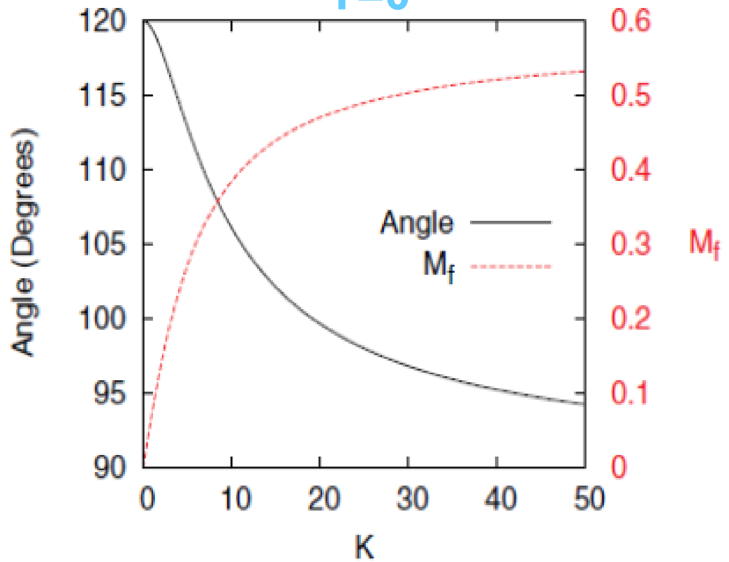
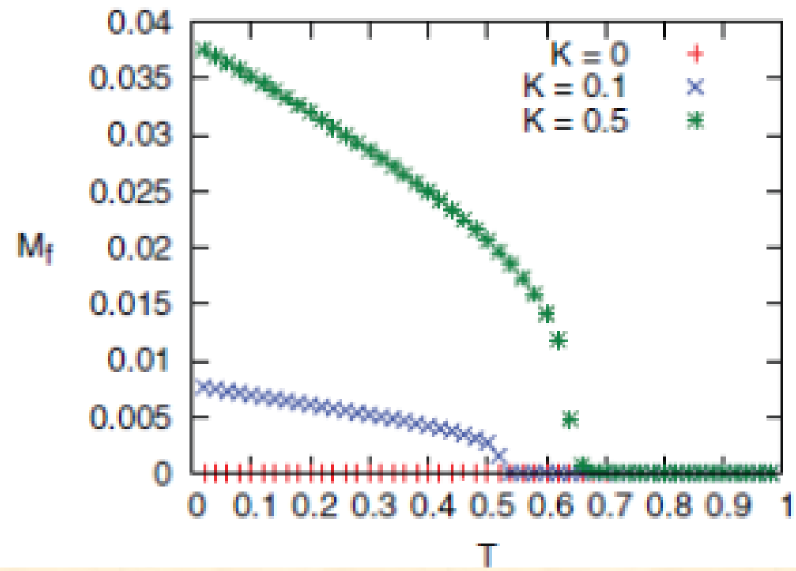


FIG. 3. (Color online) Interspin angle and magnetic moment at zero temperature vs anisotropy strength.

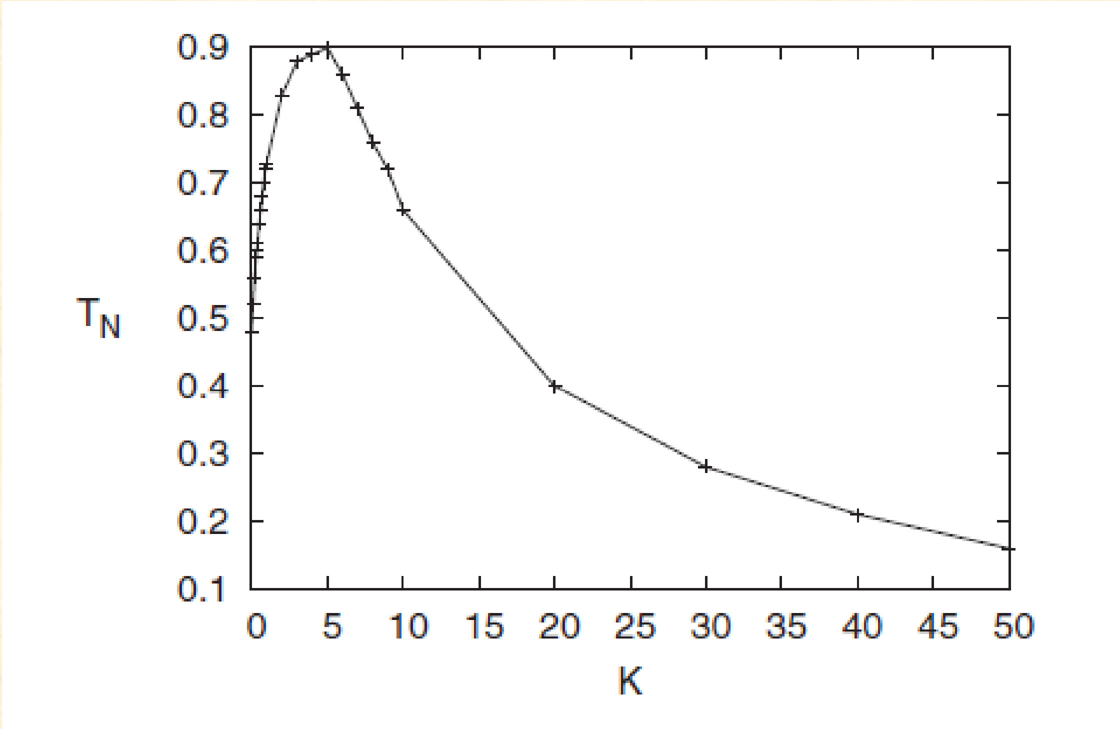


$K \rightarrow \infty$: $S_A||x$, $S_B||y$, $S_C||z$

Impact of cubic anisotropy

$K \to \infty$: $S_A || x$, $S_B || y$, $S_C || z$

Exchange term in energy is reduced to zero: No LRO.



Impact of cubic anisotropy

Now only 8 degenerate 111 ground states (8 directions of M).

- **K>0 removes the sub-lattice switching degeneracy**

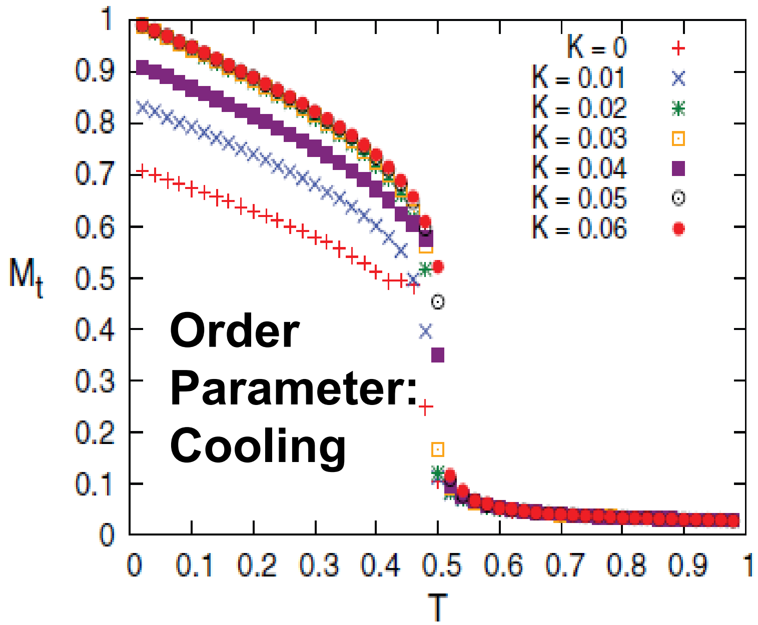
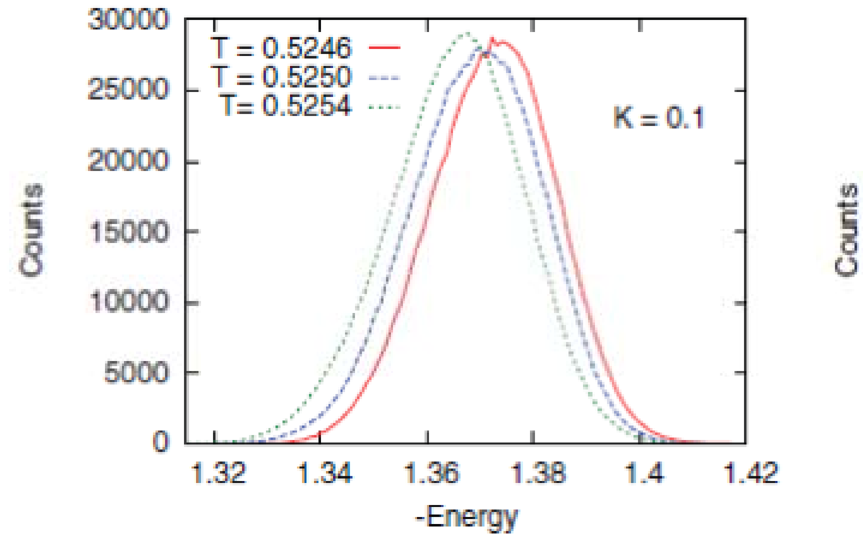


FIG. 4. (Color online) Sublattice magnetization order parameter vs temperature for small values of K from simulations with $L = 24$.

- **K>0 drives transition to be continuous**

Energy histograms near T_N

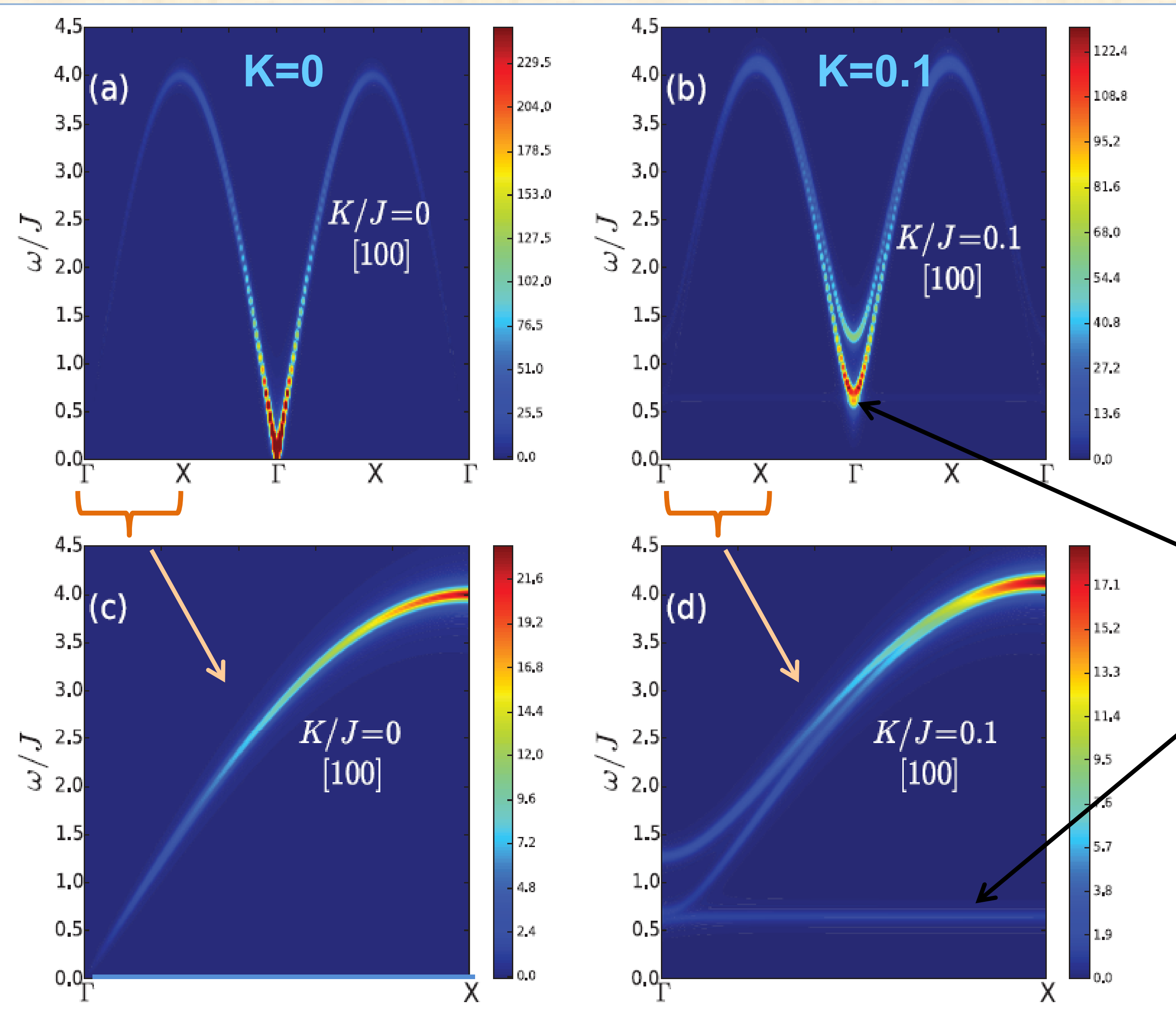


Spin Waves and Inelastic Scattering Intensity.

Impact of cubic anisotropy

DFT: K ~ 0.1

M.D. Leblanc, B.W. Southern, M.L. Plumer, and J.P. Whitehead, PRB 90, 144403 (2014).



For K=0, there remains a zero energy mode but only for q || [100]

For K>0 zero energy modes acquire a gap

Impact of cubic anisotropy

1. Degeneracies of the 120^0 spin structure are removed.

2. A finite uniform magnetization along 8 possible <111> directions is induced.

3. Transition is driven to be continuous (similar to pyrochlores).

And now,

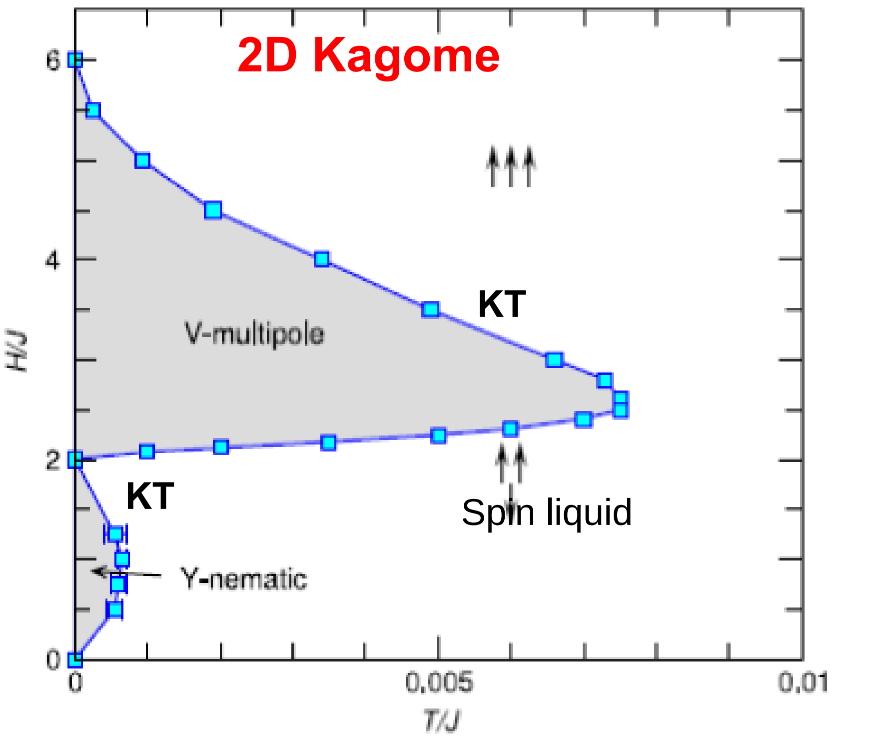
a series of preliminary MC results:

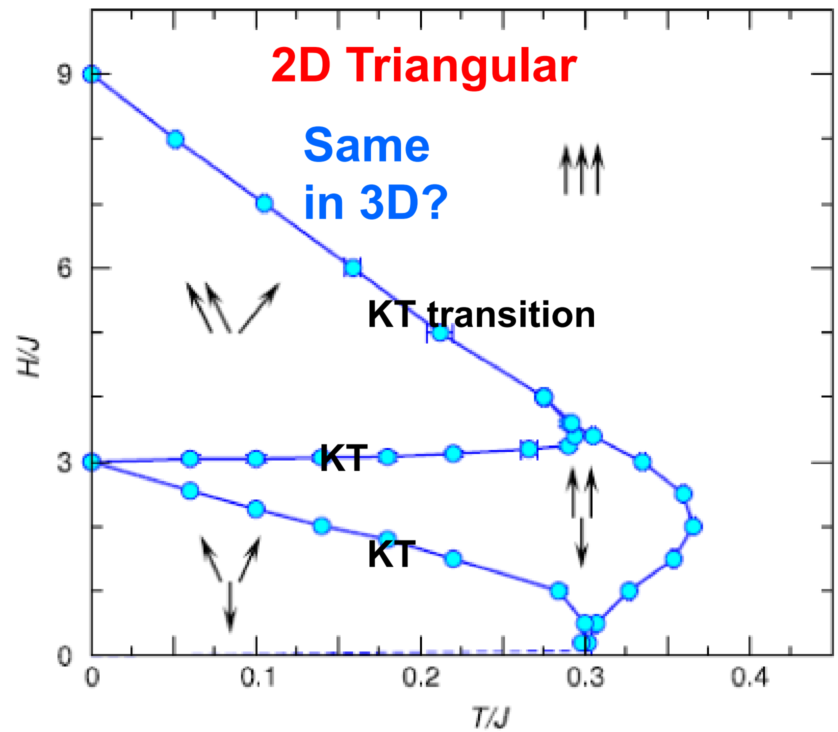
- **H-T phase diagram**
- **Thin Films**
- **2D Dipole interactions only**

Magnetic Field – Temperature phase diagram.

Monte Carlo 2D Heisenberg model (no anisotropy)

H. Hawamura et al JPSJ 54, 4530 (1985).
Gvozdikova et al JPCM 23, 164209 (2011).



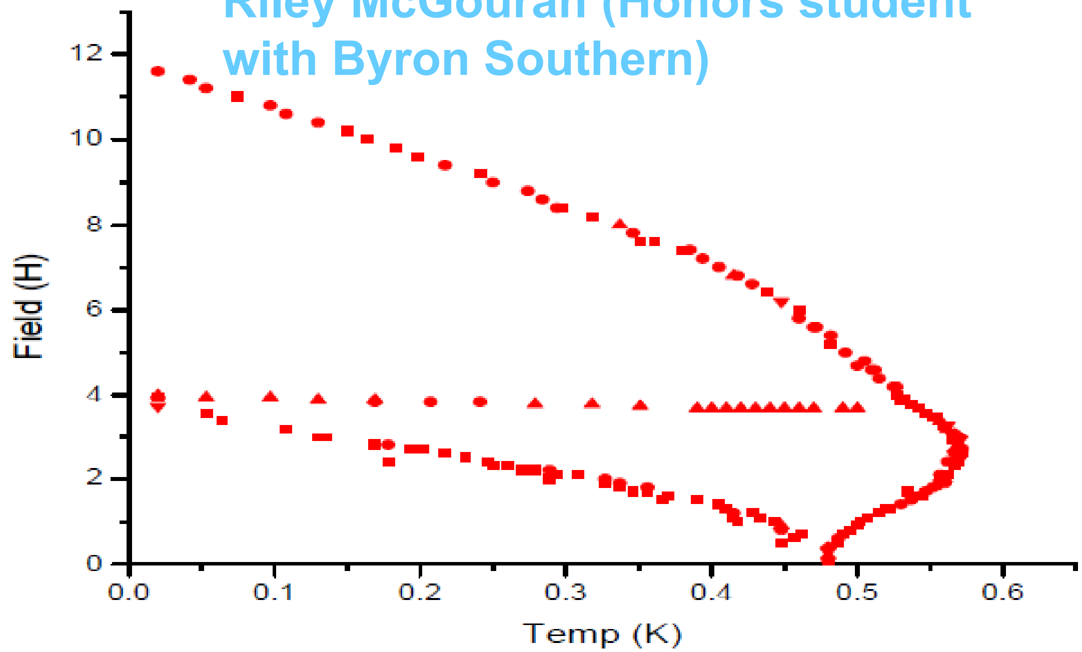


No long range dipolar order at H=0

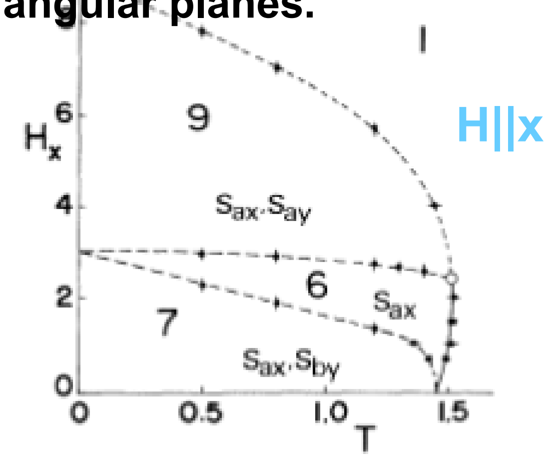
H-T Phase Diagram: 3D FCC Kagome.

- Very different from 2D Kagome.
- Very similar to 2D (and 3D?) Triangular. WHY?

Riley McGouran (Honors student with Byron Southern)



XY model. 3D hexagonal lattice. ***Ferromagnetic*** **interactions between triangular planes.**



Plumer, Mailhot and Caillé, PRB 1993

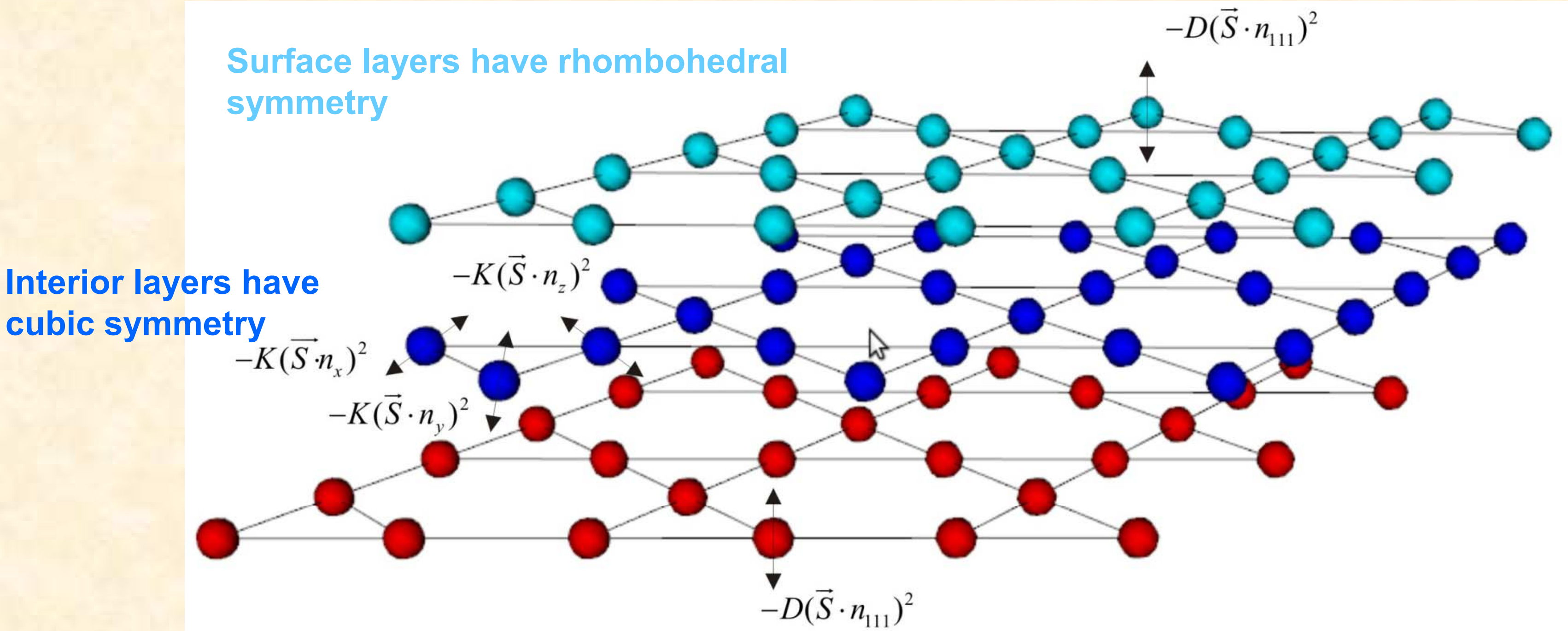
- More simulations in progress: Add anisotropy.

Thin Films: Impact of surface anisotropy $-D(\vec{S} \bullet \hat{n}_{111})^2$

Hennadii Yerzhakov. MSc student

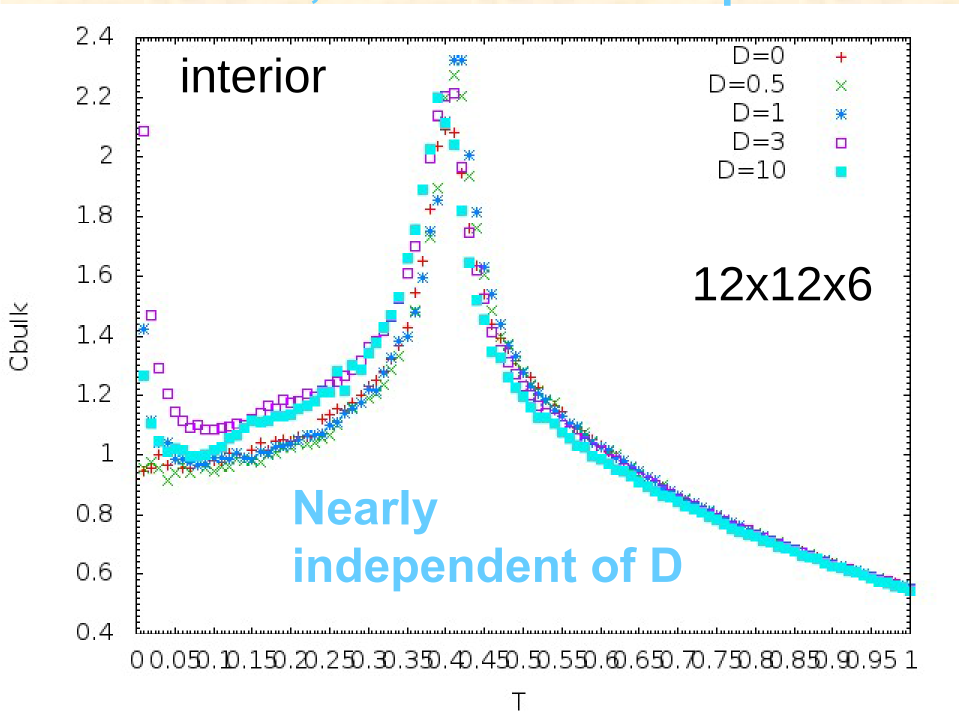
- Interior spins are subject to cubic symmetry and cubic anisotropy
- Surface spins have rhombohedral symmetry and axial anisotropy
- Surface anisotropy can be *very* large

6x3

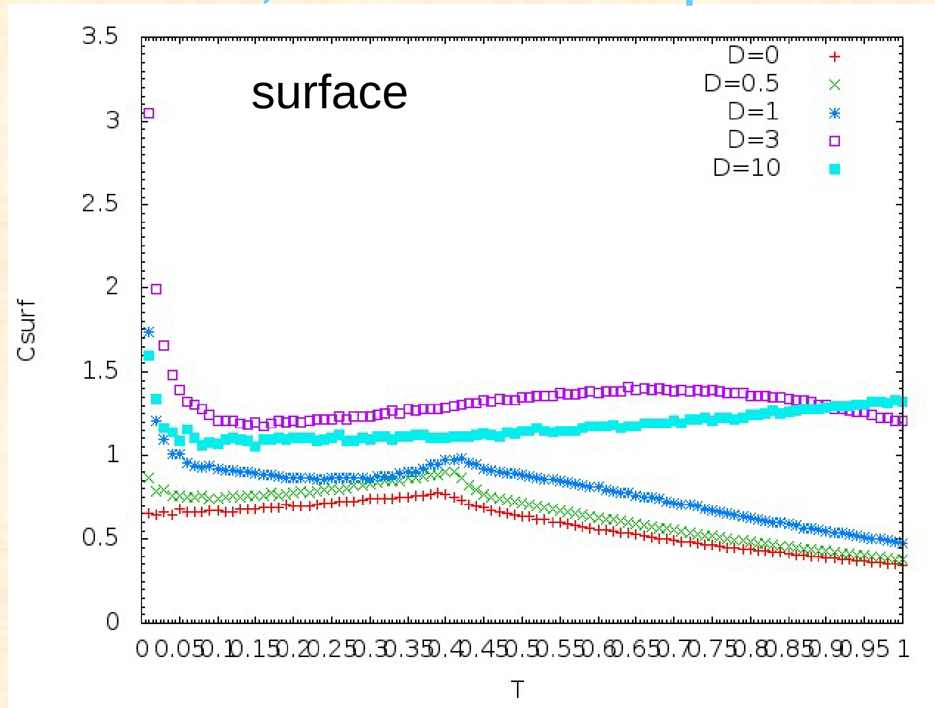


Specific Heat: Interior and Surface spins. Vary D

K=0.1, D=0 for Interior spins.



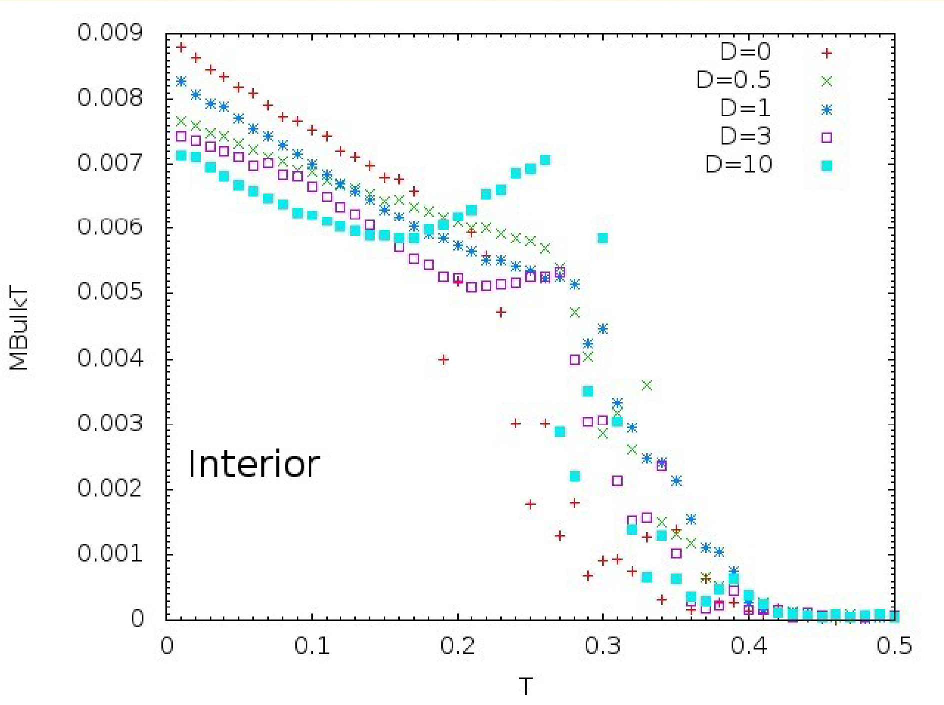
K=0, D>0 for Surface spins.

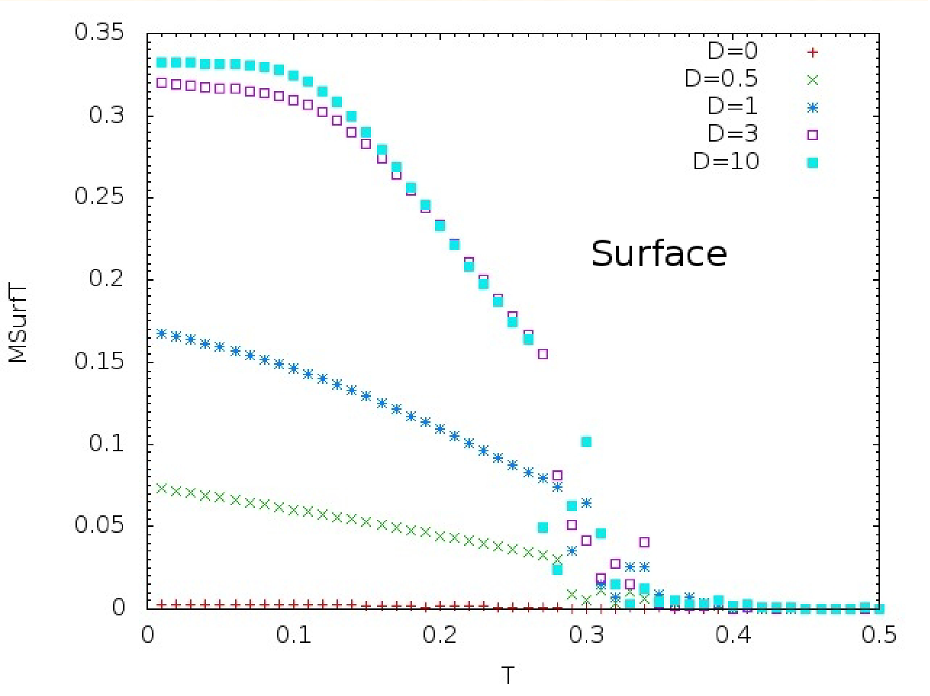


At large D surface spins do not show a sharp peak in specific heat

Magnetization

12x12x6

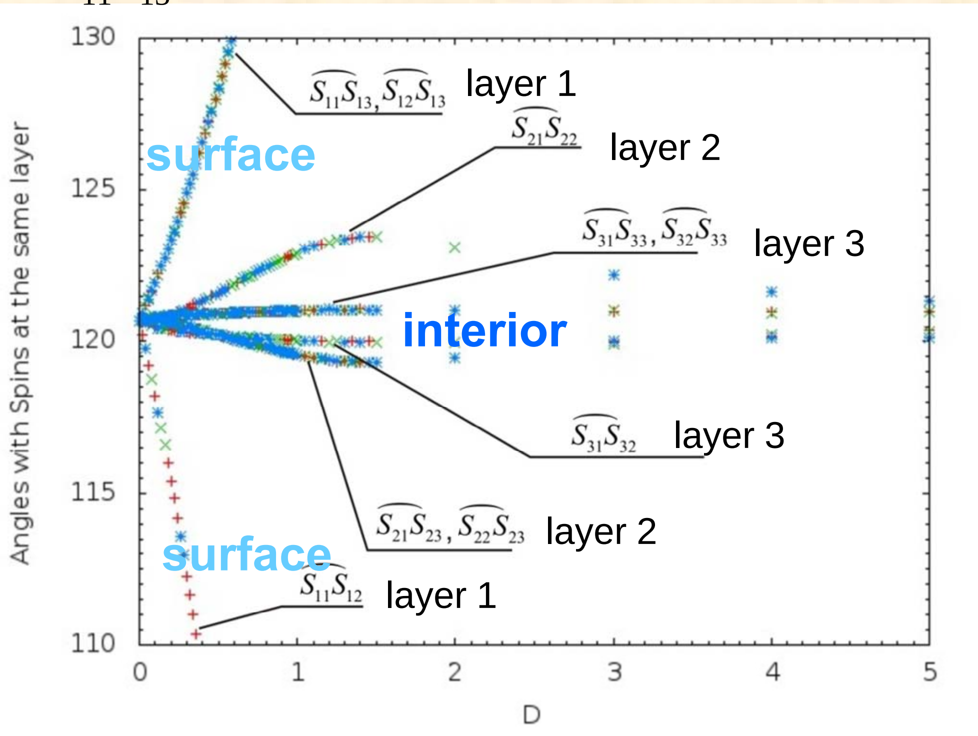




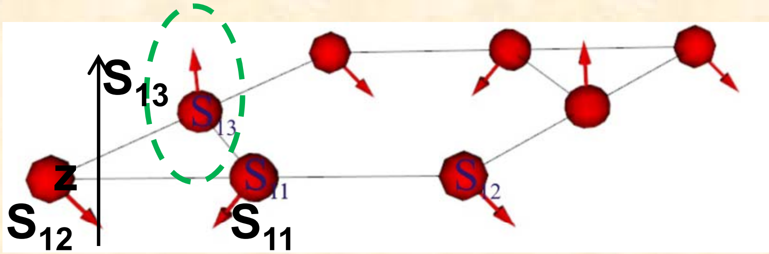
Magnetization in *Interior* is very small for any D, while at the *Surface* it almost follows order parameter (not shown).

Effect of D on Inter-spin angles and degeneracy

$\widehat{S_{11}S_{13}}$ = angle between spins 1 and 3 in a triangle on layer 1



D causes ***one*** of the three spins in a surface triangle to point up (down), the other two mostly down (up).



Distortion of the 120⁰ spin structure mostly at surface.

- When D=0 there are 8 possible ground states (four 111 planes).
- When D >0 one (111) plane is selected (that for which **D•K** is maximum).
- The ***one*** spin up/down can be selected from 3 spins on a triangle, leaving a degeneracy of 6.

Dipole Interactions

$$E = \sum_{\substack{pairs \\ ij}} \frac{\vec{m}_i \cdot \vec{m}_j}{r^3{}_{ij}} - \frac{3(\vec{m}_i \cdot \vec{r}_{ij})(\vec{m}_j \cdot \vec{r}_{ij})}{r^5{}_{ij}}$$

Mostly ignored in *basic* research on magnetic systems

- Weak compared to exchange (BUT they are long range)
- Mostly cancel out in 3D antiferromagnets.

However, they can be important for

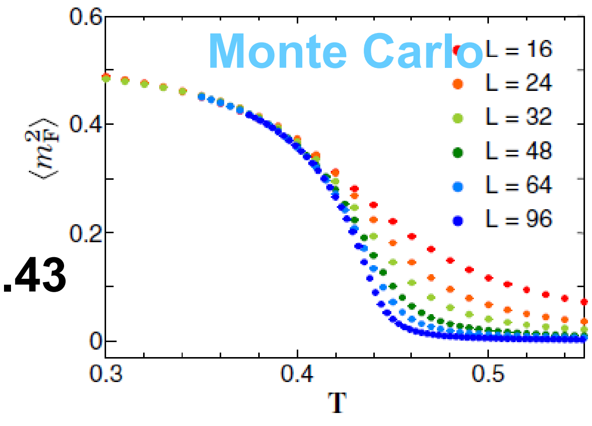
- Ferromagnets
- AFs on a frustrated lattice (e.g., pyrochlore spin ice)
- AF in thin films where geometry limits cancelation effects.

2D Kagome with only Dipole interactions

Y. Tomita, JPSJ 78, 114004 (2009)

$$E = \sum_{\substack{pairs \\ ij}} \frac{\vec{m}_i \cdot \vec{m}_j}{r^3_{ij}} - \frac{3(\vec{m}_i \cdot \vec{r}_{ij})(\vec{m}_j \cdot \vec{r}_{ij})}{r^5_{ij}}$$

Dipole interaction is long-ranged (unlike exchange).



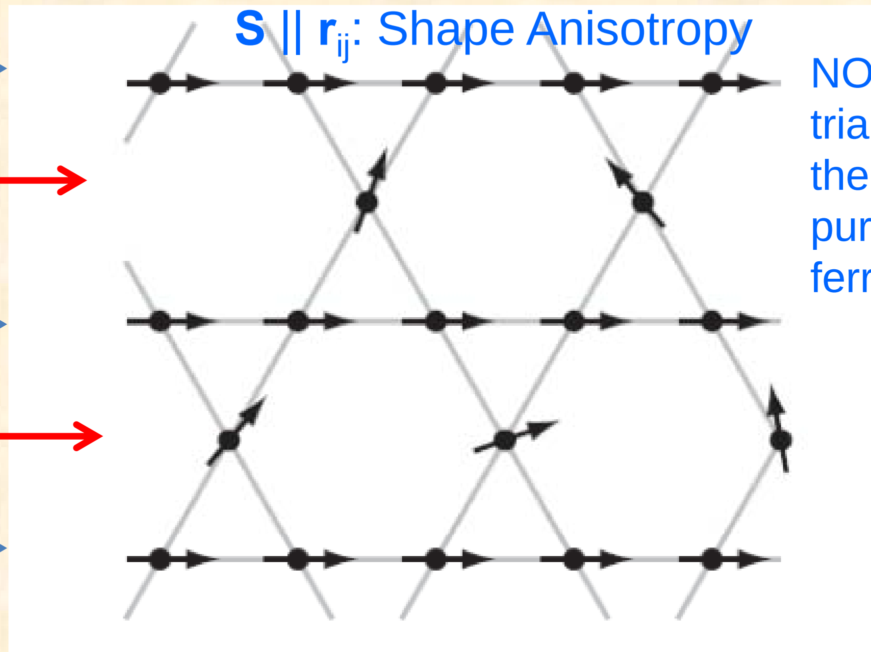
T_c=0.43

Fig. 17. (Color online) Ferromagnetic order parameters for different system sizes plotted as functions of temperature.

Ferromagnetic chains:

Disordered chains

Spins align along lattice directions (shape anisotropy)



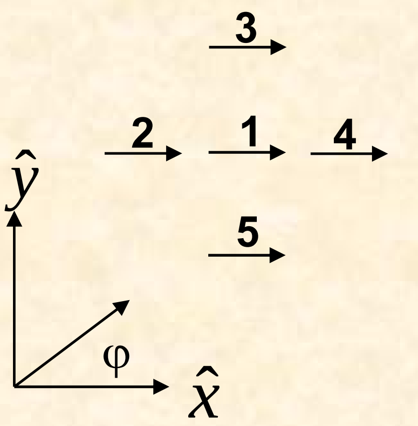
NOTE: For the triangular lattice, the spin order is purely ferromagnetic

Shape Anisotropy: A simple argument

- Dipole-dipole interaction (first terms in multipole expansion of magnetostatic energy)

$$E = \sum_{\substack{pairs \\ ij}} \frac{\vec{m}_i \cdot \vec{m}_j}{r^3_{ij}} - \frac{3(\vec{m}_i \cdot \vec{r}_{ij})(\vec{m}_j \cdot \vec{r}_{ij})}{r^5_{ij}}$$

- Consider energy of <u>dipole</u> <u>1</u> (lattice spacing $a=r_{ij}$) on a square lattice



$$\frac{a^3 E}{m^2} = (\cos\phi_{12} + \cos\phi_{13} + \cos\phi_{14} + \cos\phi_{15})$$

$$-3(\cos\varphi_1 \cos\varphi_2 + \cos\varphi_1 \cos\varphi_4 + \sin\varphi_1 \sin\varphi_3 + \sin\varphi_1 \sin\varphi_5)$$

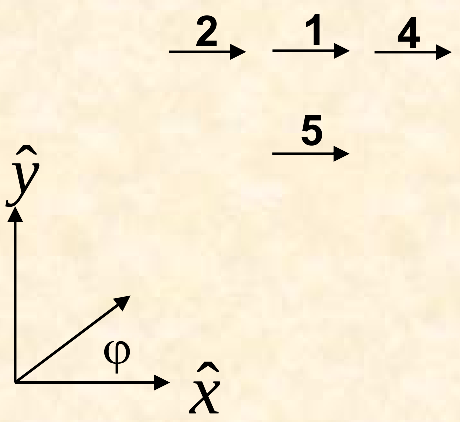
Put $\phi_i \equiv \phi$

$$= 4 - 3(2\cos^2\varphi + 2\sin^2\varphi) = -2$$

Completely isotropic.

Shape Anisotropy: A simple argument

- Create edge (remove 3)



$$\frac{\boldsymbol{a}^3\boldsymbol{E}}{\boldsymbol{m}^2} = (\cos\phi_{12} + \cos\phi_{14} + \cos\phi_{15})$$
$$-3(\cos\varphi_1 \cos\varphi_2 + \cos\varphi_1 \cos\varphi_4 + \sin\varphi_1 \sin\varphi_5)$$

Put $\phi_i \equiv \phi$

$$= 3 - 3(2\cos^2\varphi + \sin^2\varphi) = -3\cos^2\varphi$$

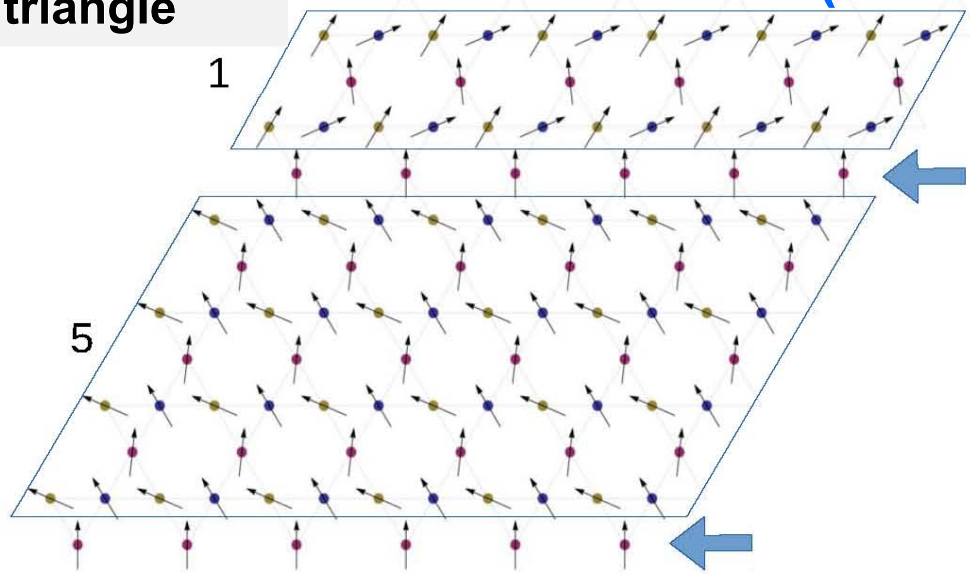
Uni-axial anisotropy induced by edge. Energetically favorable for spins to align parallel to the edge and to neighboring spins.

Ground State: T=0

Effective Field Results

Shane Holden (BSc honors student)

Sublattices A, B, C around a triangle

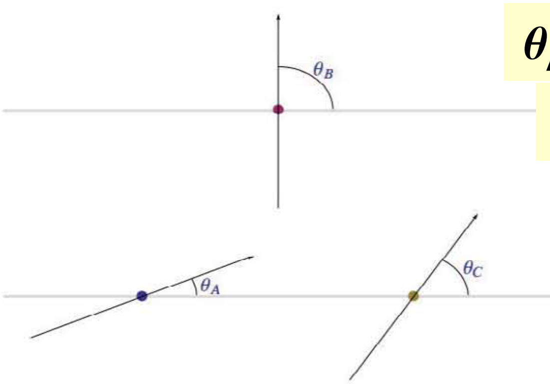


- Results show domains of a 3-sublattice system
- Each domain corresponds to one of six possible ground state
- Sublattices become ordered at low-temperatures

Domain	θ_A	θ_B	θ_C
1	23.6113	96.3887	60.0000
2	203.6114	276.3887	240.0000
3	36.3887	0.0000	-36.3887
4	216.3887	180.0000	143.6114
5	120.0000	83.6113	156.3886
6	300.0000	263.6113	336.3887

$\theta_A + \theta_B + \theta_C = n\pi$

One of $\theta_i = n\pi/3$



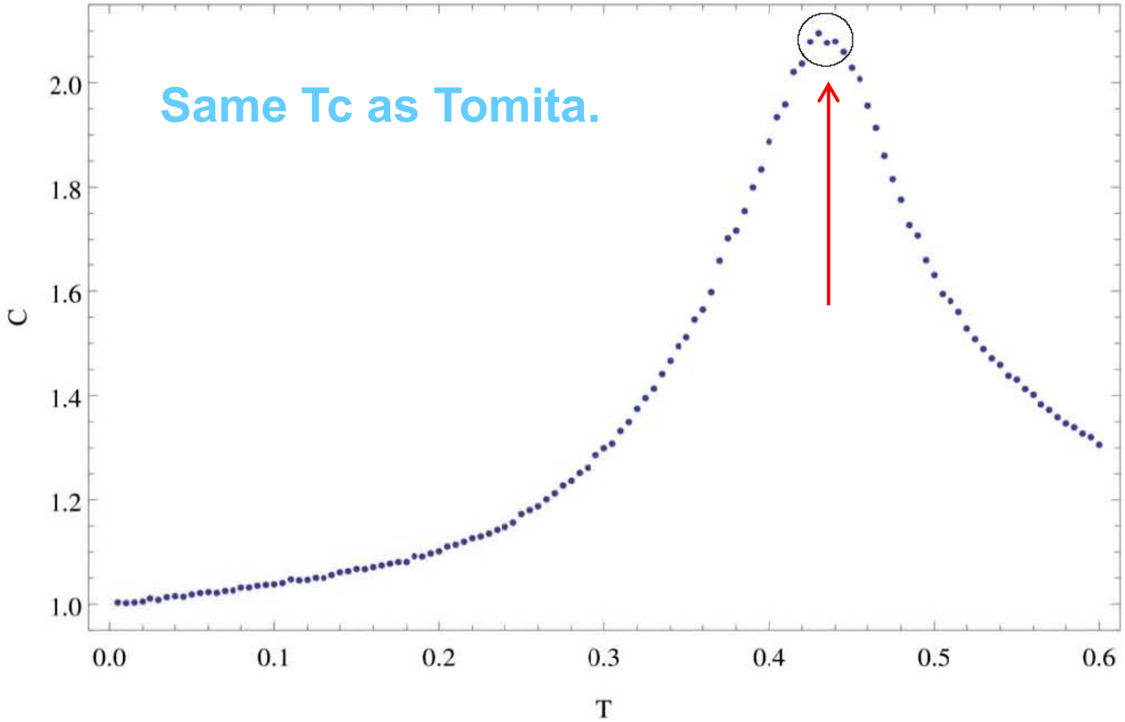
Relation between domains

Domain	θ_A	θ_B	θ_C	$\theta_A+\theta_B+\theta_C$
1	$x = 23.6113$	$120 - x$	60	1×180
2	$180 + x$	$-120 - x$	-120	-1×180
3	$y = 36.3887$	0	$-y$	0×180
4	$180 + y$	180	$-180 - y$	1×180
5	120	$z = 83.6113$	$240 - z$	2×180
6	-60	$-180 + z$	$60 - z$	1×180

Metropolis MC Results

- System undergoes a phase transition at T≈0.43 where there is a peak in the specific heat:

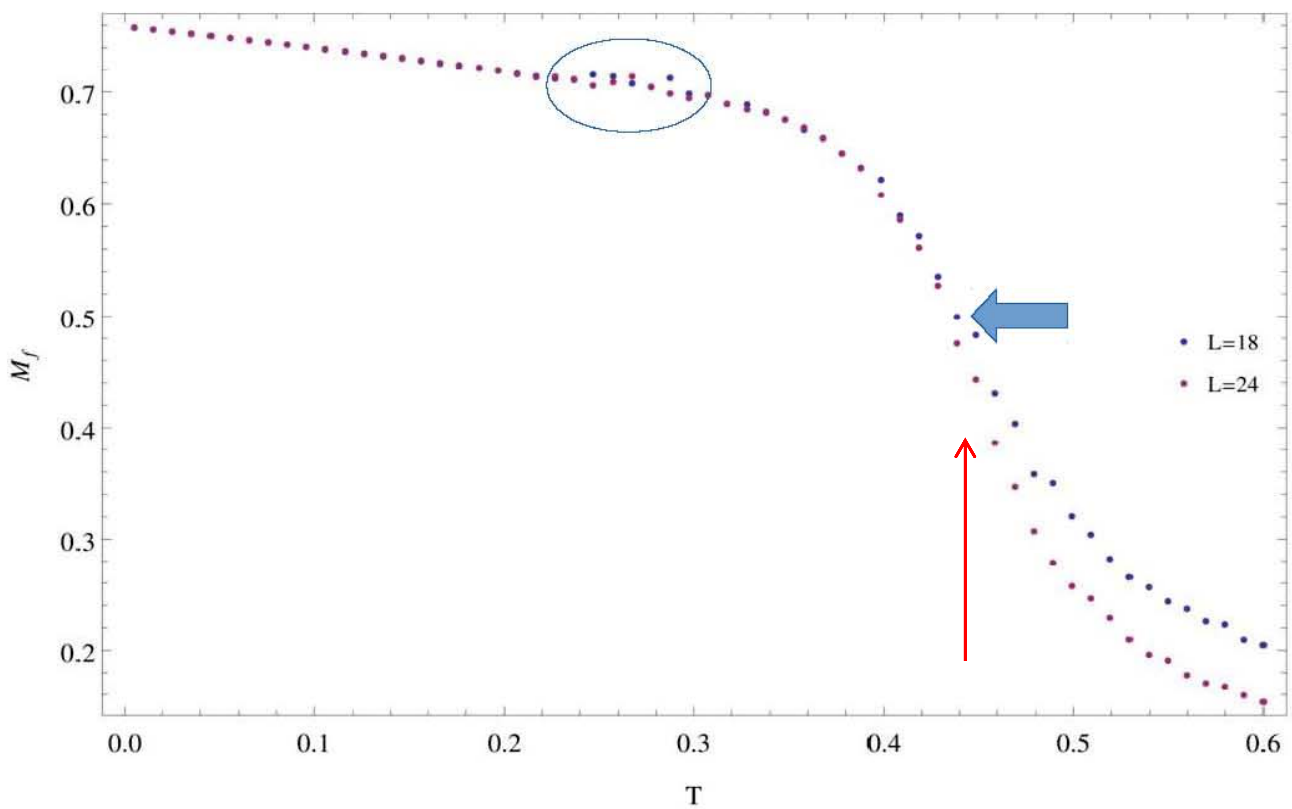
$$C = k_B \frac{\langle E^2 \rangle - \langle E \rangle^2}{(k_B T)^2}$$



Monte Carlo

-Total magnetization also suggests Tc = 0.43

- Additional feature at T ~ 0.27 ??



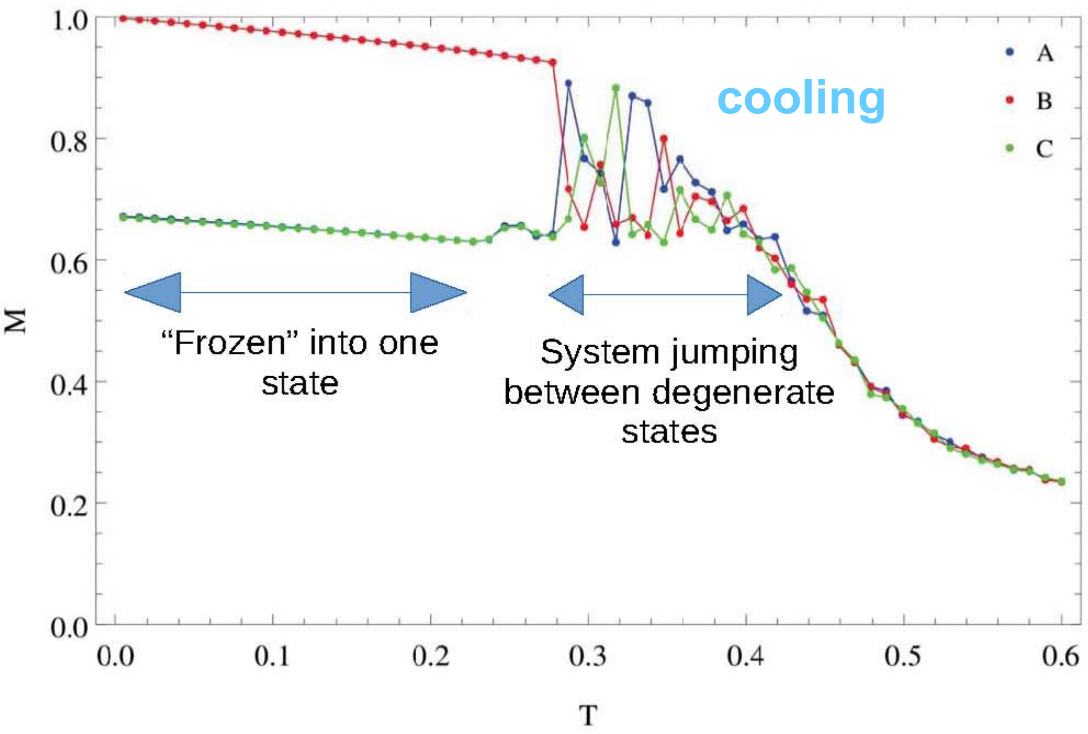
$$M_f = \frac{1}{N}\left|\left\langle \sum_i \vec{S}_i \right\rangle\right|$$

- Total magnetizations for individual sublattices show fluctuations at T≈0.3

- Fluctuations correspond to the system changing between degenerate states

- Energy cost of changing into a new state becomes too large at low temperatures causing system to become “frozen” into a degenerate state

$$M_f = \frac{3}{N} \left| \left\langle \sum_{i \subset \gamma} \vec{S}_i \right\rangle \right|$$



Magnetic Order in the FCC Kagome Lattice:

Summary and Conclusions, Part I

• 3D FCC Kagomé lattice with NN exchange only shows LRO transitions of the ‘q=0’ type for both XY and Heisenberg models.

• Kagome-type spin degeneracies persist in 3D.

• Critical fluctutations associated with the degeneracies leads to a first order transition.

• Cubic anisotropy:

- distorts 120^0 spin structure

- induces **M** || 111

-removes degeneracies and drives the transition becomes continuous.

• H-T phase diagram. Why like 2D triangular?

• Thin films: Surface anisotropy distorts 120^0

• 2D dipole interactions: 6-fold degeneracy: A new type of ‘lock-in’ phenomena below T_N?

J. Whitehead (Prof., Memorial)

B. Southern (Prof., Manitoba)

V. Hemmati (MSc, Memorial, 2012)

M. Leblanc (PhD student, Memorial)

H. Yerzhakov (MSc student, Memorial)

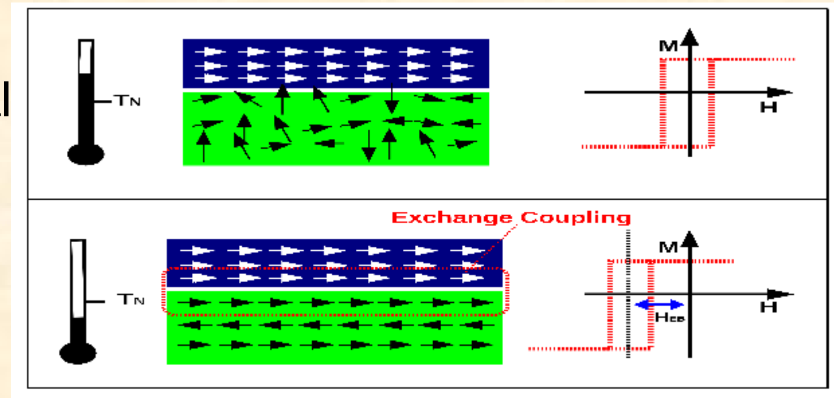
S. Holden (Honors BSc student, Memorial)

I. Saika-Voivod (Prof., Memorial)

More Summary and Conclusions: Exchange Pinning

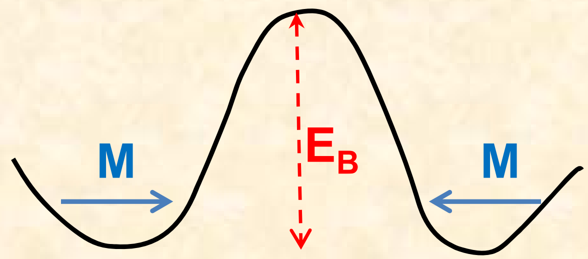
Large frustration of the Kagome structure ⇒ Other small interactions yield M≠0.

•Exchange pinning requires uni-directional magnetic moment ⇒ an effective uni-directional anisotropy.



• This is believed to arise from uni-axial anisotropy in a non-equilibrium system: Energy barrier (also from domains?) prevents magnetization from switching direction, unless at high T,

$E_B >> k_B T.$



Surface spins are pinned into a state with the direction of M fixed.

More work needs to be done on thin films:

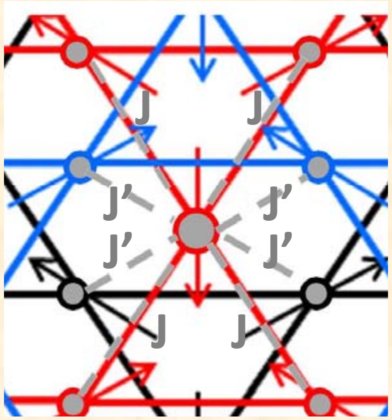
- **Surfaces with non-magnetic sites**
- **Coupling to a ferromagnetic layer**

Monte Carlo simulations of the fcc Kagomé lattice.

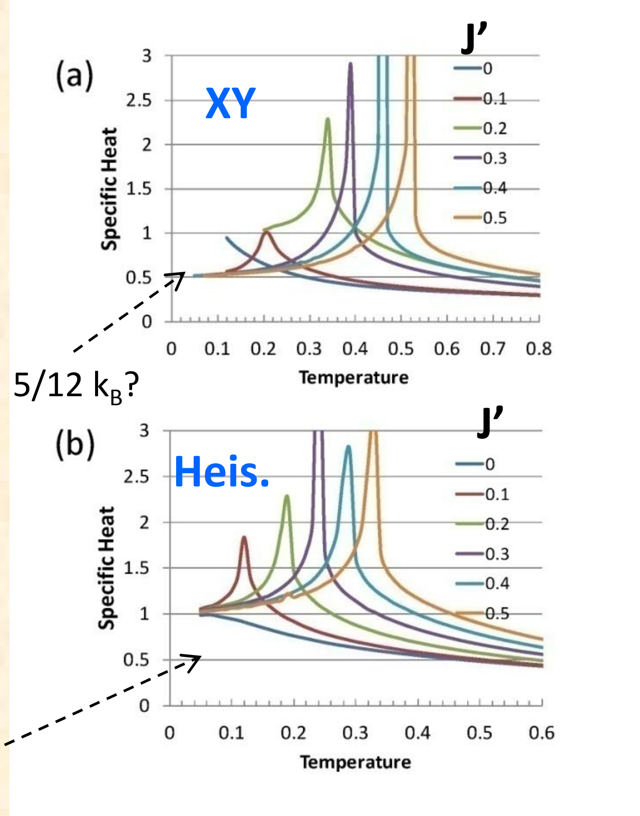
Interlayer coupling J'.

J=1

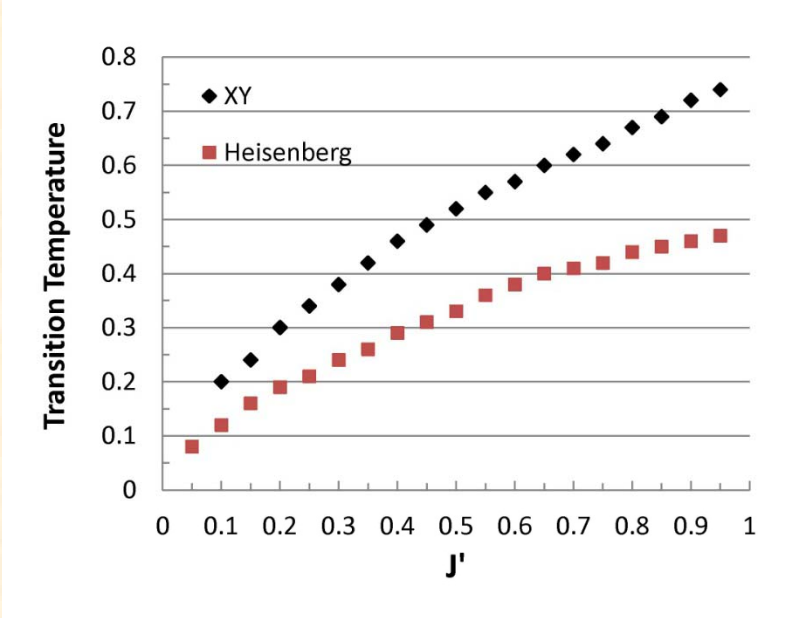
Set inter-layer to J' < 1.



Specific Heat



T_N vs J'.



Trends are similar to other quasi 2D systems.

It comes in other forms...

Relevant for sputtered thin films.

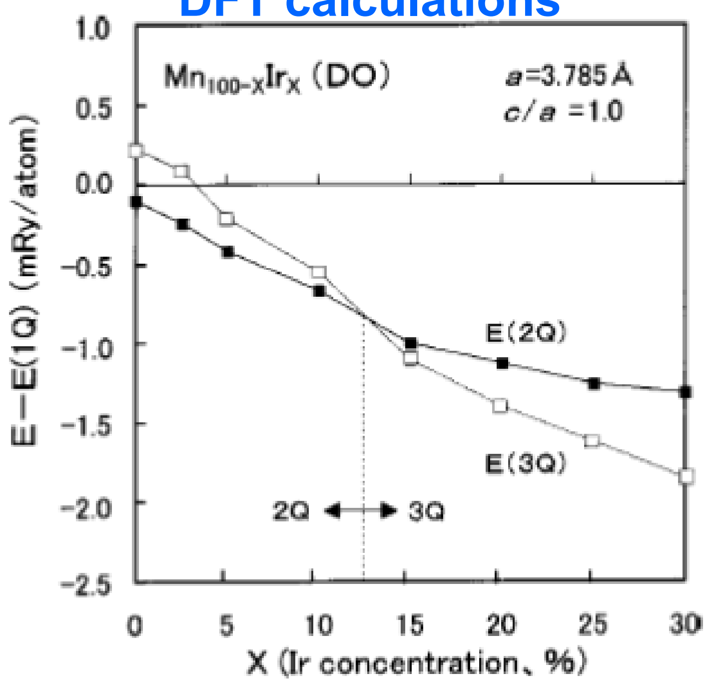
Sakuma et al, JPSJ 69, 3072 (2000); PRB 67, 024420 (2003).

Fishman et al, PRB 61, 12159 (2000).

1. **Disordered $IrMn_3$: 3Q SDW**

2. **Disordered Ir_xMn_{100-x}: 2Q SDW**

DFT calculations



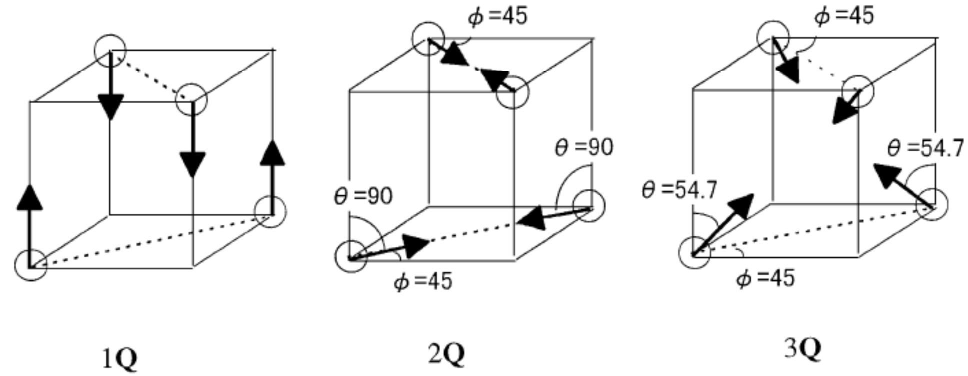


Fig. 1. Multiple-Q spin density wave structures in fcc lattice.