

Magnetic Monopoles in Spin Ice

An Introduction

Panagopoulos Georgios, ge19007

Seminar - Topic

Tuesday, 09/05/2023

School of Applied Mathematical and Physical Sciences

National Technical University of Athens

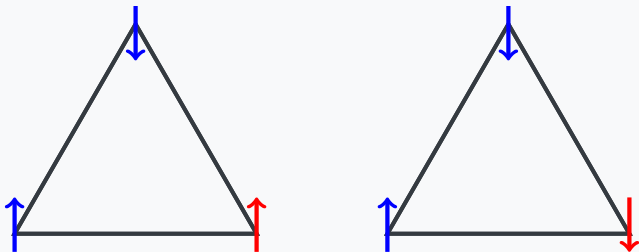
 ge19007@mail.ntua.gr

Magnetic Monopoles

- Magnetism in nature historically: Always in dipole form
- Elementary particles with magnetic charge: Magnetic Monopoles
 - Predicted by many theories
- Haven't been observed yet
- Magnetic monopoles appear as quasi-particles - emergent property of materials due to collective behavior of complex systems
- Detection and study become possible
- Applications become possible

Geometric Frustration

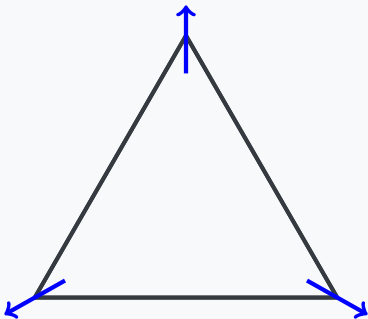
- Antiferromagnetism: Neighboring spins prefer opposite orientations



- For a given choice of 2 spins, the third can't be antiparallel to both
 → frustrated spin
- Each corner → 2 states → 6 states total with the same energy

Geometric Frustration

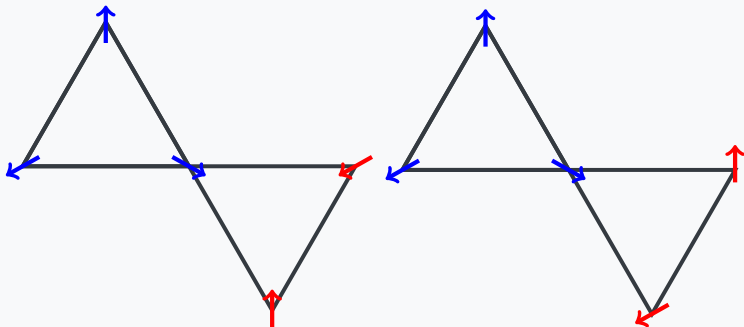
- The ground state is degenerate \rightarrow residual entropy at 0 K
- The system "compromises" to a state of least energy:



- The spins are at 120° angles \rightarrow total spin 0

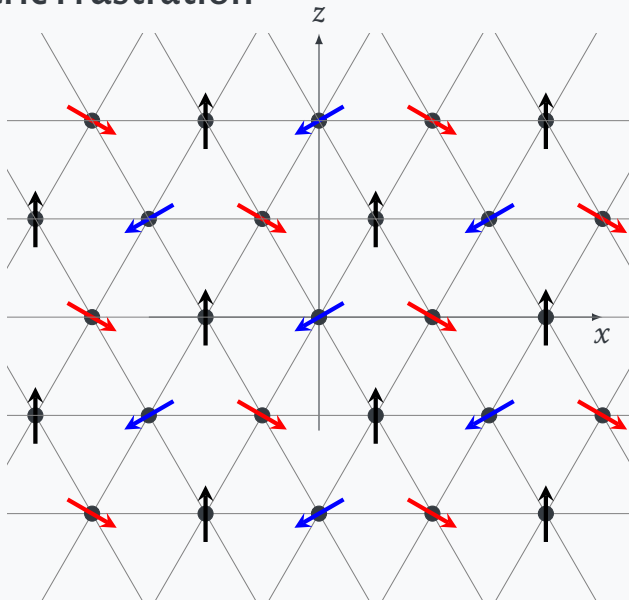
Geometric Frustration

- Consider a nearby triangle:



- There are 2 equivalent ways of satisfying the above rule
- By extension, in a crystal we have a huge ground state degeneracy

Geometric Frustration



Water Ice

- In ice, the O atoms are in the center of a tetrahedron
- All O atoms develop covalent bonds with 2 closely neighboring H atoms
- All O atoms develop weaker bonds with 2 more neighboring H atoms (hydrogen bonds between H_2O molecules) → Ice Rules

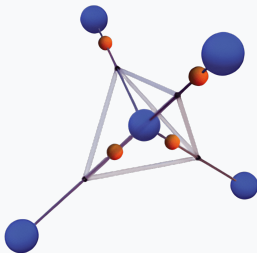


Figure 1: Tetrahedral structure of ice ¹

Water Ice

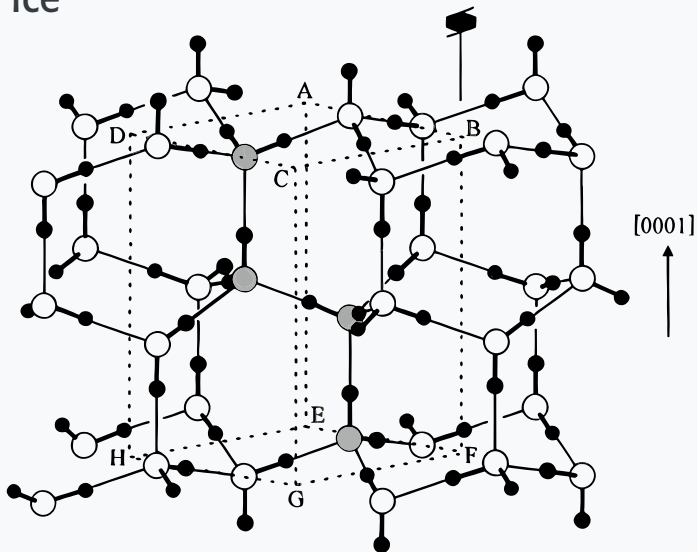
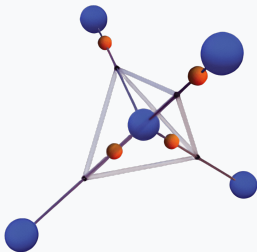


Figure 2: Periodic structure of standard ice ¹

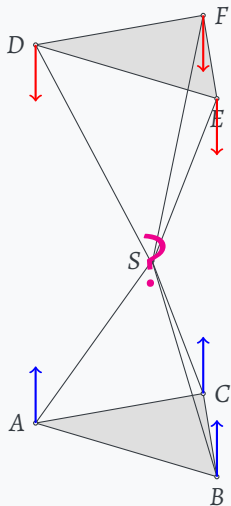
Water Ice

- Consider the placement of H atoms around an O atom in ice



- There are 6 equivalent states for every tetrahedron
- Two H atoms close (inside) & two H atoms far (outside)
- Therefore, we have a six-fold degeneracy of the ground state \rightarrow residual entropy at 0 K (Pauling, 1935²)

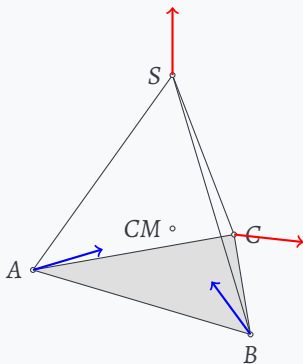
Spin Ice



- Consider a tetrahedral arrangement with ferromagnetic interactions between neighboring spins
- The spin at S is frustrated and we have a two-fold ground state degeneracy.

Spin Ice

- The system compromises to a state where 2 spins point towards to and 2 spins point away from the center of the tetrahedron



- Equivalent to the ground state of ice \rightarrow spin ice!

Spin Ice

- Ground state degeneracy \rightarrow residual entropy
- The crystal structure where this happens is the pyrochlore lattice
- FCC structure with 4 atom tetrahedral basis formed by materials of the type $A_2B_2O_7$
- A, B are usually rare earths or transition metals and they both form the pyrochlore structure
- Characteristic examples: $Dy_2Ti_2O_7$ (dysprosium titanate) & $Ho_2Ti_2O_7$ (holmium titanate)

Spin Ice

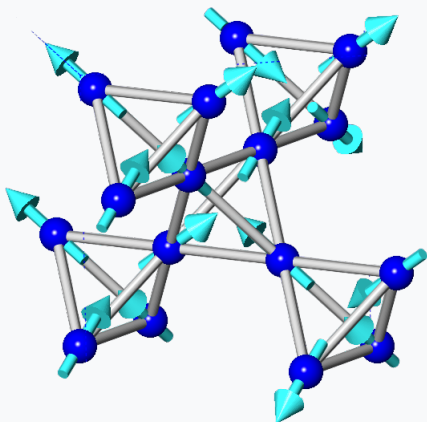


Figure 3: Spin Ice pyrochlore structure³

Spin Ice

Nearest-Neighbor Spin Ice Model

- NNSIM is the simplest model where we consider ferromagnetic Heisenberg interactions between neighboring spins:

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad (1)$$

where $J > 0$ means ferromagnetic interaction

- On the pyrochlore lattice $\vec{S}_i \cdot \vec{S}_j = -\frac{1}{3}\sigma_i\sigma_j$ and thus⁴:

$$H = \frac{J}{3} \sum_{\langle i,j \rangle} \sigma_i\sigma_j = J_{nn} \sum_{\langle i,j \rangle} \sigma_i\sigma_j \quad (2)$$

where $\sigma_i = \pm 1 \rightarrow$ and $J_{nn} > 0$, which is an Ising *antiferromagnetism* model!

Spin Ice

Nearest-Neighbor Spin Ice Model

- NNSIM reproduces the ground state degeneracy of spin ice
- However, it is crude, especially for $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$
- In reality, the interactions are antiferromagnetic in the Heisenberg model, i.e. ($J_{nn} < 0$). How?
- Dy^{+3} and Ho^{+3} have a large magnetic moment $\sim 10\mu_B$
- We have ignored a dipole interaction term \rightarrow Dipolar Spin Ice Model (DSIM)

Spin Ice

Dipolar Spin Ice Model

- The new Hamiltonian is⁴

$$H = J_{nn} \sum_{\langle i,j \rangle} \sigma_i \sigma_j + D r_{nn}^3 \sum_{i>j} \left[\frac{\vec{S}_i \cdot \vec{S}_j}{|\vec{r}_{ij}|^3} - \frac{3(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{|\vec{r}_{ij}|^5} \right] \quad (3)$$

where $D = \frac{\mu_0 \mu^2}{4\pi r_{nn}^3}$, r_{nn} the distance between NN and r_{ij} the distance between any two spins

- The second term is the dipole interaction. For NN, this term is $D_{nn} = \frac{5D}{3}$
- We can define an effective NN energy scale⁵:

$$J_{eff} = J_{nn} + D_{nn} \quad (4)$$

Spin Ice

Dipolar Spin Ice Model

- If $J_{eff} > 0$ the effective interaction is ferromagnetic (NNSIM), even if the actual interaction between nearest neighbors is antiferromagnetic ($J_{nn} < 0$)
- However, further neighbor interactions are important \rightarrow we expect the degeneracy to be lifted
- It does happen, but it's very weak \rightarrow quasi-degenerate states
- In reality, there is a unique ground state

Spin Ice

Dipolar Spin Ice Model

- At $\sim 0.18mK$ first order phase change from quasi-degenerate states, Long range order \rightarrow total magnetization 0

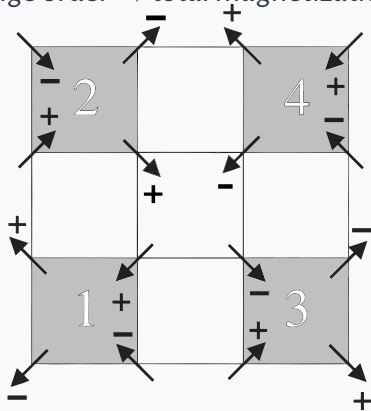


Figure 4: Top down projection of the Dipolar Spin Ice Model ground state.
The total magnetization is 0⁵

Summary

- In some materials with the pyrochlore structure there is magnetic frustration of spins
- The ground state of such crystals obeys the Ice Rules
- The NNSIM is a simple model that gives reasonably good results. A more accurate model is the Dipolar Spin Ice model
- But where are the monopoles?

Magnetic Monopoles in Spin Ice

Dumbbell Model

- Consider each dipole moment to be a monopole-antimonopole pair (dumbbell)
- All monopoles-antimonopoles are in the center of a tetrahedron:

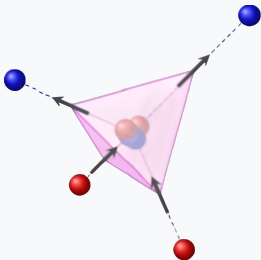


Figure 5: Dumbbell model: A magnetic dipole moment (spin) can be viewed as two opposite magnetic charges ⁴

- A diamond lattice is formed by these magnetically neutral spots

Magnetic Monopoles in Spin Ice

Dumbbell Model

- DSIM: Excitation from a quasi-degenerate (Pauling) state \rightarrow spin flip \rightarrow Ice Rules are broken
- DM: Same excitation corresponds to swapping a monopole with an antimonopole

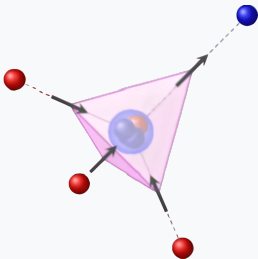


Figure 6: Dumbbell model: Magnetic charge appears as a result of crystal excitations caused by spin flips⁴

Magnetic Monopoles in Spin Ice

Dumbbell Model

- Excitations cause concentrations of magnetic charge to appear in neighboring tetrahedra
- Flipping chains of spins \rightarrow move magnetic charges away from each other at large distances. The chains of flipped spins are an analogue of Dirac Strings
- The interaction between monopoles is Coulombic⁶:

$$V(r_{ij}) = \begin{cases} \frac{\mu_0}{4\pi} \frac{q_i q_j}{r_{ij}} & r_{ij} \neq 0 \\ v_0 q_i q_j & r_{ij} = 0 \end{cases} \quad (5)$$

where the magnetic charge takes values $q_m = \pm \frac{\mu}{a_d}$, a_d the distance between positions in the diamond lattice

Magnetic Monopoles in Spin Ice

Dumbbell Model

- The corresponding Hamiltonian can be written as⁶

$$H = \frac{\mu_0}{4\pi} \sum_{\alpha < \beta} \frac{Q_\alpha Q_\beta}{r_{\alpha\beta}} + \frac{v_0}{2} \sum_{\alpha} Q_\alpha^2 \quad (6)$$

where Q_α the total magnetic charge in a lattice position and v_0 is a constant that reproduces the ferromagnetic coupling of NN

- Are the monopoles unconfined? As the dirac string length grows, the energy cost must be bound \rightarrow monopoles move freely in the crystal
- Ensured by the quasi-degenerate Pauling states

Magnetic Monopoles in Spin Ice

Dumbbell Model

- A closed path of flipped spins (worm) leads to a different quasi-degenerate crystal state
- Worms can have arbitrary shapes and lengths, due to the geometry → infinite number of dirac strings connecting two monopoles
- Therefore, dirac strings are energetically insignificant → monopole interaction is purely Coulombic^{7,8}
- Dirac Strings are observable → no quantization of magnetic charge

Magnetic Monopoles in Spin Ice

Dumbbell Model

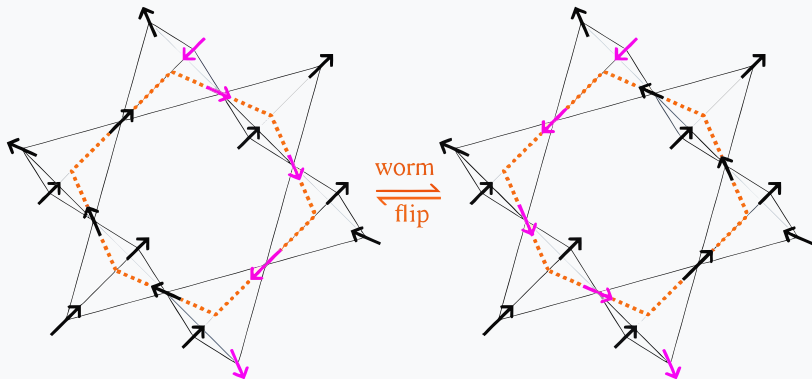


Figure 7: Closed path of flipped spins (worm) ⁹

Magnetic Monopoles in Spin Ice

Dumbbell Model

- Interaction between monopoles is purely Coulombic \rightarrow energy between two monopoles at distance r is⁶

$$E(r) = 2\frac{2\nu_0\mu^2}{a_d^2} + \frac{\mu_0}{4\pi} \frac{\left(\frac{2\mu}{a_d}\right) \cdot \left(-\frac{2\mu}{a_d}\right)}{r} \quad (7)$$

where the first term is the monopole-antimonopole creation energy cost and the second term is the magnetic Coulomb interaction

- For $r \rightarrow \infty$ the energy is finite and thus the monopoles are deconfined

Application: Parallel Computing

Spintronics

- Conventional semiconductor electronics are based on the charge property of electrons
- Spintronics (spin transport electronics) are based on the property of spin and can be used for non-volatile memory in combination with conventional systems
- Spintronics are good for intrinsically parallel computation systems which are very efficient, like Quantum Computers or the human brain¹⁰
- Spin Ice systems are also spin based and fit into the same broad category with spintronics → spin ice based parallel computation systems

Application: Parallel Computing

Artificial Spin Ice

- Inspired by natural spin ice, we can make larger scale artificial spin ice systems
- Artificial Spin Ice consists of tiny ferromagnets on the *nm* scale, whose magnetization is fixed on a given direction
- We can arrange these ferromagnets such that magnetic frustration and magnetic monopoles arise
- We can build logic gates based on the transfer of magnetic charge in such systems
- Operation close to the Landauer limit, i.e. to the theoretical limit for maximal efficiency (and thus least energy consumption)¹¹

Application: Parallel Computing

Artificial Spin Ice

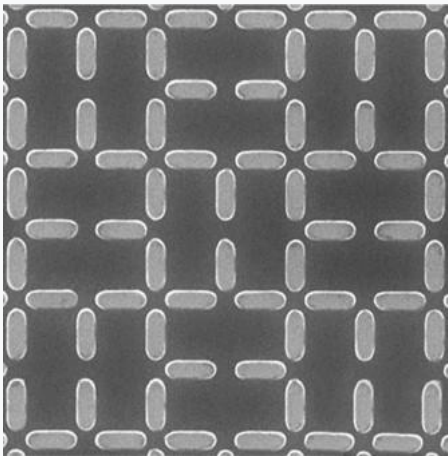


Figure 8: Artificial Spin Ice: Shakti Lattice¹²



Bibliography

- ¹ C. Nisoli, “Frustration(s) and the ice rule: from natural materials to the deliberate design of exotic behaviors”, in (Springer Cham, Nov. 2018), pp. 57–59.
- ² L. Pauling, “The structure and entropy of ice and of other crystals with some randomness of atomic arrangement”, *Journal of the American Chemical Society* **57**, 2680–2684 (1935).
- ³ Mjppgngras, *Portion of the pyrochlore lattice showing magnetic moments (arrows) obeying the two-in, two out spin ice rule*, Sept. 2013.
- ⁴ L. Jaubert and P. Holdsworth, “Magnetic monopole dynamics in spin ice”, *Journal of physics. Condensed matter : an Institute of Physics journal* **23**, 164222 (2011).



Bibliography

- ⁵ R. G. Melko and M. J. P. Gingras, “Monte carlo studies of the dipolar spin ice model”, *Journal of Physics: Condensed Matter* **16**, R1277–R1319 (2004).
- ⁶ C. Castelnovo, R. Moessner, and S. Sondhi, “Spin ice, fractionalization, and topological order”, *Annual Review of Condensed Matter Physics* **3**, 35–55 (2012).
- ⁷ C. Castelnovo, R. Moessner, and S. L. Sondhi, “Magnetic monopoles in spin ice”, *Nature* **451**, 42–45 (2008).
- ⁸ C. H. Marrows, “Experimental studies of artificial spin ice”, in *Spin ice*, edited by M. Udagawa and L. Jaubert (Springer International Publishing, Cham, 2021), pp. 455–478.
- ⁹ L. Jaubert, “Topology of the vacuum”, in (Oct. 2021), pp. 117–141.
- ¹⁰ M. Di Ventura and Y. V. Pershin, “The parallel approach”, *Nature Physics* **9**, 200–202 (2013).



Bibliography

- ¹¹ F. Flicker, *The magick of matter the magick of matter*, (Profile Books, London, England, Nov. 2022).
- ¹² Y. Lao, F. Caravelli, M. Sheikh, J. Sklenar, D. Gardeazabal, J. D. Watts, A. M. Albrecht, A. Scholl, K. Dahmen, C. Nisoli, and P. Schiffer, “Classical topological order in the kinetics of artificial spin ice”, *Nature Physics* **14**, 723–727 (2018).

Thank you for your attention!