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.

\[ \text{Mn} \quad [\text{Ar}] 4s^2 3d^5 \quad \text{Mn}^{2+} \quad \uparrow \uparrow \uparrow \quad t_{2g} \]

Z = 25

Local atomic physics
(e.g. spin-orbit, crystal fields) => wide variety of magnetism
Experimental Identification

- electrically insulating $\rho \sim e$

- Curie susceptibility

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

Signature of free moments

$\chi^{-1}$ vs $T$

$\Theta_{cw}$ $T_N$ $T$

Ferromagnetism $\uparrow \uparrow \uparrow \uparrow \uparrow$
Let's calculate the net magnetic moment of a system of electrons in a solid.

Magnetization

\[ M = \frac{\mu}{V} \]

\[ E = -\mu \cdot B \]

Lorentz force

\[ \vec{F} = q \left( \vec{E} + \vec{v} \times \vec{B} \right) \]

\[ \vec{F} + \vec{v} \quad \text{No work done} \]

\[ E \neq E(B) \]

Classically, magnetization = 0!

Quantum Mechanics Necessary for Magnetism

(Bohr - van Leuven Theorem)

Niels Bohr 1911
Hendricka Johanna von Leuven 1919
No thermal equilibrium magnetization in classical systems.

Basic Idea

\[ Z \text{ for } N \text{ particles of charge } q \]

\[ Z \sim \int \cdots \int \exp \left( -\beta E(\mathbf{r}_i, \mathbf{p}_i) \right) \, d\mathbf{r}_1 \cdots d\mathbf{r}_N \]  
\[ \downarrow \quad \text{moments} \]
\[ d\mathbf{p}_1 \cdots d\mathbf{p}_N \]

6N dimensional phase space
(3N positions, 3N particles)

\[ B \neq 0 \quad \mathbf{p} \rightarrow \mathbf{p} - q \mathbf{A} \]

Limits of integral \(-\infty \rightarrow +\infty\)

Shift absorbed by shifting origin of momentum integration

\[ Z \neq Z(B), \quad F \neq F(B). \]
Result: Intuitively surprising

Classical electrons

Quantum Mechanics Needed!

Interaction between spins

Heisenberg Model

\[ H = \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \]

\( J < 0 \) FM

\( J > 0 \) AFM

\( \chi \sim \frac{A}{T + T^*} \)
AFM: A Brief History

\[ \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \] (Néel).

Problem: \[ \uparrow \downarrow \uparrow \downarrow \] not ground state
\((\vec{m} \text{ is not a conserved order parameter})\)

Landau

\[ \text{singlet} \quad \frac{1}{\sqrt{2}} \left\{ \left| \uparrow \uparrow \right> - \left| \downarrow \downarrow \right> \right\}. \]

Bethe's exact solution of \( s = \frac{1}{2} \) AFM

power-law (critical)

\[ \downarrow \]

philosophically extended to higher \( d \)?
\((\text{No LRO}).\)
Magnetic Moments of Neutrons

MnO (NaCl)

X-rays chemical unit cell

Neutrons 23.5 K

80 K

\[ a = 4.43 \, \text{Å} \]

\[ a = 8.85 \, \text{Å} \]

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

\[ \langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle \propto \mathbf{H}_i^2 \times \mathbf{Q} \cdot (\mathbf{R}_i - \mathbf{R}_j) \]

\[ \mathbf{Q} = \left( \frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a} \right) \]
Anderson / Kubo Semiellassical Theory

Analogy with quantum harmonic oscillators

(Zero-point energy neglected previously)

AFM = Semiellassical Spins + Zero Point Fluctuations

\[ \delta S^2 \]

Fast, slow degrees of freedom

Reduction in sublattice magnetization O \( \left( \frac{1}{T^2} \right) \)

\[ \delta M \sim \int d^d q \left\{ n(q) + \frac{1}{2} \int \frac{1}{w_q} \right\} \]

\[ \delta M \sim \int d^d q \frac{1}{w_q^2} \quad T \gg w \]

\[ \delta M \sim \int d^d q \frac{1}{w_q} \quad T \ll w \]
We can get a feeling for this w/ SHO.

**Equipartition Theorem**

\[
\frac{1}{2} m \omega^2 \langle x^2 \rangle \sim kT
\]

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

Classical

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

\[
\langle x^2 \rangle \sim \frac{1}{\omega}
\]

Quantum

---

AFM

\text{d-dimensional rhombohedral lattice}

\[ T = 0 \]

\[ d = 1 \quad \times \]

\[ d \geq 2 \quad \checkmark \]

\[ w_q \sim \theta \]

\[ \text{Nell order OK} \]

\[ T \neq 0 \quad d \geq 3 \]

\[ \text{Nell order OK} \]
Neutrons - excellent agreement with zero point fluctuations in $\bar{\Lambda}$

2D Heisenberg model

$T = 0$ Neel
$T \neq 0$ Disordered (PM)

Aside: 1973 Anderson Distinct absence

of 2D $s = \frac{1}{2}$ AFMs

Unr. d, low spin frustrated systems

Could quantum fluctuations $\Rightarrow$

destroy LRO?

1987 La$_2$CuO$_4$ 2D $s = \frac{1}{2}$ AFM

Doped semimetallic $\Rightarrow$ superconducting state

Suggestion (Anderson)

Large q. fluctuations $\Rightarrow$ destroy magnetism

"Spin Liquid" + charge

New type of superconduct?
Frustration

Empirically \( x^{-1} \)

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

(e.g. 5-10)

Heisenberg systems?
e.g. Kagome

![Diagram of a Kagome lattice with arrows indicating local degeneracy (soft mode).]

Frustration $\Rightarrow$ large ground-state degeneracy

(why corner-sharing?)

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

$$ F = D - K $$

\[ \text{total # of DOF} - \text{# degrees of freedom in the ground state} \]
linear algebra $\Rightarrow$ system of $K$ equations

for $D$ variables

$\downarrow$

solution space $F = D - K$

Heisenberg Hamiltonian

$$H = \frac{J}{2} \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j$$

$J < 0$

(AFM)

cluster of $q$ spins

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

ground states $\Leftrightarrow$ states with $L = 0$.

Heisenberg $n = 3$

$L_i + L_2 + \ldots + L_n = 0$

total spin of unit independent of $q$
Spins w/ n components

n constraints/and

q spins/unit

n components

\[ F = \frac{\# \text{ degeneracy of fractional}}{\text{spin/unit}} \]

\[ F = (n-1)q - n \]

\[ K = n \]

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

\[ \text{gs. degeneracy} = \frac{N}{2} \left[ n(q-2) - q \right] \]
Heisenberg model on pyrochlore lattice

\[ D = \frac{N}{2} \]

Spin Ice

Historically first frustrated system \( \rightarrow \) ice.

Entropy measured by Gianque et al.

1956 Anderson

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

1997 Holmium sulfate

Ising on pyrochlore.