Structure Factor

- In spin ice, there is no incipient ordered state: feature in correlations is more subtle than a peak
- Coarse-graining argument: correlations are governed by *effective free energy*

$$H_{\text{eff}} = \int d^3r \, \frac{c}{2} |\vec{b}|^2$$

- Need to calculate

$$\langle b_\mu(r) b_\nu(r') \rangle = \frac{1}{Z} \int [d\vec{b}(r)] \boxed{\delta[\vec{\nabla} \cdot \vec{b}]} b_\mu(r) b_\nu(r') \, e^{-\beta H_{\text{eff}}[\vec{b}]}$$

Structure factor

- Fourier $$H_{\text{eff}} = \sum_k \frac{c}{2} |\vec{b}_k|^2$$
- Constraint $$\vec{\nabla} \cdot \vec{b} = 0 \qquad b_z = -(k_x b_x + k_y b_y)/k_z$$

$$H_{\text{eff}} = \sum_k \frac{c}{2} B_k^\dagger \begin{pmatrix} 1 + \frac{k_x^2}{k_z^2} & \frac{k_x k_y}{k_z^2} \\ \frac{k_x k_y}{k_z^2} & 1 + \frac{k_y^2}{k_z^2} \end{pmatrix} B_k \, , \quad B_k = \begin{pmatrix} b_x \\ b_y \end{pmatrix}$$

- Structure factor

$$\langle b_\mu(r) b_\nu(r') \rangle = \frac{1}{N} \sum_k \langle b_\mu^*(k) b_\nu(k) \rangle e^{ik\cdot(r-r')}$$

Gaussian integrals

- General rule

$$\beta H = \frac{1}{2}\sum_{ij} K_{ij} x_i x_j$$

$$\langle x_i x_j \rangle = \frac{1}{Z}\int [\prod_k dx_k] x_i x_j e^{-\beta H}$$

$$= \left[K^{-1}\right]_{ij}$$

- Proved in many many references...

Proof

- Generating function

$$\langle e^{\sum_i q_i x_i} \rangle = \frac{1}{Z} \int [\prod_k dx_k] e^{-\frac{1}{2}\sum_{ij} K_{ij} x_i x_j + \sum_i q_i x_i}$$

- Shift

$$x_i \to x_i + \sum_j [K^{-1}]_{ij} q_j$$

- Result

$$\langle e^{\sum_i q_i x_i} \rangle = e^{\frac{1}{2}\sum_{ij} [K^{-1}]_{ij} q_i q_j}$$

- Differentiating twice gives $\langle x_i x_j \rangle = \left[K^{-1}\right]_{ij}$

Gaussian integrals

- General rule: invert the quadratic form

$$\langle b_\mu^*(k) b_\nu(k)\rangle = \frac{k_B T}{c} \begin{pmatrix} 1+\frac{k_x^2}{k_z^2} & \frac{k_x k_y}{k_z^2} \\ \frac{k_x k_y}{k_z^2} & 1+\frac{k_y^2}{k_z^2} \end{pmatrix}^{-1}$$

- With some algebra

$$\langle b_\mu^*(k) b_\nu(k)\rangle = \frac{k_B T}{c} \left(\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2} \right)$$

- We could have guessed this!

$$\sum_\mu k_\mu \langle b_\mu^*(k) b_\nu(k)\rangle = 0$$

Power law correlations

- Neutrons

$$\mathcal{S}(k) = \sum_{\mu\nu} (\delta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2}) \mathcal{S}_{\mu\nu}(k)$$

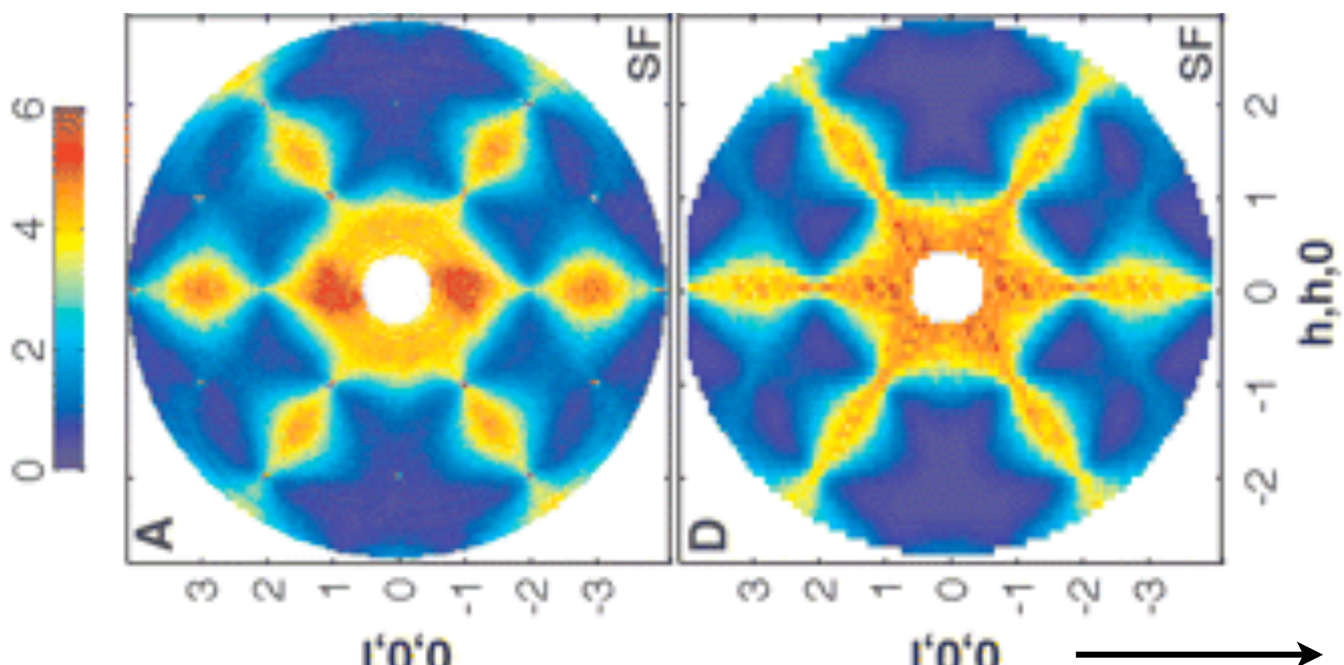
- Measured near a reciprocal lattice vector

$$\mathcal{S}(K_{002} + k) = \mathcal{S}_{xx}(K + k) + \mathcal{S}_{yy}(K + k)$$

$$\approx 2 - \frac{k_x^2 + k_y^2}{k^2} = 1 + \frac{k_z^2}{k^2}$$

- Not a peak but a singularity

pinch points in $Ho_2Ti_2O_7$



k_z

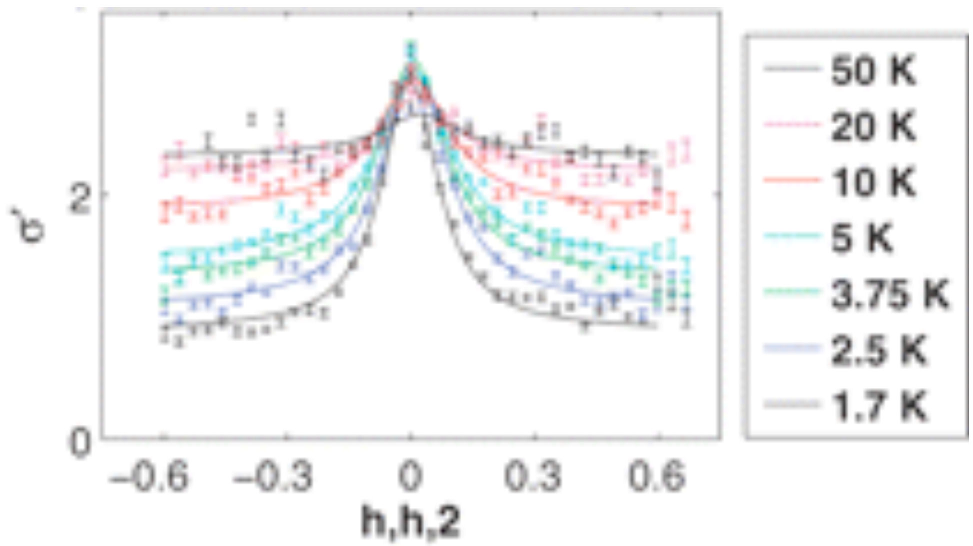
experiment theory

T. Fennell *et al*, 2009

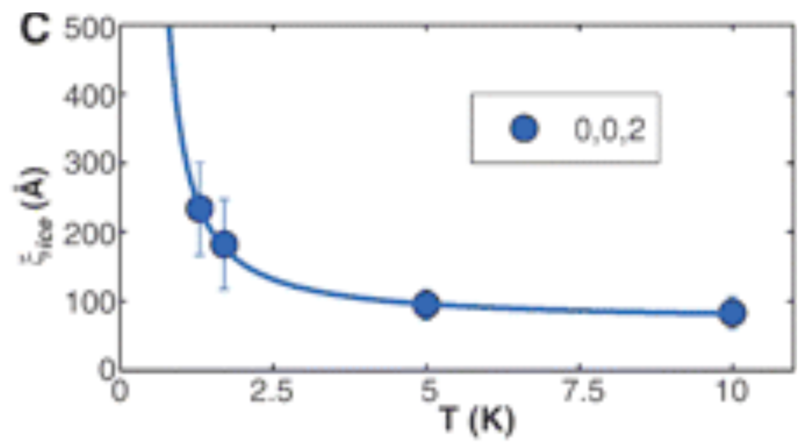
$$\mathcal{S}(K_{002}+k) \sim \frac{k_z^2}{k^2}$$

vanishes for k_z=0

Quality of singularity



pinch point sharpens
with lower T

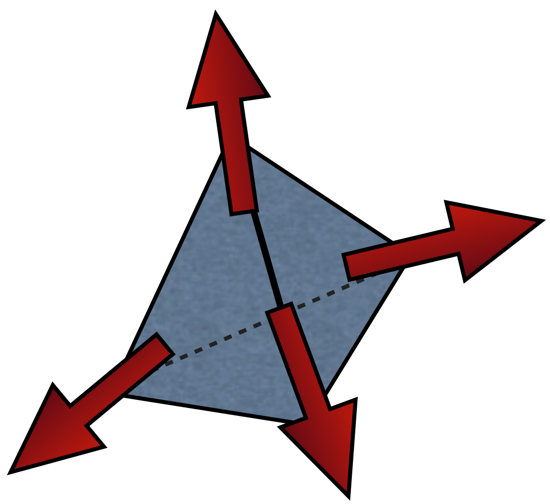


"Correlation length" for
rounding of pinch point

Roughly $\xi \sim e^{1.8K/T}$

Defects

- The ice rules constraint is not perfectly enforced at $T>0$
- Primitive defect is a "charged" tetrahedron with $\sum_i \sigma_i = \pm 1$.



costs energy $2J_{eff}$

What to call it?

- Consider Ising "spin"

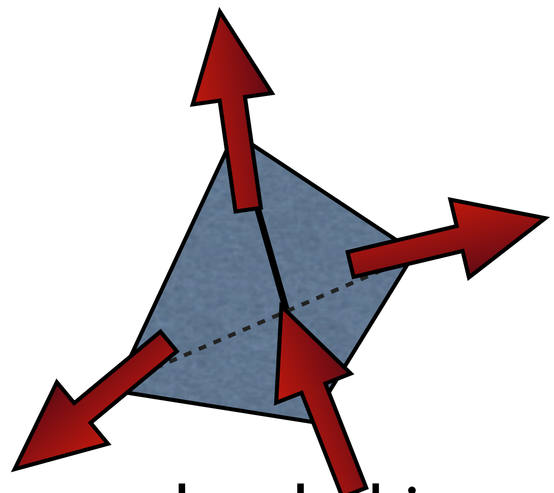
$$S^z_{\mathrm{TOT}} = \sum_i \sigma_i = \frac{1}{2}\sum_t S^z_t$$

- Single flipped tetrahedron has $S^z_{\mathrm{TOT}} = \pm 1/2$
  - "spinon"? (M. Hermele *et al*, 2004)
  - But S^z is not very meaningful in spin ice
- Use magnetic analogy: *magnetic monopole*

Magnetic monopoles

Castelnovo *et al*, 2008

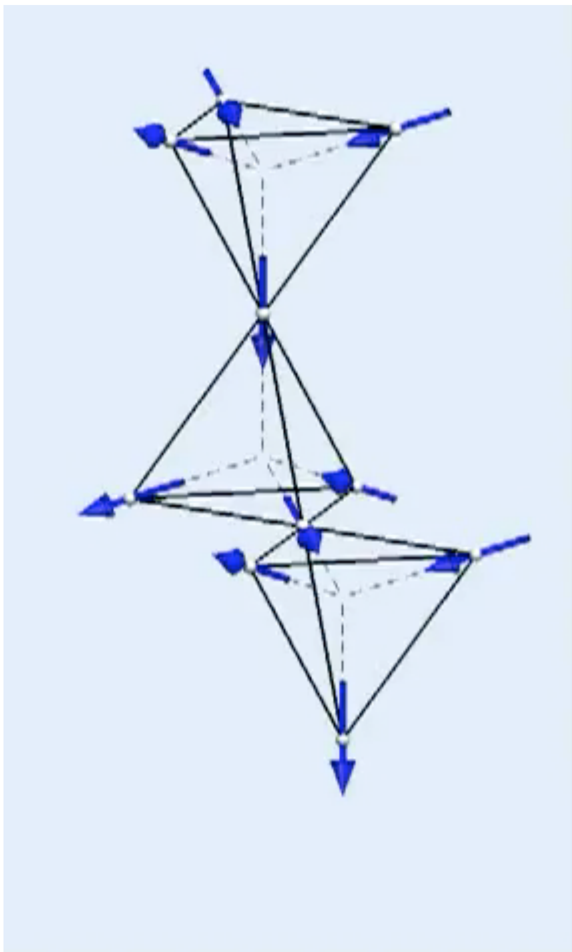
- Defect tetrahedra are sources and sinks of "magnetic" flux



div b = 1

- It is a somewhat non-local object
  - Must flip a semi-infinite string of spins to create a single monopole
  - Note similarity to 1d domain wall

String



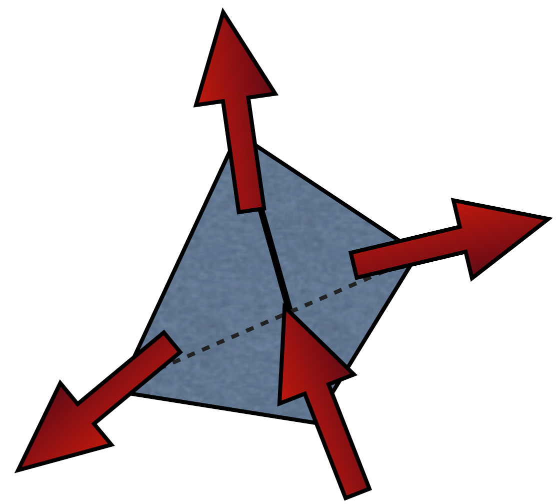
stolen (by somebody else on youtube)
from Steve Bramwell

- Note that the string is tensionless because the energy depends only on $\sum_i \sigma_i$ on each tetrahedra
    - In an ordered phase, this would cost energy
- Once created, the monopole can move by single spin flips

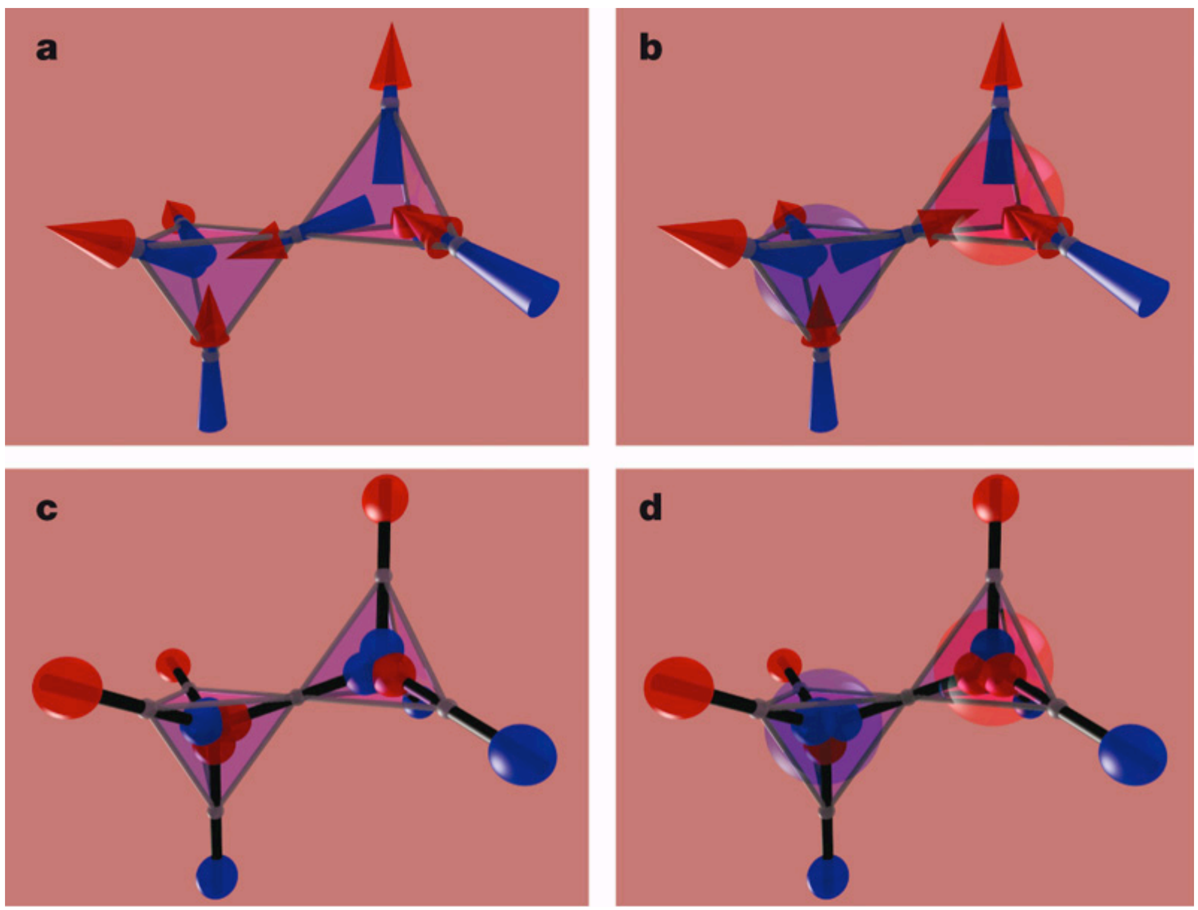
Monopoles are “real”

Castelnovo *et al*, 2008

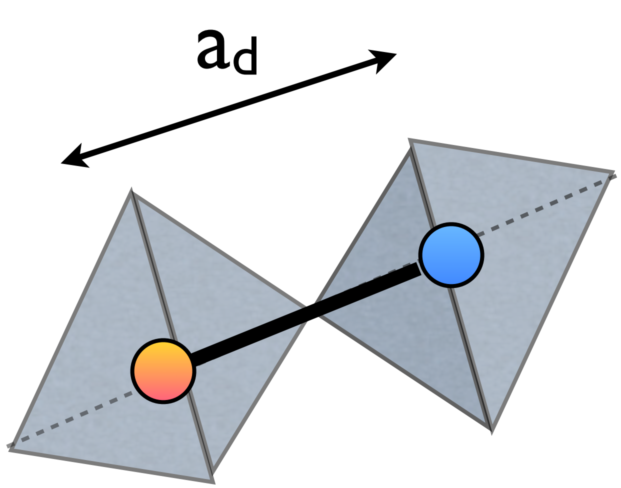
- Monopoles actually are sources for (internal) magnetic field
  - Magnetization $M \propto b$
  - hence $\mathrm{div}\, M \sim \mathrm{div}\, H \sim q\, \delta(r)$
- Actual magnetic charge is small



Monopoles for dumbbells



Dumbbell model



magnetic charge ±q $q = \mu / a_d$

Dy, Ho $\mu \approx 10 \mu_B$

potential
$$V_{qq} = \frac{\mu_0}{4\pi} \frac{q_a q_b}{r_{ab}}$$
$$= \frac{\mu_0}{4\pi} \frac{\mu^2}{a_d^2} \frac{1}{r_{ab}}$$

Coulomb
$$V_{ee} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{r}$$