Why spin ice obeys the ice rules

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Overview

• The history of (nearest-neighbour) spin ice
  - Pauling’s entropy
  - Anderson’s mapping
  - Experimental discovery of Ho$_2$Ti$_2$O$_7$ by Bramwell+Harris
  - Ramirez’ entropy experiment

• Spin ice: the real Hamiltonian
  - Dipolar spin ice (Bangalore group)
  - Self-screening (Waterloo group)

• Why spin ice obeys the ice rules
  - projective equivalence and the model dipoles
  - emergent vs. intrinsic gauge structure
  - dipolar spins are ice because ice is dipolar
From a tetrahedron to the Pauling entropy $S_0$

Consider Ising spins $\sigma_i = \pm 1$ with antiferromagnetic $J > 0$:

$$\mathcal{H}_{tet} = J \sum_{\langle ij \rangle} \sigma_i \sigma_j = \frac{J}{2} \left( \sum_{i=1}^{4} \sigma_i \right)^2 + \text{const}$$

- Number of ground states: $N_{gs} = \binom{4}{2} = 6$ for one tetrahedron

$$\mathcal{H}_{pyro} = \sum_{tet} \mathcal{H}_{tet} = \frac{J}{2} \sum_{tet} \left( \sum_{i \in tet} \sigma_i \right)^2$$

- Pauling estimate: ground-state constraints independent

$$N_{gs} = 2^n \left( \frac{6}{16} \right)^{n/2} = \left( \frac{3}{2} \right)^{n/2} \Rightarrow S_0 = \frac{1}{2} \ln \frac{3}{2}$$
Spin ice \textit{Anderson 1956}

- $\text{Ho}_2\text{Ti}_2\text{O}_7$ (and $\text{Dy}_2\text{Ti}_2\text{O}_7$) are pyrochlore Ising magnets which do not order at $T \ll \Theta_W$ \textit{Bramwell+Harris}

- Residual low-$T$ entropy: Pauling entropy for water ice $S_0 = (1/2) \ln(3/2)$ \textit{Ramirez et al.}:
Spin ice and the ice rules

\[ H = -E \sum_i \left( \hat{d}_{\kappa(i)} \cdot S_i \right)^2 + J \sum_{\langle ij \rangle} S_i \cdot S_j = -(J/3) \sum_{\langle ij \rangle} \sigma_i \sigma_j \]

- Spins, \( S_i \), are forced to point along local [111] axes, \( \hat{d}_{\kappa(i)} \)
  \( \Rightarrow \) anisotropy, \( E \), generates Ising pseudospins: \( S_i = \sigma_i \hat{d}_{\kappa(i)} \)
- There are four sublattices, \( \kappa \), with \( \hat{d}_\kappa \cdot \hat{d}_{\kappa'} = -1/3 \)
  \( \Rightarrow \) \( J \) for pseudospins changes sign!
- Ground states have \( \sum \sigma_i = 0 \) for each tetrahedron
- These are the two-in, two-out states (Bernal-Fowler ice rules)
Dipolar spin ice: the real Hamiltonian

- The ice model is not the correct microscopic starting point
- Real interactions, $D$, are mainly dipolar: long-ranged!

$$D_{ij} = \frac{S_i \cdot S_j - 3(S_i \cdot \hat{r}_{ij})(S_i \cdot \hat{r}_{ij})}{r_{ij}^3}$$

- **Question:** Why is Pauling entropy (from nearest-neighbour model) measured in dipolar spin ice??? Siddharthan+Shastry

- Simulations including truncated Bangalore group and especially Ewald-summed Waterloo group dipolar interactions give reasonable agreement with experimental data.
‘Self-screening’ of dipolar interaction \textit{Gingras et al.}

- **Crucial observation**: Spectra of n.n. and dipolar interactions are very similar in mean-field

“In other words, there must be an almost exact symmetry fulfilled in this system when long-range dipolar interactions are taken into account. However, the same long-range nature of these interactions renders it difficult to construct a simple and intuitive picture of their effects ...” \textit{den Hertog+Gingras, PRL 2000}
Enforcing the ice rules by projection: $\mathcal{P}$

- Degeneracy $\Rightarrow$ local zero-energy modes $\Rightarrow$ flat bands

- At low $T$, only modes in flat bands are populated
  - deforming finite-energy bands without consequence
  - can replace $\mathcal{J}$ by a projector, $\mathcal{P}$
    $\Longrightarrow$ all non-zero modes cost the same energy
  - must keep eigenvectors the same!
Our model dipolar interaction: $\mathcal{P}$

\[ \mathcal{D} = \frac{8\pi}{3} \mathcal{P} + \Delta \quad \text{with} \quad \Delta \sim O(1/r^{5}) \]

- Ice rules imply conservation law for $S_{i}$
  \[ \sum_{i \in \text{tet}} \sigma_{i} = 0 \Leftrightarrow \nabla \cdot S = 0 \Rightarrow S = \nabla \times A \]

- Ground states differ by reversing spins around closed loop, for which average $\langle S \rangle = 0$

- upon coarse-graining: low average $\langle S \rangle$ preferred $\Rightarrow E \sim (\nabla \times A)^{2}$
  $\Rightarrow$ artificial magnetostatics
**Intrinsic vs. emergent gauge structure**

- Magnetostatic interaction, $\mathcal{D}$, between real dipoles also
  \[ \nabla \cdot \mathbf{B} = 0 \text{ and } E \sim (\nabla \times \mathbf{A})^2 \]
- Nonetheless: geometric coincidence that $\mathcal{D} \propto \mathcal{P}$ (only Ising)
- almost flat lines for Gd$_2$Ti$_2$O$_7$ probably similar origin
- Ising ground states of $\mathcal{J}$ and $\mathcal{P}$ the same $\Rightarrow$ Ramirez expt!

\[ |0\rangle = \sum_{\mu=1,2} \sum_{q} a_\mu(q) |v_\mu(q)\rangle \]
- only made out of modes $|v_\mu(q)\rangle$ in flat bands $\mu = 1, 2$
- $|S| = 1 \Rightarrow$ nonlinear constraints on amplitudes $a_\mu(q)$, which need not be resolved (we know the ground states!)

- $\mathcal{D}$ and $\mathcal{P}$ differ at lowest $T$; $\mathcal{J}$ and $\mathcal{P}$ at any $T > 0$
Reconstructing $D = \frac{8\pi}{3} P + \Delta$: note the gap

\[
\begin{array}{c|c}
\mathcal{J} & \mathcal{P} \\
\mathcal{P} + \Delta_{nn} & \mathcal{P} + \Delta_{nn} + \Delta_{fn}
\end{array}
\]
**How to distinguish $\mathcal{D}$, $\mathcal{P}$ and $\mathcal{J}$**

### $\mathcal{D}$ vs. $\mathcal{P}$:
- $\Delta$ gives weak dispersion to flat bands
  $\Rightarrow$ ordering expected at low $T$
  Bangalore+Waterloo groups
- ordering not observed experimentally

### $\mathcal{J}$ vs. $\mathcal{P}$:
- Long-range $\mathcal{P}$ – long-range correlations even at high $T$:
  $$\langle S_i S_j \rangle \propto -\frac{\mathcal{P}_{ij}}{T} \sim \frac{1}{Tr^3}$$
- Short-range $\mathcal{J}$ – short-range correlations at any $T > 0$:
  $$\xi \propto \exp(2J/3T)$$
Why spin ice obeys the ice rules

Projective equivalence of emergent and intrinsic gauge structure

• Ground states of n.n. $J$ and model dipole $P$ identical
• Real dipole $D$ deviates from $P$ only at short distances
• Finite-$T$ properties differ

Dipolar spins are ice because ice is dipolar

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