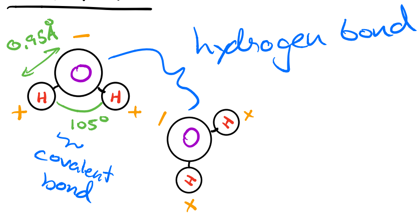
A Brief Introduction to (Quantum) Spin Ice

Laumann 9/4/19

Water Ice

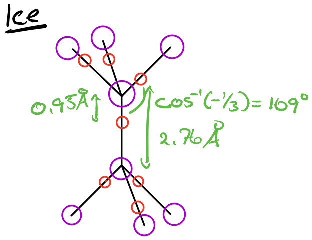


H_2O is shaped like a boomerang.

Strongly polarized.

forms O–H···O hydrogen bonds.

Ice



In ice, each O hydrogen bonds 4 neighbors.

2 H's close to O, 2 far. "2-in, 2-out"

Bernal, Fowler 1933

Even if O's form regular crystal, many possible orientations for H_2O molecules. ⇒ residual entropy.

Pauling (1935) estimated this configurational entropy:

Estimate 1 (orientation is d.o.f., bonds give constraints)

1) $6 = \binom{4}{2}$ orientations of each molecule

2) $1/2$ chance that adj. molecules agree

$$\# \text{ of configs} = 6^{N_{H_2O}} (1/2)^{N_e} = \left(6 \cdot \frac{1}{4}\right)^{N_{H_2O}} = \left(\frac{3}{2}\right)^{N_{H_2O}} \qquad N_e = 2N_{H_2O}$$

Estimate 2 (bond is d.o.f., molecule gives constraint)

1) 2 H positions per edge

2) $\frac{6 \text{ configs}}{16 \text{ possible}}$ for each molecule

$$\# = 2^{N_e} (6/16)^{N_{H_2O}} = (3/2)^{N_{H_2O}}$$

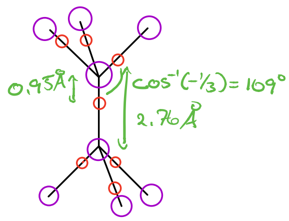
Comments ① Local constraint counting → shouldn't be exact.

② $S_{\text{Pauling}} = N \ln 3/2 \sim 0.405 N$

$S_{\text{expt}} \sim 0.44 N$ (from 1935) 10% agreement!

Spin Ice

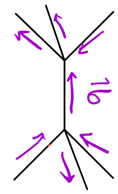
Magnetic materials where ice rules emerge for spin d.o.f.



Replace hydrogen ⟶ bonds by Ising spins pointing along bonds

2 level
easy axis

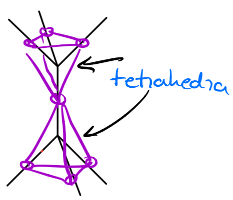
spin points to H



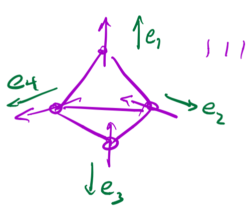
Ice states satisfy "2-in, 2-out"

Where does this happen?

Lattices with corner-sharing tetrahedra and easy-axis Ising spins



Magnetic atom at midpoints of 4 bonds surrounding O's in original water ice



On tetrahedron, all spins interact with same strength.

$$J_0 \sum_{i,j \in \triangle} \bar{\sigma}_i \cdot \bar{\sigma}_j = J_0 \Big(\sum_{i \in \triangle} \bar{\sigma}_i \Big)^2 + \text{constant}$$

$$\bar{\sigma}_i = \pm \bar{e}_i = \sigma_i \bar{e}_i \qquad \text{easy axis + Ising}$$

Q? Should J_0 be FM (<0) or AF (>0)?

for 2in-2out, ferromagnetic! $\bar{e}_i \cdot \bar{e}_j = -1/3$

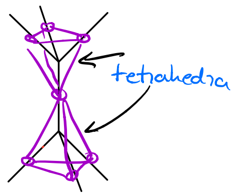
Short calculation: $\underbrace{-\tfrac{2}{3} J_0}_{J>0} \Big(\sum_i \sigma_i \Big)^2$

∴ minimize $\sum_i \sigma_i$: 2 in - 2 out

Notice $\sum_i \sigma_i = \sum_i \bar{\sigma}_i \cdot \hat{e}_i = (\text{div } \bar{\sigma})_\triangle$ is lattice divergence of spin field @ tetrahedron.

outward

Lattice of Tetrahedra



$$H = J_0 \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j = J_0 \sum_{\substack{\text{tetrahedra} \\ \alpha}} \sum_{ij \in \alpha} \vec{\sigma}_i \vec{\sigma}_j$$

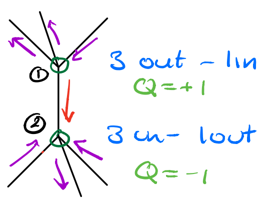
$$= J \sum_{\alpha} (\text{div } \vec{\sigma})_{\alpha}^2 \quad + \quad \text{constant}$$

Ground state: $\text{div}\,\vec{\sigma} = 0 \iff$ 2in − 2out everywhere

Ice States!

Excitations

Flip a spin relative to an ice state:



$$\Delta E = J \Big(\sum_{①} \sigma_i\Big)^2 + J \Big(\sum_{②} \sigma_i\Big)^2$$

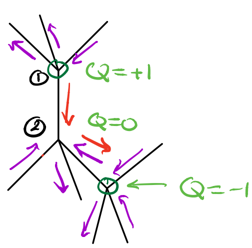
$$= J(+2)^2 + J(-2)^2 = 4JQ^2 + 4JQ^2$$

$$\equiv 2\Delta$$

Energy cost Δ on two tetrahedra with ice rule violations.

Define $Q_{\alpha} = \text{div}_{\text{lattice}} \frac{\vec{\sigma}}{2}$ "charge" on site α

Flip another spin:

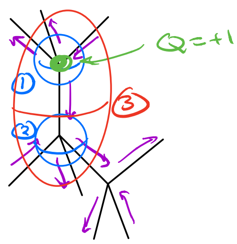


Moves violation, no ΔE.

Charges energetically free to move independently

Classical fractionalization of underlying spin.

Gauss' Law



The definition

$$Q_\alpha = \frac{1}{2}(\mathrm{div}\,\bar{\sigma})_\alpha$$

is Gauss' law in "lattice differential" form.

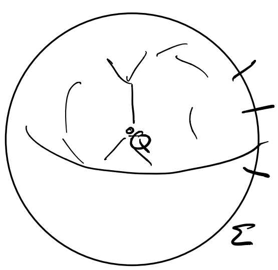
It says $\bar{\sigma}$ flux out of ① is charge 1 $\left(\frac{3\text{out} - 1\text{in}}{2}\right)$

$\bar{\sigma}$ flux out of ② is 0. $(2\text{out} - 2\text{in})$

Since internal flow cancels,

$\bar{\sigma}$ flux out of ③ is 1 $\frac{(4\text{out} - 2\text{in})}{2}$

More generally, "lattice integral" form



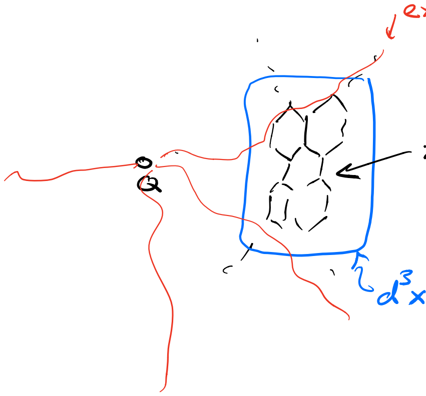
$$Q_{\text{inside}} = \frac{1}{2}\oint_{\Sigma} \bar{\sigma}\cdot d\bar{a} \underset{\text{lat}}{=} \frac{1}{2}\sum_{\substack{\text{bonds}\\ \text{on surface}}} \sigma_i\,(\overset{\text{outward}}{\pm})$$

holds for every configuration.

Thus, it also holds averaging over all $\bar{\sigma}$ states consistent w/ Q:

$$Q_{\text{inside}} = \frac{1}{2}\oint_{\text{lattice}} \langle\bar{\sigma}\rangle\cdot d\bar{a}$$

Coarse graining:



really local magnetization

calling it $\tilde{\bar{E}}$ to emphasize Gauss

$\tilde{\bar{E}}(x) \sim$ Average $\langle\bar{\sigma}_i\rangle$ over $d^3x \gg a^3$

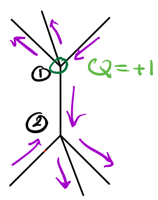
Expect coarse grained Gauss' law:

$$\oint \tilde{\bar{E}}\cdot d\bar{a} = \tilde{Q}_{\text{inside}}$$

In isotropic lattice:

$$\tilde{\bar{E}} \propto Q\,\frac{\hat{r}}{R^2}$$

<u>Entropic Interactions</u>



Consider spin ice with a charge at ①:

3 out - 1 in has $4/16 < 6/16$ local configs

Entropy from tetrahedron ① $\Delta S \sim \ln 2/3 < 0$

Away from charge, all tetrahedra satisfy 2 in - 2 out

<u>but</u> $\langle \vec{\sigma} \rangle \propto \vec{\tilde{E}} \neq 0$

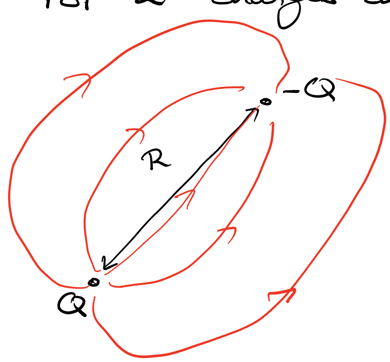
Estimate using coarse grained theory for small $\vec{\tilde{E}}$:

$$\Delta S = -\int d^3x \;\; \alpha \vec{\tilde{E}}^2 + \cdots$$

scalar

suppression from local $\langle \vec{\sigma} \rangle$ bias in d^3x

Put 2 charges in:



$\vec{\tilde{E}}$ physical dipole field

But ΔS is like energy in usual E&M

$$\Delta S_{int}(R) \propto \frac{Q^2}{R} \qquad (\text{large } R)$$

Attractive entropic interaction is pure Coulomb in nearest-neighbor model!

At finite T, should really consider free energy: $F_{INT} \propto -\frac{TQ^2}{R}$

Dipolar Spin Ice and Magnetic Monopoles (Castelnovo, Moessner, Sondhi 08)

If $\bar\sigma$ carries real magnetic moment:

$$\bar\mu = g\mu_B\bar\sigma$$

then "charges" Q produce monopole fields in $\bar M = \langle\bar\mu\rangle = m\frac{\hat r}{R^2}$

Similarly the macroscopic $\bar H$ field satisfies

$$\bar\nabla\times\bar H = \bar J_f = 0$$

$$\bar\nabla\cdot\bar H = -\bar\nabla\cdot\bar M = -Q\delta(\bar r)$$

$$\Longrightarrow \quad \bar H = -m\frac{\hat r}{R^2}$$

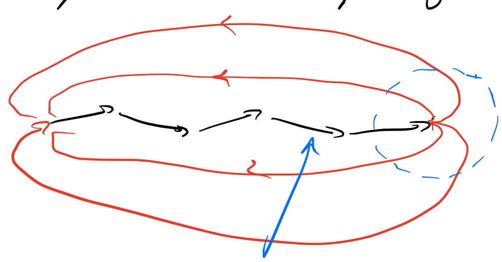
So "charges" carry physical magnetic monopole field!

lec1

Comments:

1) Literature splits on calling Q magnetic monopoles
"electric" charges
spinons

2) Physical m not quantized by Dirac argument (H, not B)



Monopole field

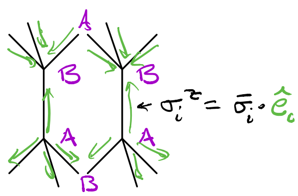
Spin chain "Dirac string" → not fundamental
fluctuating

3) Dipole-dipole coupling $\bar\mu_i\frac{(\mathbb{1}-3\hat r_{ij}\hat r_{ij})}{r^3}\bar\mu_j$ maps to effective energetic Coulomb interaction between Q's
↳ spin ice picture still OK.

Quantum Spin Ice (μ-scopics)

3^{rd} Law of Thermodynamics: $S(T\to 0)\to 0$

Something has to lift GS entropy



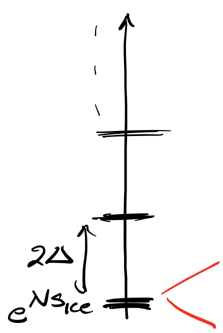
Crystal symmetry and/or time reversal protects on-site Ising doublet,

$$H = J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \; + J_\perp \sum_{\langle ij \rangle} \left(\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+ \right)$$

XY QSI

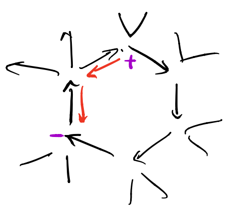
$\pm$ wrt local axis
(orient say A→B everywhere)
on Pyrochlore

Simplest symmetry allowed interaction



How lifted?

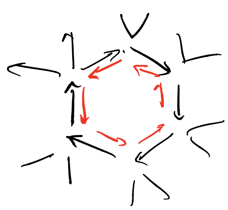
Perturbation Thy on Ice manifold:



$J_\perp$ term creates 2 charges → pays 2Δ

If charge exists, hops @ no cost
(by 2 sites)

Leading term in degen pert thy is ring exchange $g \sim \frac{J_{\pm}^3}{\Delta^2}$



$$\mathcal{H}_{eff} = g \sum_{\hexagon} \sigma^+ \sigma^- \sigma^+ \sigma^- \sigma^+ \sigma^- + h.c.$$

- Think of σ^z as E field on bond
- Ring exchange causes resonance in alternating E loops

↳ cos curl A in lattice QED

Emergent Local U(1) Symmetry

In ice manifold, $(\bar{\nabla} \cdot \bar{\sigma})_\alpha = \sum_{i \in \alpha} \sigma^z = 0$, so:

$$G(\theta_\alpha) = \underbrace{e^{i\theta_\alpha \sum_{i\in\alpha} \sigma^z}}_{\text{local } U(1) \text{ symmetry}} |ice\rangle = |ice\rangle$$

local U(1) symmetry → conservation of 2in-2out

Notice

$$G: \sigma_i^+ \longrightarrow e^{i\theta_\alpha} \sigma_i^+ e^{i\theta_{\alpha'}} \qquad \sigma_i^+ \simeq e^{iA_i}$$

So ring exchange is "gauge invariant" lattice Wilson loop.
$\sim \cos(\text{curl}\, \bar{A})$

Pure U(1) Lattice Gauge Theory!

for pure g model → deconfined compact QED phase.

Emergent photon	$\bar{a}$	⟷	linearly dispersing transverse of spin ice excitations
Charges	Q	⟷	half of spin flip gapped by Δ
Magnetic monopoles	M	⟷	gapped of order g

[Evidence: – analysis of RK point in related dimer models]
– perturbative formal lattice gauge thy mapping
– ED + QMC: deconfined for $\frac{J_\perp}{J} < \sim \frac{1}{10}$