Frustrated Spin Systems

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References

1- "*Lecture Notes on Electron Correlations and Magnetism*", P. Fazekas, World Scientific (1999).

2- "*Introduction to Frustrated magnetism , Material, Experiments, Theory*", edited by C. Lacroix, P. Mendels, and F. Mila, Springer (2010).

3- " *Frustrated Spin Systems*", edited by H. T. Diep, World Scientific (2004).

4- "Spin Liquid in Frustrated Magnets ", L. Balents, Nature 464, 199 (2010).

Outline

- Brief introduction to magnetism and magnetic exchanges.
- Magnetic orders
- Magnetic Frustration
- Order by disorder
- Spin Ice
- Magnetic monopoles in spin Ices
- Some examples

What is the Origin of Magnetism?

1. Magnetic moment of electron

   Orbital magnetic moment+ Spin magnetic moment

   $$\mu = \mu_L + \mu_s = -\mu_B (L + 2S) \qquad \mu_B = \frac{e\hbar}{2m_e}$$

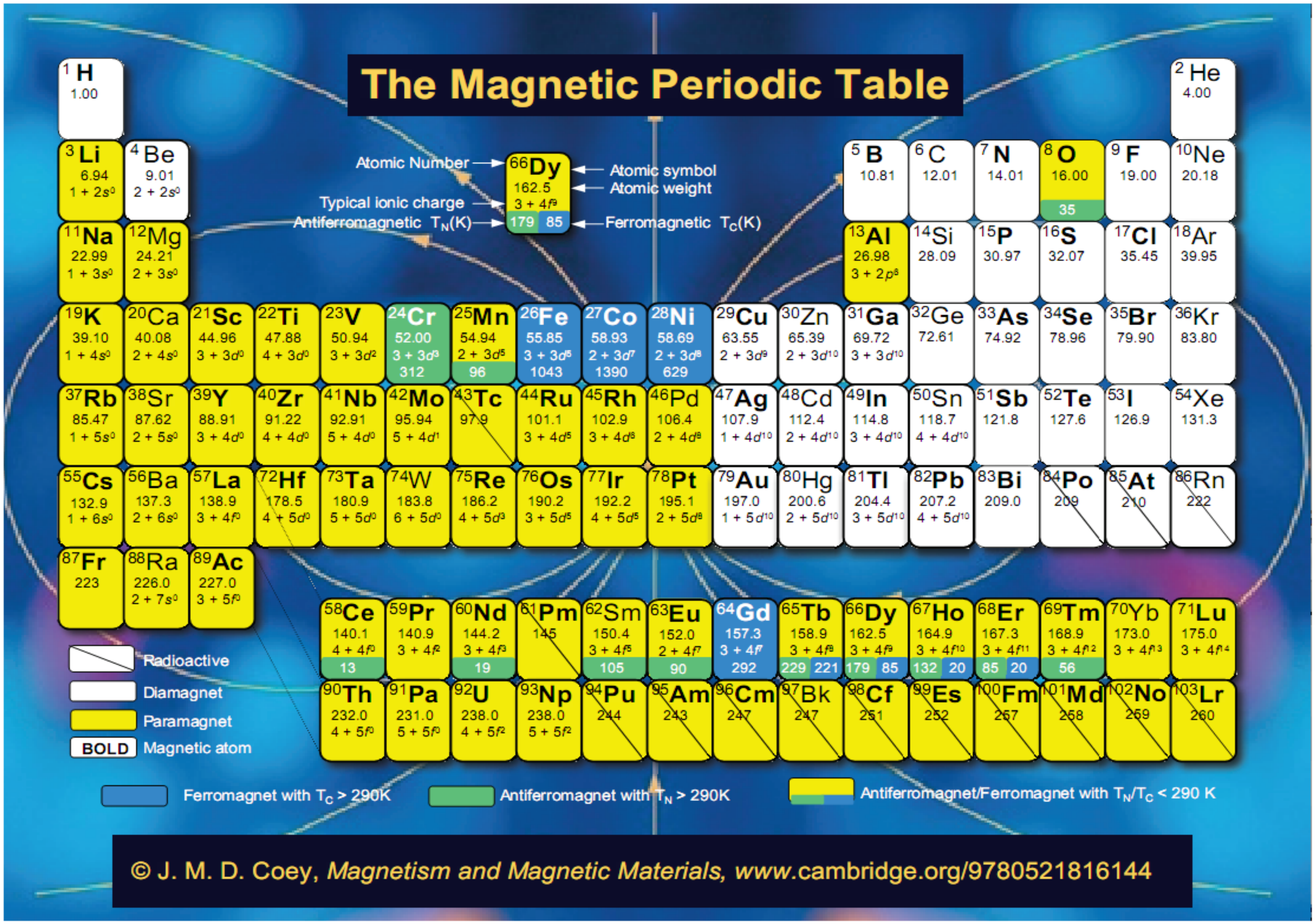
2. Quantum mechanical indistinguishbility

   (many body wave function should be anti-symmetric)

3. Coulomb interactions between electrons

   (example: Hund's rules for atoms and ions)

79 elements are magnetic in atomic form, however only a few of them (16) are magnetic in solid form



Types of Magnetic Exchange

Exchange interactions are due to the coulomb repulsion of electrons and can be classified as:

- Direct exchanges
- Indirect exchanges

Direct Exchange

- Exchange of two electrons between two atomic orbitals by the repulsive coulomb potential.

- FM for orthogonal orbitals.

(example : first Hund's rule for filling the atomic shells)

- Could be AF for non-orthogonal overlapping orbitals.

(example : Hydrogen molecule H_2)

Indirect Exchanges

1. Super exchange :

   (exchange between to 3d orbitals is mediated by cations like oxygen ions, short range, FM or AF)

2. RKKY exchange :

   (rare earths ,exchange between 4f electrons is mediate by 6s or 5d conduction electrons, long range, oscillating sign)

3. Double exchange :

   (FM, mixed valence compounds , Manganites)

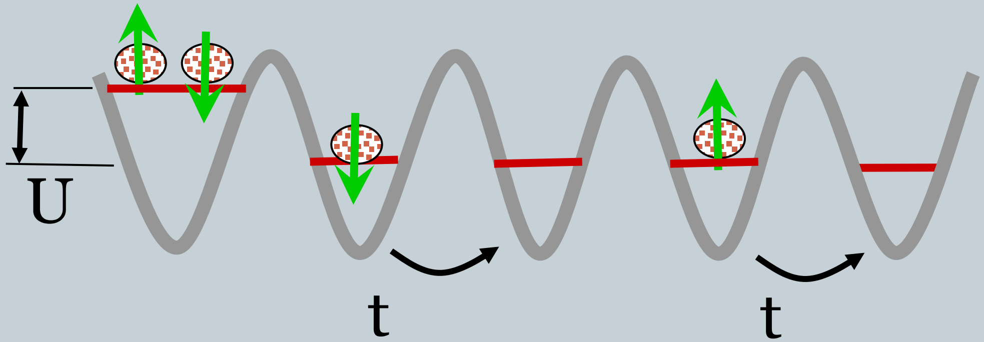
4. Itinerant magnetism :

   (3d metals such as Fe, Ni, Co)

Fermionic Hubbard Model

- The simplest model for describing the strongly correlated materials:

$$H = -t \sum_{\langle i,j \rangle, \alpha} (c_{i\alpha}^{\dagger} c_{j\alpha} + c_{j\alpha}^{\dagger} c_{i\alpha}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

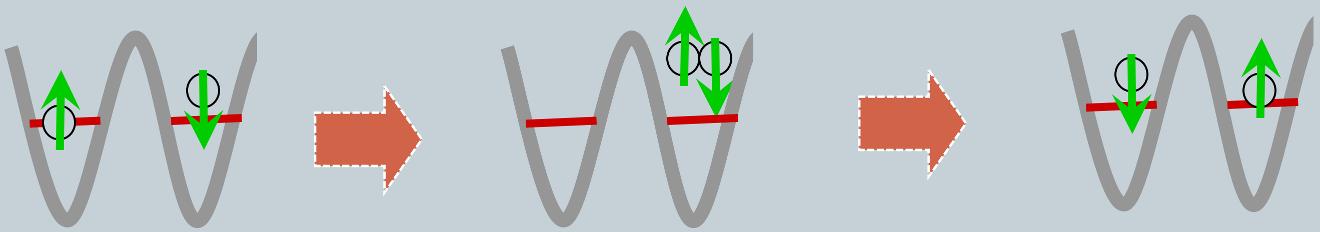


Phenomena Predicted in Hubbard Model

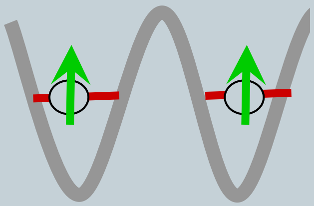
- Superexchange and Antiferromagnetism (P.W. Anderson)
- Itinerant ferromagnetism. Stoner instability (J. Hubbard)
- Incommensurate spin order. Stripes (Schulz, Zaannen, Emery, Kivelson, White, Scalapino, Sachdev, ...)
- d-wave pairing (Scalapino, Pines,...)
- d-density wave (Affleck, Marston, Chakravarty,Laughlin,...)

Superexchange and Antiferromagnetism in Hubbard Model: Large U Limit

- In Singlet state virtual hoppings gain kinetic energy
- Second order perturbation : $\Delta E_s = -4\frac{t^2}{U}$



- In Triplet states virtual hoppings are forbidden
  then : $\Delta E_t = 0$



Effective Hamiltonian

- At half filling, to lowest perturbation order, the effective Hamiltonian is the nearest neighbor antiferromagnet Heisenberg model:

$$H_{eff} = 4\frac{t^2}{U}\sum_{\langle i,j\rangle} S_i . S_j + O(\frac{t^4}{U^3})$$

- Higher order terms would be the next neighbor AF Heisenberg interactions as well as terms consisting of more than two spin interactions (i.e ring exchanges).

Relativistic effects

- Spin-Orbit coupling introduces anisotropic terms to Effective spin Hamiltonian which leads to non-collinear states:

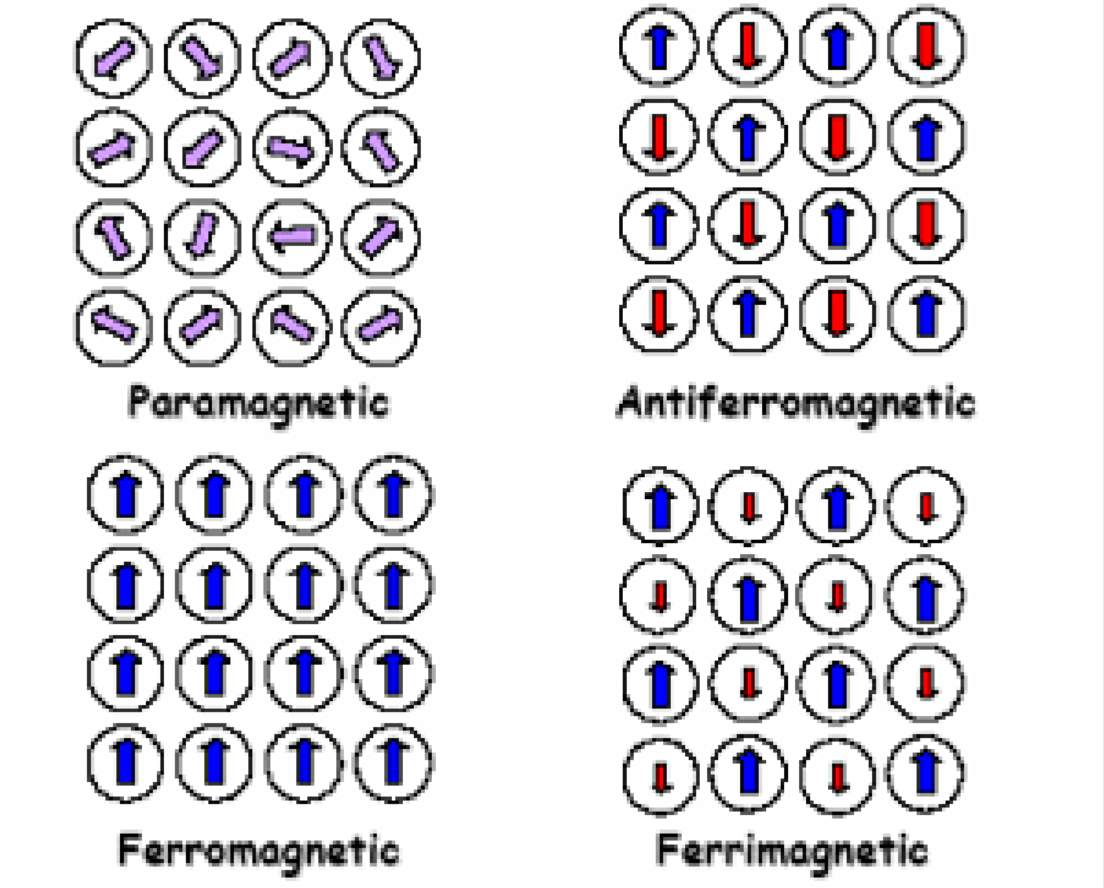
1- Dzyaloshinsky-Moriya (DM) Interaction:

$$\vec{D}.(S_i \times S_j)$$

2-Single ion anisotropy:

$$(S_i.\vec{D})^2$$

Types of Magnetic Orderings



Spin – Spin Correlation and magnetic orders

- Long –range magnetic order: $\lim_{r\to\infty}\langle S(0).S(r)\rangle \neq 0$

  Example: Ferromagnets , Anti-ferromagnets

- Quasi long-range order : $\lim_{r\to\infty}\langle S(0).S(r)\rangle \approx r^{-\eta}$

  Example: Critical points, 2D planar spin systems

- Short-range order : $\lim_{r\to\infty}\langle S(0).S(r)\rangle = \exp(-\frac{r}{\xi})$

  Example : Paramagnets (fluctuating spins),

  Spin glasses (spin freezing)

What Prevents Long-range Ordering?

- Low dimensionality:

  strong fluctuations (thermal or quantum) in one and two dimensions suppress the long-range order.

- Frustration :

  competing exchange interactions or lattice geometry prevents long-range orderings.

  Local interactions and the global energy can not be minimized simultaneously, which leads to degeneracy in the classical ground state.

Low Dimensionality

- **Mermin-Wagner theorem:** One and two dimensional classical Spin systems with short range exchange interactions do not order at any finite temperature due to thermal fluctuations. (2D -XY model is an exception)

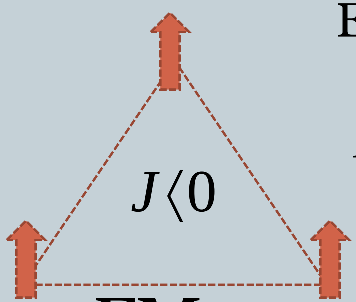
- Quantum Heisenberg chains (exactly solvable):

  $s = 1/2$ chain : quasi long-range ordering, no spin gap

  $s = 1$ chain: short-range ordering, spin gap

Types of Frustration

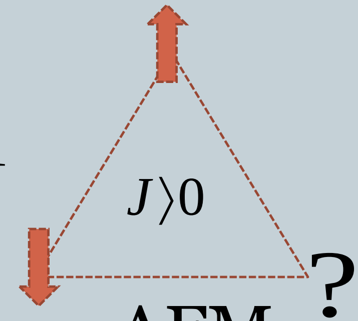
- Geometrical frustration:



FM

Example: Ising model

$$H = J\sum_{\langle i,j\rangle} S_i.S_j, S = \pm 1$$

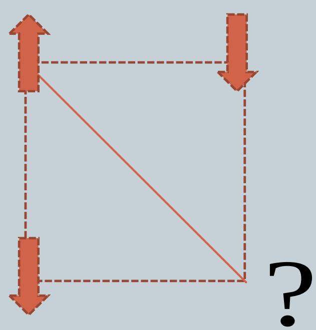


AFM

- Competing interactions:

$$H = J_1\sum_{\langle i,j\rangle} S_i S_j + J_2\sum_{[i,j]} S_i S_j$$

$$J_1 > 0, J_2 > 0$$

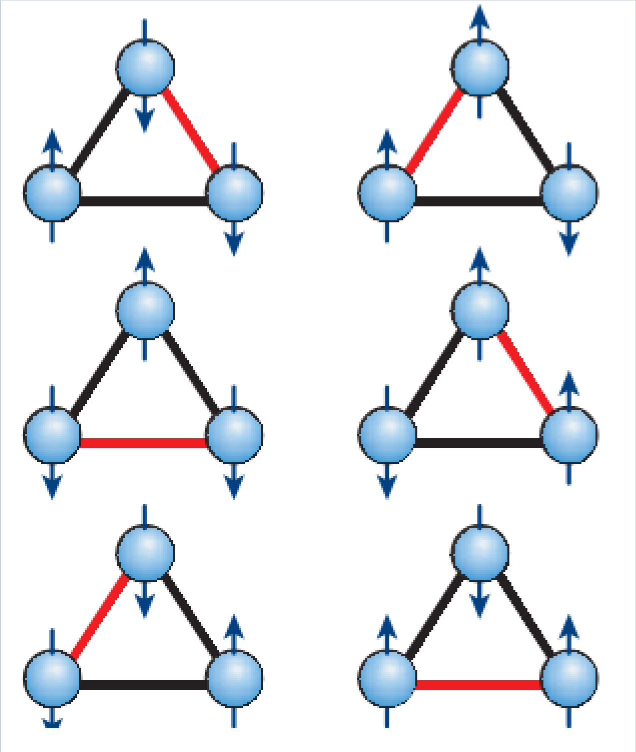


Classical Degeneracy of Ground State in Geometrically Frustrated Magnets

- The ground state of classical AF Ising model on triangular lattice is six-fold degenerate.

No lang-range order,
However fluctuations are restricted to the ground state manifold.

Cooperative paramagnet or
Classical spin liquid.



Measure of Frustration

- At high temperatures, DC magnetic susceptibility of local- moment magnets generally has a Curie-Weiss form :

$$\chi \approx \frac{1}{T - \theta_{CW}}$$

θ_{CW} is the Curie-Wiess temperature and is a measure of exchange interactions. For frustrated magnets the freezing temperature is much less than curie-Weiss temperature:

$$T_f \langle\langle | \theta_{CW} |$$

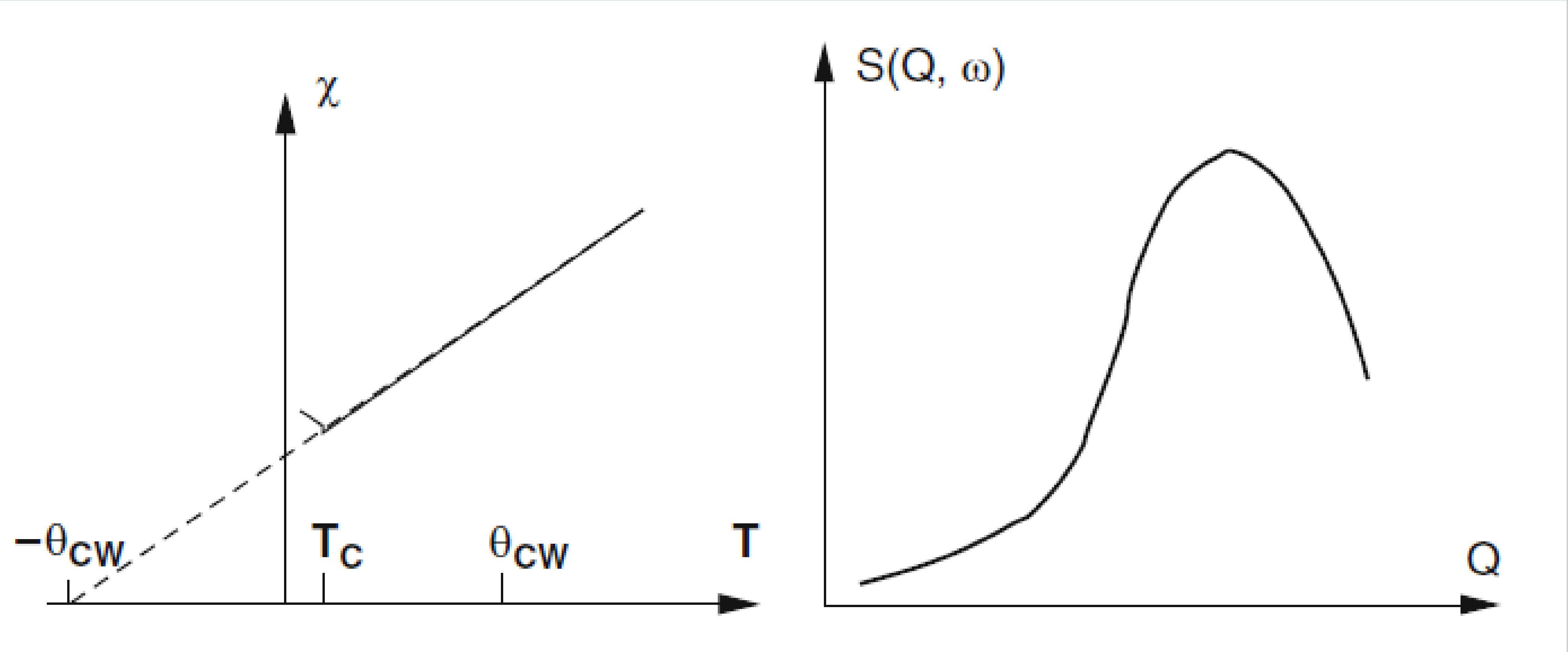
classical Spin liquid:

$$T_f \langle T \langle | \theta_{CW} |$$

Frustration parameter:
(Ramirez)

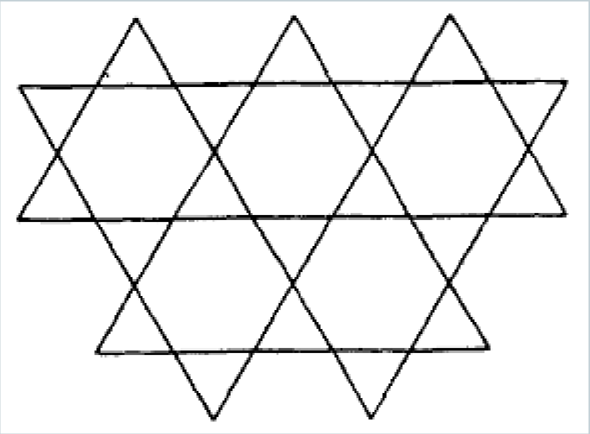
$$f = \frac{|\theta_{CW}|}{T_f}$$

Typical behavior of Susceptibility and Dynamical Structure factor in frustrated magnets

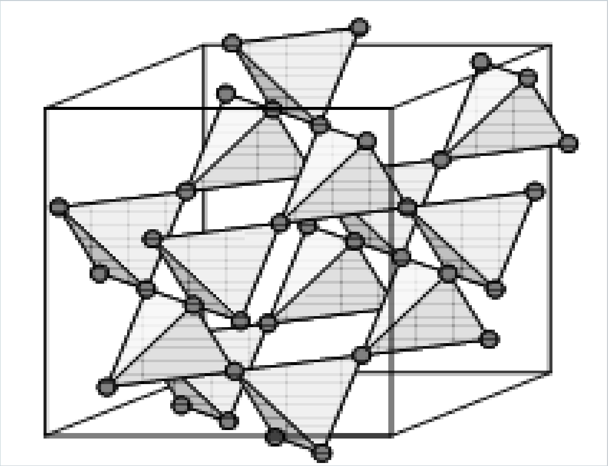


Examples of Geometrically Frustrated Magnets

- 2D: Kagome lattice :



- 3D: Pyrochlore lattice

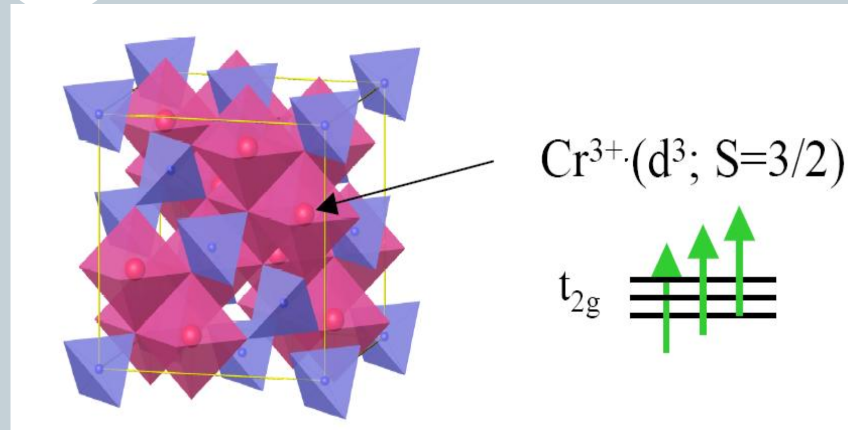


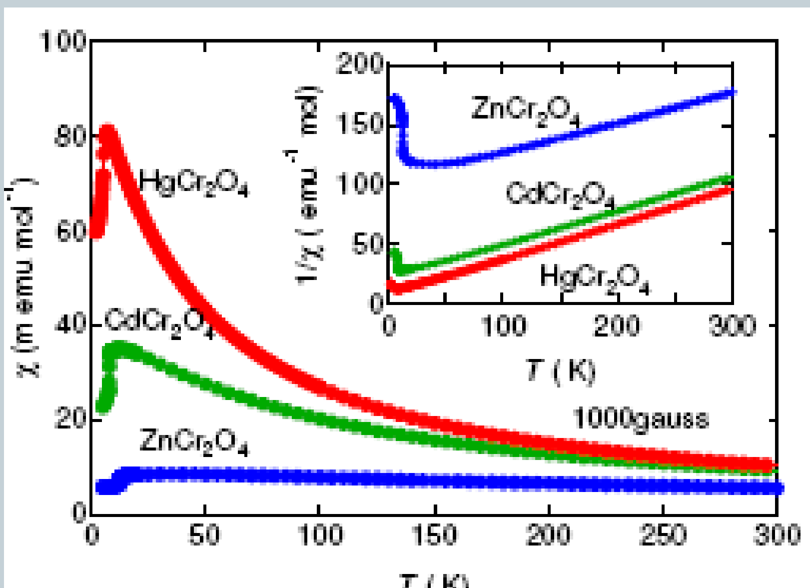
Examples of Real Pyrochlore Magnets

- Chromium spinels

  ACr_2O_4

  $(A = Zn, Cd, Hg)$





$$-\Theta_{CW} = 390K, 70K, 32K$$

$$T_c = 12K, 7.8K, 5.8K$$

$$f = 32.5, 9, 5.5$$

Anti-ferromagnetic Heisenberg model on a single tetrahedron

- for $J > 0$ the ground state is achieved when $L = 0$.

$$\mathcal{H} = J \sum_{\text{pairs}} \mathbf{S}_i \cdot \mathbf{S}_j \equiv \frac{J}{2} |\mathbf{L}|^2 + c$$

with

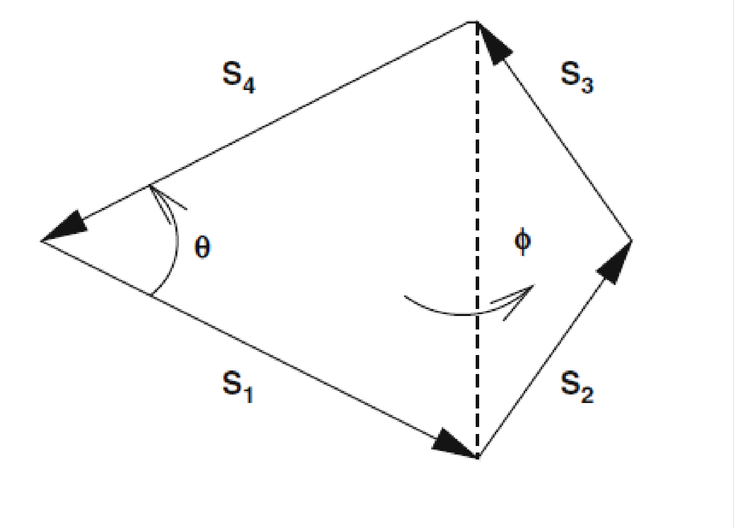
$$\mathbf{L} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4$$

Number of equations=3

number of components=8

Total degrees of freedom=5

Internal degrees of freedom=5-3=2



AFM Heisenberg model on the Pyrochlore lattice

- $N_s \equiv$ Number of spins $= 2\ N_c$
- $N_c \equiv$ Number of units
- $F = 2\ N_s$
- $D = N_c$
- Geometric frustration leads to extensive degeneracy

$$\mathcal{H} = J \sum_{\text{bonds}} \mathbf{S}_i \cdot \mathbf{S}_j \equiv \frac{J}{2} \sum_{\text{units}} |\mathbf{L}_\alpha|^2 + c$$

Total number of degrees of freedom:

$$F = 2 \times (\text{number of spins})$$

Constraints satisfied in ground state:

$$K = 3 \times (\text{number of units})$$

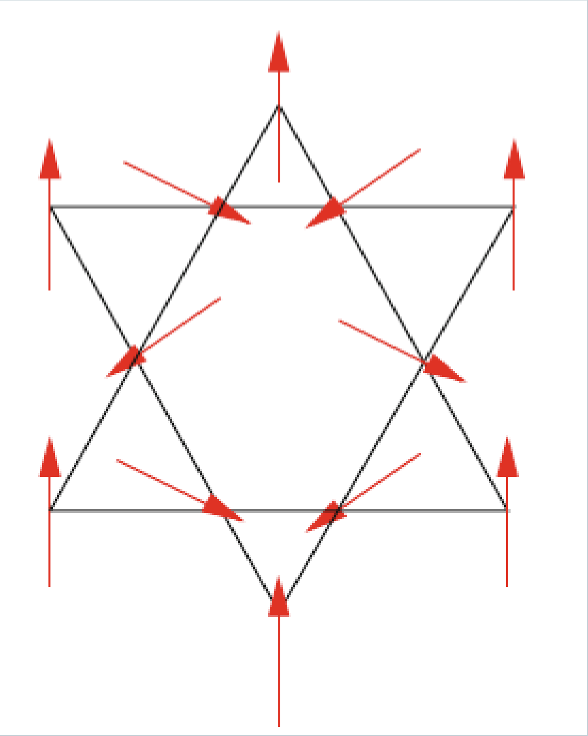
Ground state dimension:

$$\boxed{D = F - K}$$

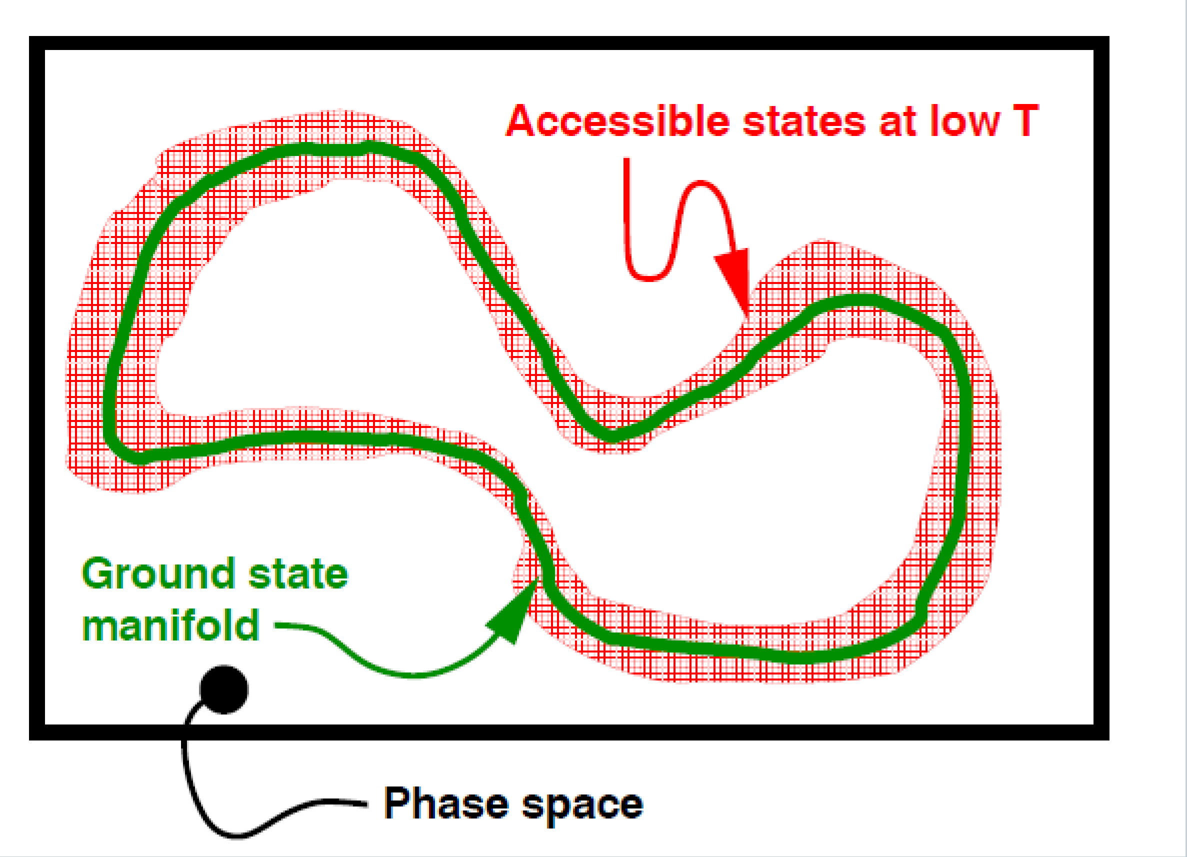
AFM Heisenberg model on Kagome lattice

- Illustration of ground state degeneracy:

  spins on the central hexagon can be rotated together by any angel about the axes defined by the outer spins



Behavior of a frustrated system at low temperature

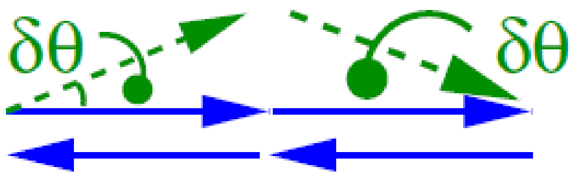


Order by Disorder

- Thermal or Quantum fluctuations may limit the phase space, hence inducing order.

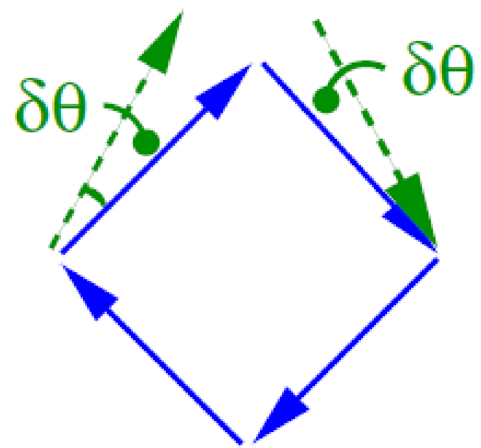
Soft modes

Some states have soft modes



$$E = \frac{J}{2}|\mathbf{L}|^2 \propto (\delta\theta)^4$$

Others don't



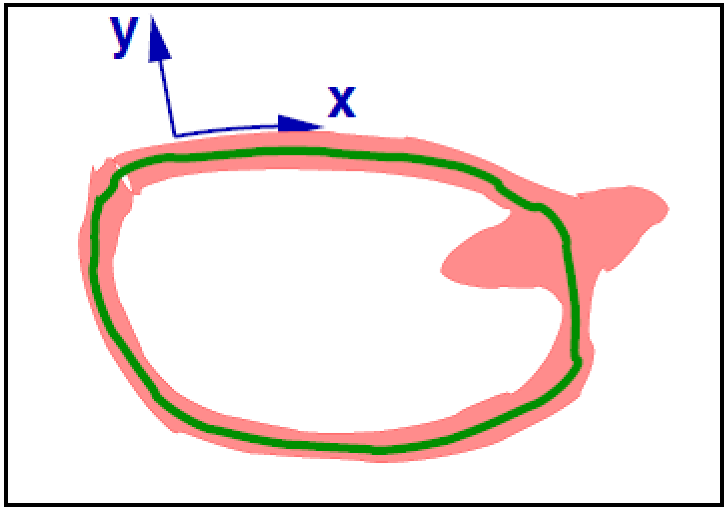
$$E = \frac{J}{2}|\mathbf{L}|^2 \propto (\delta\theta)^2$$

Ground state selection by thermal fluctuations

Thermal fluctuations

Probability distribution on ground states

$$\int \mathrm{d}y\ \mathrm{e}^{-\omega y^2/k_\mathrm{B}T} \propto \sqrt{\frac{k_\mathrm{B}T}{\omega}}$$



$$P(\mathbf{x}) \propto \prod_l \left(\frac{k_\mathrm{B}T}{\omega_l(\mathbf{x})}\right)$$

Thermal fluctuations

kagome $\longrightarrow$ coplanar

pyrochlore $\longrightarrow$ disordered

Linear spin wave theory

- Holstein-Primakoff transformation:

$$S_i^z = S - a_i^\dagger a_i$$
$$S_i^+ = (2S)^{1/2} a_i + \dots$$
$$S_i^- = (2S)^{1/2} a_i^\dagger + \dots,$$

- Quadratic magnon Hamitonian:

$$\mathcal{H} = J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z = JS \sum_{ij} \left[a_i^\dagger a_j + a_j^\dagger a_i \right] - \mu \sum_i a_i^\dagger a_i$$

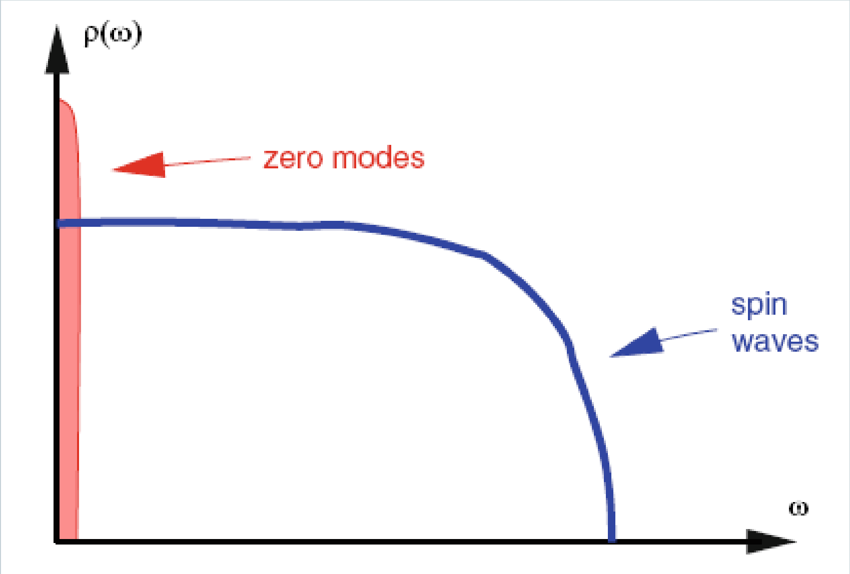
$$\mu \equiv zJS - h$$

Ground state selection by quantum fluctuatios

The quantum zero point energy in SW approximation, for a given configuration X in the ground State manifold is given by:

$$\mathcal{H}_{\text{eff}}(\mathbf{x}) = \frac{1}{2}\sum_{l} \hbar\omega_l(\mathbf{x})$$

The ground state is a set of configurations on which the above zero point energy is minimum.



Example

- For the Heisenberg anti-ferromagnets at large S the selected ground state by quantum fluctuations are:

i) Coplanar on the Kagome lattice,

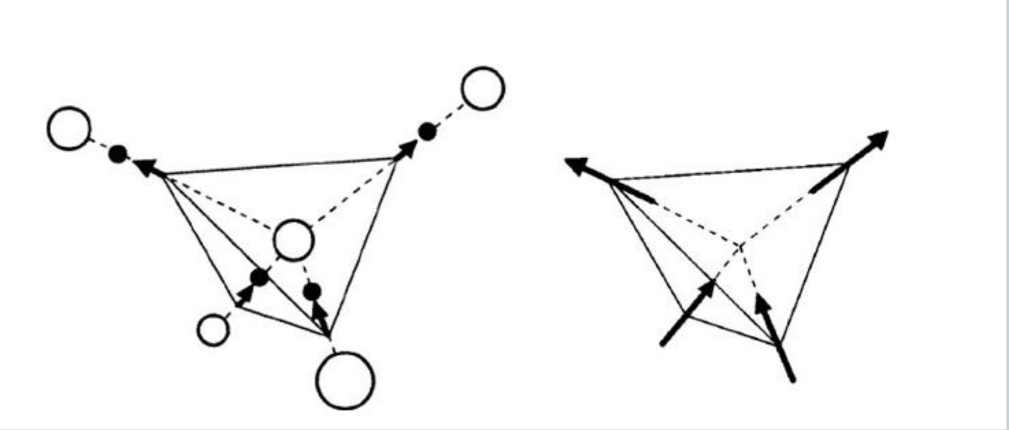
(A. V. Chubukov, Phys. Rev. Lett. 69, 832 (1992))

ii) Collinear on the pyrochlore lattice.

(C. L. Henley, Phys. Rev. Lett. 96, 47201 (2006))

In both examples 1/3 modes are soft.

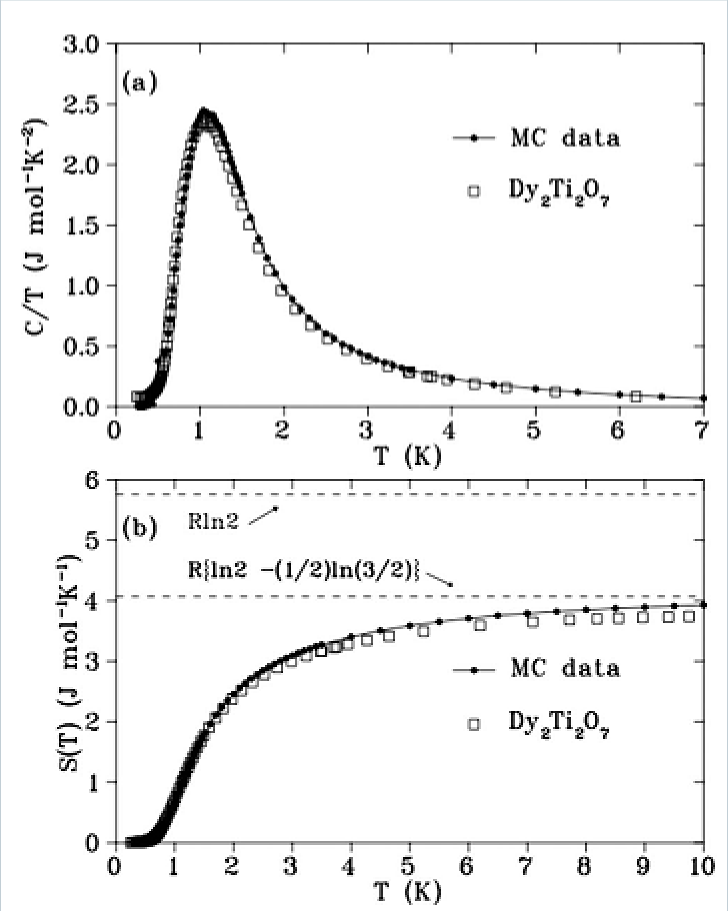
Spin Ice



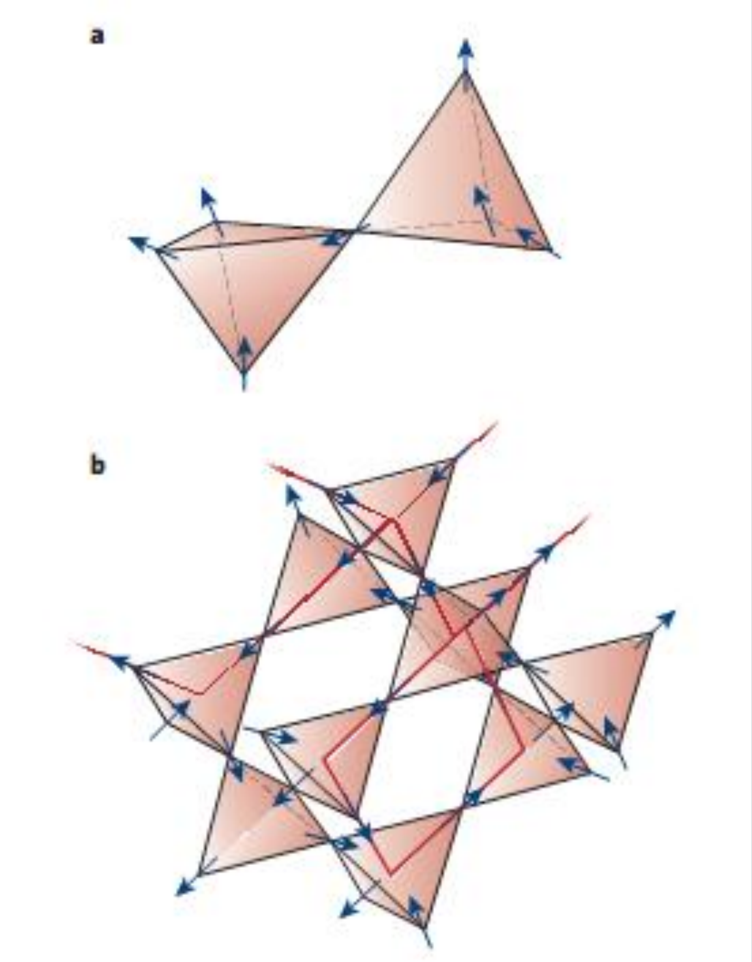
$$H = -J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \Delta \sum_i (\hat{z}_i \cdot \boldsymbol{S}_i)^2$$

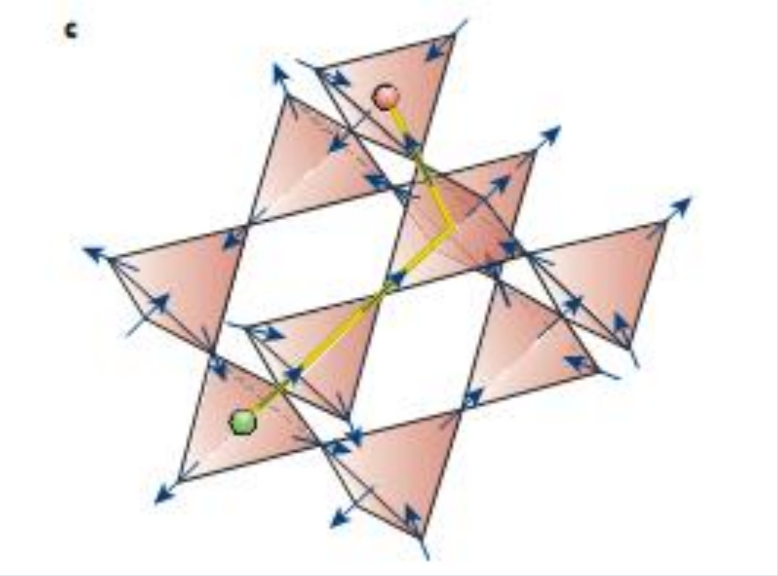
$$H = -J \sum_{\langle ij \rangle} \boldsymbol{S}_i^{\hat{z}_i} \cdot \boldsymbol{S}_j^{\hat{z}_j} + D r_{\mathrm{nn}}^3 \sum_{i>j} \frac{\boldsymbol{S}_i^{\hat{z}_i} \cdot \boldsymbol{S}_j^{\hat{z}_j}}{|\boldsymbol{r}_{ij}|^3} - \frac{3(\boldsymbol{S}_i^{\hat{z}_i} \cdot \boldsymbol{r}_{ij})(\boldsymbol{S}_j^{\hat{z}_j} \cdot \boldsymbol{r}_{ij})}{|\boldsymbol{r}_{ij}|^5}.$$

Residual Entropy in Spin Ices



Artificial magnetic fields and magnetic monopoles in spin ice





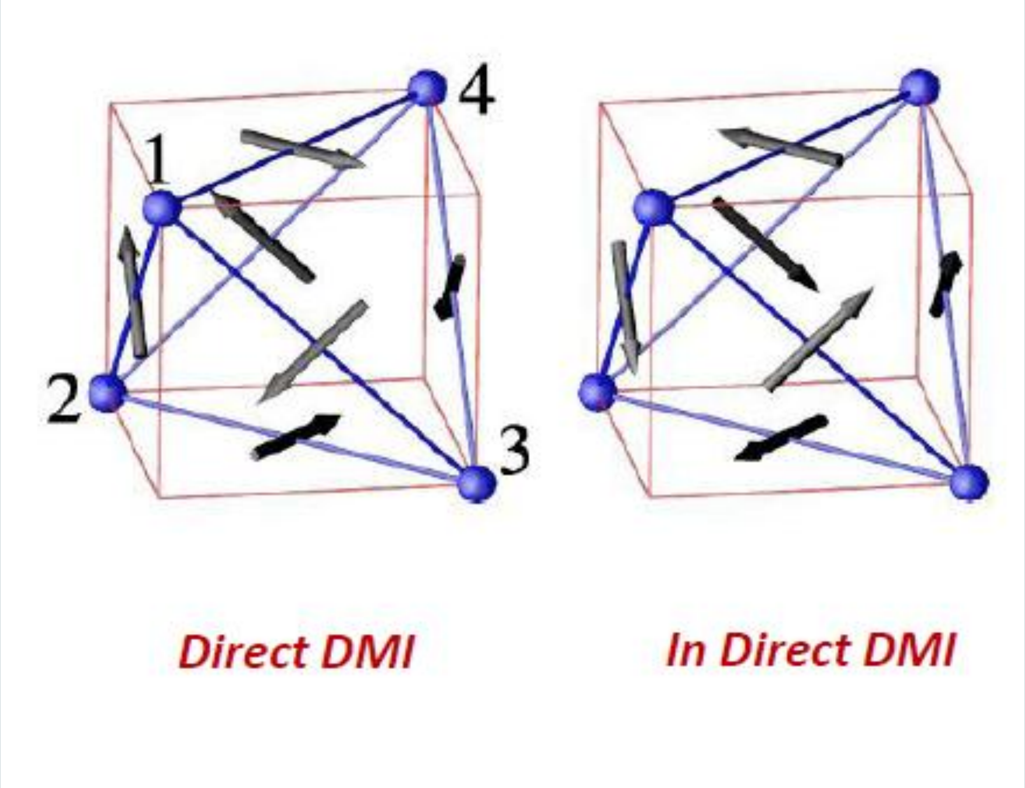
Conclusion

- Geometrical frustration generates macroscopic degeneracies which avoid long-range order.
- Thermal or Quantum fluctuations may help the system to select a definite ground state.
- Emergence of novel excitations such as magnetic monopoles

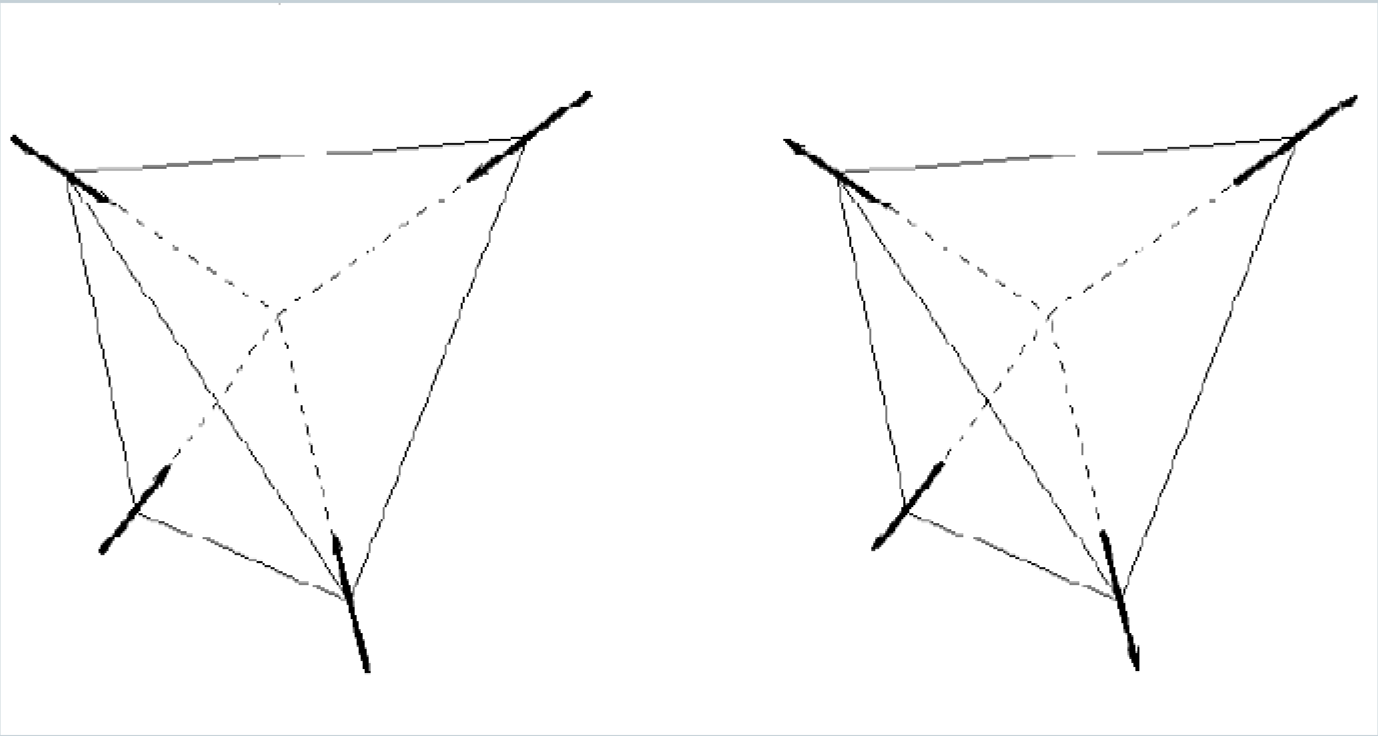
DM Interaction on Pyrochlore AFM

- FeF3 in pyrochlore structure:
  - The Magnetic Fe^{+3} ions are in d^5 electronic configuration with a totally symmetric ground state with no net angular momentum.
  - Anti-ferromagnetic exchange interactions between nearest neighbors
  - System is highly frustrated, hence any small amount of anisotropy will be important in determining the ground state of the system
  - The observed low-temperature phase consists of four sublattices oriented along four [111] directions (All-in All-out state)

D-Vectors



Direct DM leads to All-in All-out GS



Monte Carlo Simulation

- The phase transition from disorder to all-in all-out ordered state is second order for $D/J>0.05$.

- The phase transition from disorder to all-in all-out ordered state is second order for $D/J<0.05$.

- Then $D/J \sim 0.05$ would be a Tri-Critical point.

THANKS FOR YOUR ATTENTION