1/28

Introduction to Classical Frustrated Magnetism

Let's unpack the title

- Magnets
  - Focus on systems with well-defined local moments
  - Almost isolated ions with partially filled shells.
  - Magnetism arises from Hund's rule e.g.

$$\uparrow\ \uparrow\ e_g$$

$$\text{Mn} \quad [\text{Ar}]\, 4s^2\, 3d^5 \qquad Mn^{2+} \quad \uparrow\ \uparrow\ \uparrow$$

$$t_{2g}$$

$Z = 25$

Local atomic physics
(e.g. spin orbit, crystal fields) $\Rightarrow$
wide variety of magnetism

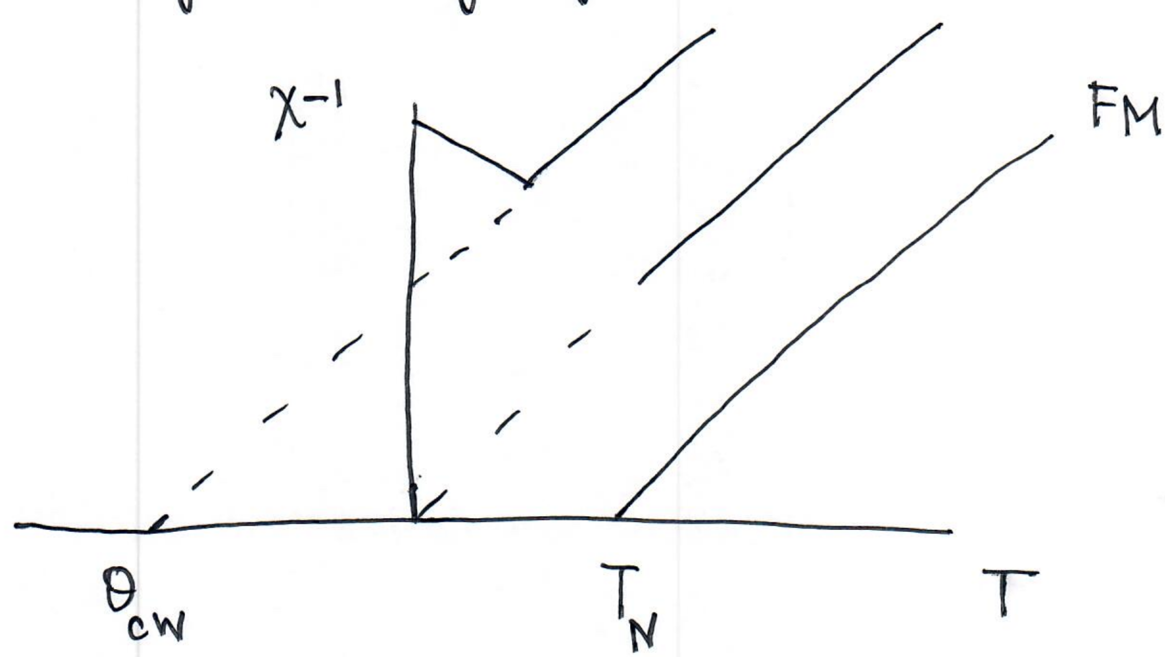
Experimental Identification

- electrically insulating $\rho \sim e^{E_g/T}$

- Curie susceptibility

$$\chi = \lim_{H \to 0} \frac{M}{H}$$

Signature of free moments



Ferromagnetism $\uparrow \uparrow \uparrow \uparrow$

Let's calculate the net magnetic moment of a system of electrons in a solid

Magnetization

$$M = \frac{\vec{\mu}}{V} \qquad E = -\vec{\mu} \cdot \vec{B}$$

Lorentz force $\vec{F} = q(\vec{E} + \vec{v} \times \vec{B})$

$\vec{F} \perp \vec{v}$ No work done.

$E \neq E(B)$

classically magnetization = 0!

Quantum Mechanics Necessary for Magnetism

(Bohr - van Leeuwen Theorem)

Niels Bohr 1911

Hendrika Johanna von Leeuwen 1919

No thermal equilibrium magnetization in classical systems.

Basic Idea

Z for N particles of charge q

$$Z \sim \int\int\int \exp - \beta E(r_i, p_i) \, dr_1 \dots dr_N \, dp_1 \dots dp_N$$

$r_i \rightarrow$ position

$p_i \rightarrow$ momenta

6N dimensional phase space

(3N positions, 3N particles)

$B \neq 0 \qquad p \rightarrow p - qA$

Limits of integral $-\infty \rightarrow +\infty$

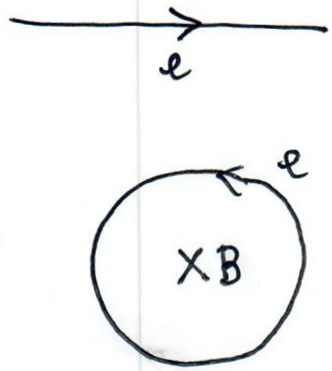
shift absorbed by shifting origin of momentum integration

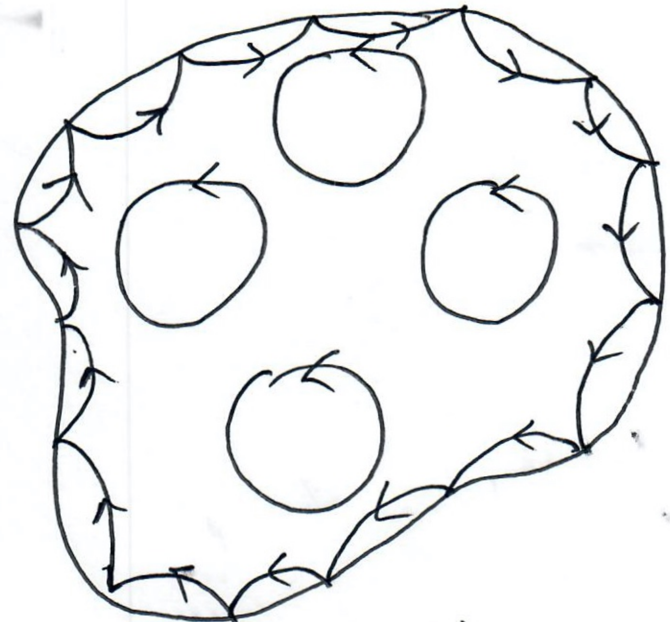
$\Downarrow$

$Z \neq Z(B), \quad F \neq F(B).$

Result Intuitively Surprising

classical electrons





Quantum Mechanics Needed!

$\vec{M} = 0.$

Interaction between Spins

Heisenberg Model

$$H = J \sum_{ij} \vec{S}_i \cdot \vec{S}_j$$

$J < 0$ FM

$J > 0$ AFM

$$\chi \sim \frac{A}{T \mp T^*}$$

AFM : A Brief History

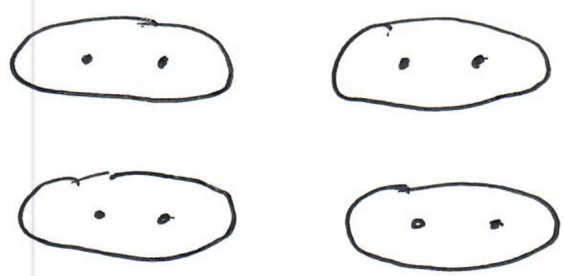
$\uparrow \downarrow \uparrow \downarrow \uparrow \downarrow$ (Néel).

Problem: $\uparrow\downarrow\uparrow\downarrow$ <u>not</u> ground state

($\vec{m}$ is not a conserved order parameter)

Landau

singlet $\frac{1}{\sqrt{2}} \left\{ |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right\}$.



Bethe's exact solution of $s = 1/2$ AFM

power-law (critical)

$\Downarrow$

philosophically extended to higher d?

(No LRO).

Magnetic Moments of Neutrons $\Rightarrow$ Magnetic Moments of Electrons.

MnO (NaCl)

X-rays chemical unit cell $a = 4.43$ Å

Neutrons 235 K $a = 4.43$ Å

80 K $a = 8.85$ Å

Spins parallel in [111] plane / antiparallel in adjacent ones.

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \propto M_i^2 \cos \vec{Q} (\vec{R}_i - \vec{R}_j)$$

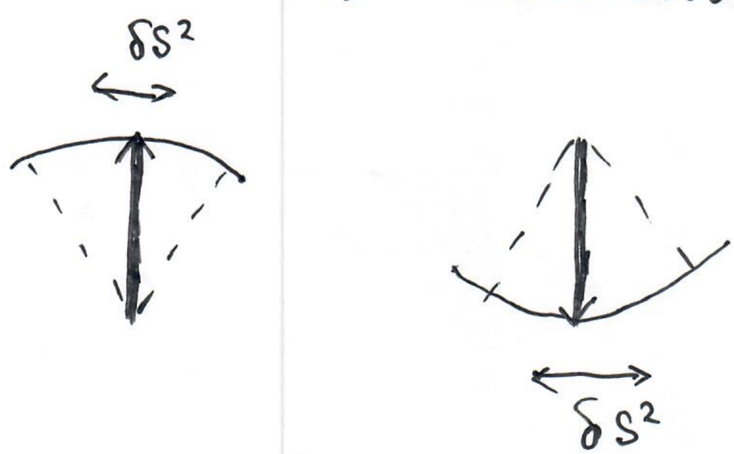
$$\vec{Q} = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a} \right).$$

1952 Anderson / Kubo Semiclassical Theory

Analogy with quantum harmonic oscillators

(zero-point energy neglected previously)

AFM = Semiclassical Spins + Zero Point Fluctuations



Fast, slow degrees of freedom

Reduction in sublattice magnetization $O\left(\frac{1}{zS}\right)$

$$\delta M \sim \int d^d q \left\{ n(\omega_q) + \frac{1}{2} \right\} \frac{1}{\omega_q}$$

$T \gg \omega$ $\qquad$ $T \ll \omega$

$$\delta M \sim \int d^d q \, \frac{T}{\omega_q^2} \qquad \delta M \sim \int \frac{d^d q}{\omega_q}$$

We can get a feeling for this w/ SHO.

Equipartition Theorem

$$\frac{1}{2} m\omega^2 \langle x^2 \rangle \sim kT \qquad \text{classical}$$

$$\langle x^2 \rangle \sim \frac{kT}{\omega^2}$$

$$\frac{1}{2} m\omega^2 \langle x^2 \rangle \sim \hbar\omega$$

$$\langle x^2 \rangle \sim \frac{1}{\omega} \qquad \text{quantum}$$

AFM d-dimensional hypercubic lattice $\omega_q \sim q$

$T = 0$ $d = 1$ ✗

$d \geq 2$ ✓ Neel order OK

$T \neq 0$ $d \geq 3$ Neel order OK

Neutrons - excellent agreement with zero point fluctuations in $\vec{M}$

2D Heisenberg model

$T = 0$ Neel

$T \neq 0$ Disordered (PM)

Aside: 1973 Anderson Distinct <u>absence</u> of 2D $s = 1/2$ AFMs

low d, low spin frustrated systems

could quantum fluctuations $\Rightarrow$ destroy LRO?

1987 $La\,Cu\,O_4$ 2D $s = 1/2$ AFM

Doped semimetallic $\rightarrow$ superconducting state

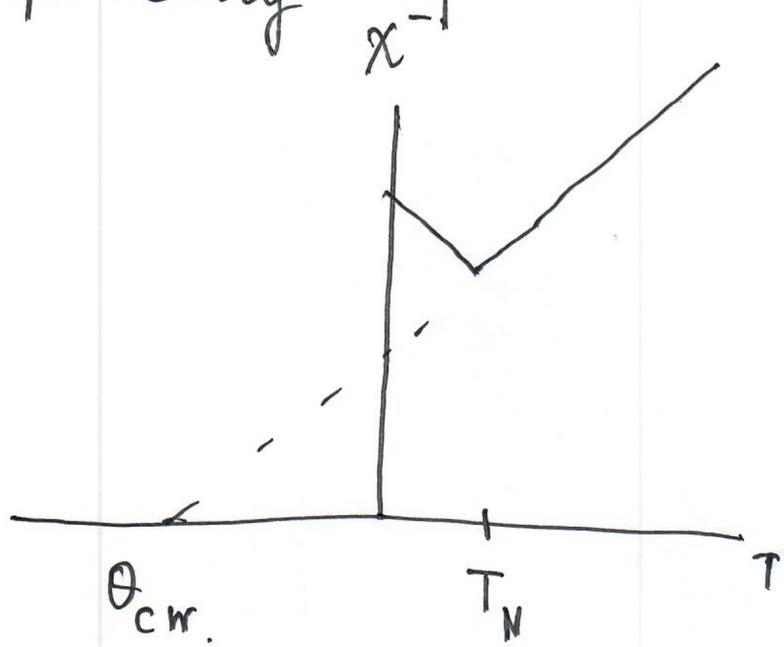
Suggestion (Anderson) Large q. fluctuations $\Rightarrow$ destroy magnetism

"Spin Liquid" + charge

new # type of Superconductor?

Frustration

Empirically

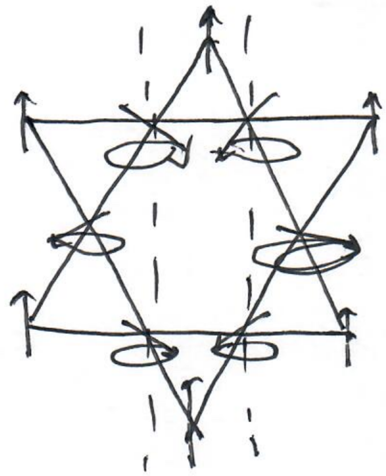


$$f = \frac{|\theta_{cw}|}{T_N} \gg 1.$$

(e.g. 5–10)

Heisenberg systems?

e.g. Kagome



local degeneracy
(soft mode)

Frustration $\Rightarrow$ large ground-state degeneracy

(why corner-sharing ?)

Continuous spins $\Rightarrow$ simple counting argument ("Maxwellian")

$$F \;=\; D \;-\; K$$

F		D		K
$\parallel$		$\parallel$		$\parallel$
# degrees of freedom in the ground state		total # DOF		constraints

(linear algebra $\Rightarrow$ system of K equations for D variables
$\downarrow$
solution space $F = D - K$)

Heisenberg Hamiltonian

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \qquad J < 0 \ (AFM)$$

$\downarrow$ cluster of q spins

$$H = \frac{J}{2} \left(\sum_{i=1}^{q} S_i \right)^2$$

$$= \frac{J}{2} \vec{L}^2 \qquad L = \sum_{i=1}^{q} S_i$$

total spin of unit

ground-states $\Leftrightarrow$ states w $\vec{L} = 0$.

Heisenberg $n = 3$ $\quad L_1 + L_2 + \ldots L_n = 0$

independent of q

Spins w/ n components

$\Downarrow$

n constraints / unit

$\left(\begin{array}{l} n = 2 \ xy \\ n = 3 \ \text{Heisenberg} \end{array} \right)$

q spins / unit

n components

$F = \# \ \dfrac{\text{degrees of freedom}}{\text{unit}}$

share corners

$$F = (n-1) q - n$$

$\downarrow$

$\#$ global rotations

$$K = n$$

$\downarrow$

gd. state constraint

$$D = F - K = \frac{N}{2} \left[(n-1) q - 2n \right]$$

$\downarrow$

gs. degeneracy

$$= \frac{N}{2} \left[n(q-2) - q \right]$$

Heisenberg model on pyrochlore lattice

$$D = \frac{N}{2}\left[6 - 4\right]$$

$$\Downarrow$$

$$\underline{D = N}$$

Spin Ice

Historically first frustrated system $\Rightarrow$ ice.

Entropy measured by Giauque et al.

1956 Anderson

Ice rules work for specific types of pyrochlore systems w/ Ising DOFs.

1997 Holmium Titanate

Ising on pyrochlore.