Novel Orders from Geometric Frustration

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• Fa Wang
• Frank Pollman
• Arun Paramekanti, Roger Melko, A. Burkov, L. Balents, D. N. Sheng.

1. Spin phonon induced colinear order and magnetization plateaus in triangular & kagome antiferromagnets. Applications to CuFeO$_2$

2. Extended Supersolid Phase of Frustrated Bosons on the triangular lattice.
   Fa Wang, Frank Pollmann, A.V., arXiv:0809.1667
Geometric Frustration

- Frustration ~ degeneracy of classical ground states.

\[ E = J \sum_{i,j \text{neighbors}} S_i S_j \]

\[ J > 0, S_i = \pm 1 \]

(Classical Spin)

Frustrated systems occur *commonly* in nature: Eg. ICE: Proton site frustration.

**Triangular Lattice:**

\[ \text{# of ground states} = \mathcal{C}_0.323N \]

(N sites)

**Interest:**
- Can realize novel ordered and liquid phases

**Applications:**
- Frustrated spin system - Complex orders can lead to multi-ferroic behavior.
Geometrical Frustration in Ice

[CONTRIBUTION FROM THE CHEMICAL LABORATORY OF THE UNIVERSITY OF CALIFORNIA]

The Entropy of Water and the Third Law of Thermodynamics. The Heat Capacity of Ice from 15 to 273°C.

BY W. F. GIAUQUE AND J. W. STOUT

Residual Entropy of Ice (1936):

\[ S_0 = 0.82 \pm 0.05 \text{cal/mol } ^0\text{K} \]

Idea: **Hydrogens** remain disordered giving entropy

\[ S_{Pauling} = 0.806 \text{cal/mol } ^0\text{K} \]
Geometric Frustration & Relief

Outline

1. Frustration relief by residual interactions
   - eg. complex orders from lattice couplings

   Here – CuFeO₂

2. Selection by quantum/thermal fluctuations

   Here - supersolid order by disorder.

3. Quantum spin liquids.  Strong tunneling

   Candidates Eg. Na₄Ir₃O₈; ‘hyperkagome’; no order T>1% J
Complex Orders From Frustration

- Eg. Cu FeO$_2$ a triangular lattice multiferroic.
  - $S=5/2$, $L=0$. Expect ISOTROPIC spin interactions and 120° state
Complex Orders From Frustration

- **Cu FeO$_2$**
  - Co-linear zigzag state seen.
  - Complex phase diagram in a field including
    - Multiferroic spiral phase
    - 1/5, 1/3 magnetization plateau states.

Also Ferroelectric: P
(Multi-ferroic)
Spin Lattice Coupling

$$E = \sum_{i,j\text{nbhrs}} (J + \partial_i J \cdot [\delta r_i - \delta r_j]) \mathbf{S}_i \cdot \mathbf{S}_j$$

$$+ K \sum_i \delta r_i^2$$

Change in $J$

Integrating out phonons:

$$H = J \left[ \sum_{<ij>} \tilde{S}_i \cdot \tilde{S}_j - c \sum_i \tilde{F}_i^2 \right]$$

$$\tilde{F}_i = \sum_{<ij>} e_{ij} \tilde{S}_i \cdot \tilde{S}_j$$

$$c = \frac{\alpha^2 JS^2}{2K}$$

Restoring force

Generates $(\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{S}_j \cdot \mathbf{S}_k)$ terms

Tchernyshyov et al., Penc et al., Bergmann et al. for pyrochlore

Generally - Phonons enhance colinear order:

Fa Wang and AV, PRL '08.
Magnetization Plateaus and CuFeO$_2$

Spin-Phonon model:

$$H = J \left[ \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j - c \sum_i \vec{F}_i^2 \right]$$

$$\vec{F}_i = \sum_{<j>} \hat{e}_{ij} \vec{S}_i \cdot \vec{S}_j \quad c = \frac{\alpha^2 JS^2}{2K}$$

Good agreement with known phases of Triangular magnet CuFeO$_2$.

Prediction for 1/3 plateau structure.

$\frac{1}{3}$ state

Fa Wang and AV, PRL 2008
Complex Phase Structure of Frustrated Systems

- Violations of “Gibbs Phase Rule” (4 phases meet at a point – due to frustration)
  - \( E_1 - E_2 = E_2 - E_3 = 0 \) (requires 2 parameters)
  - \( E_4 - E_3 = E_4 - E_1 = 0 \) (accidental degeneracy – frustration)

Spin-phonon Phase Diagram in a field
Order by Quantum Fluctuations. Example: Super-solid order from quantum fluctuations

Spin-boson mapping:

\[ S^z = \pm 1/2 \]

\[ n = 1 \]

\[ S^z = -1/2 \]

\[ n = 0 \]

Spin-boson mapping:

\[ H = J_z \sum_{i,j} S_i^z S_j^z \rightarrow J_z \sum_{i,j} (n_i - \frac{1}{2})(n_j - \frac{1}{2}) \]

Repulsion

Quantum Fluctuation: Boson hopping

Bosons on the Triangular lattice:

\[ H = -t \sum_{ij} b_i^* b_j + b_i^* b_j \]

\[ + J_z \sum_{ij} (n_i - 1/2)(n_j - 1/2) \]

\[ t=0 \text{ highly frustrated} \]

Supersolid order on the triangular lattice

\[ H = -t \sum_{ij} b_j^* b_i + b_i^* b_j + J_z \sum_{ij} (n_i - 1/2)(n_j - 1/2) \]

Case 1. If \( t >> J_z \)
uniform superfluid

Case 2. If \( J_z >> t \)
Expect a solid. Charge order (m)

No sign problem – large system sizes can be studied with Quantum Monte Carlo

Melko, Paramekanti, Burkov, A.V., Sheng and Balents, PRL 06; Haiderian and Damle; Wessel and Troyer
Supersolid order on the triangular lattice

\[ H = -t \sum_{ij} b_i^* b_j + b_i^* b_j + J_z \sum_{ij} (n_i - 1/2)(n_j - 1/2) \]

Case 1. If \( t \gg J_z \)
uniform superfluid

Case 2. If \( J_z \gg t \)
Charge order \((m)\) AND superfluid \((\rho_s)\)
high & low density

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![Graphs showing \( \rho_s \) and \( m^2 \) vs. \( 1/L \) for different values of \( J_z \).]
Origin of Super-solidity

Consider: $J_z >> t$

$|\psi_\alpha\rangle = \begin{cases} \text{Classical Ising States} & \text{Constrained Hilbert space:} \\ \text{Constraint: One frustrated bond per triangle} \\ = \text{hardcore dimers on Honeycomb lattice (2 to 1 map)} \end{cases}$

Quantum Dynamics leads to selection of solid order and superfluid ground state
Triangular Lattice bosons with *Frustrated* Hopping

\[ H = + t \sum_{ij} b_i^* b_j + b_i^* b_j + J_z \sum_{ij} (n_i - 1/2)(n_j - 1/2) \]

Natural sign for spin model – XXZ anti-ferromagnet on triangular latt.

**Sign Problem** – cannot use Quantum Monte Carlo.

- However, in the limit \( J_z >> t \), a ‘Marshall sign’ type unitary transformation exists – that reverses the sign.

\[ H = + t \sum_{ij} P(b_i^* b_j + b_i^* b_j)P \]

\[ UHU^+ = - t \sum_{ij} P(b_i^* b_j + b_i^* b_j)P \]

Triangular Lattice bosons with *Frustrated* Hopping

- **Unitary transformation:** $U|\text{dimer}\rangle = i^{N_{\text{brown}}} |\text{dimer}\rangle$
  - Diagonal in $S_z$ (or density) basis.
  - Thermodynamics of $+t$ and $-t$ models identical in large $J_z$ limit
- **Immediate Implications for $+t$**
  - Ground state also has same solid order ($U$ diagonal in density basis) as $-t$
  - Same superfluid density as $-t$ (free energy with vector potential: $F[A]$ identical)
  - Also a *SuperSolid*
Triangular Lattice bosons with *Frustrated* Hopping

- Nature of Supersolid order: obtained using a variational wavefunction approach (Sen et al. for the unfrustrated case)

- Correlation functions evaluated using Grassman techniques invented to solve dimer stat-mech problems.

**FIG. 4:** Supersolid LRO from the variational wavefunction in the strong repulsion limit. Greyscale shows density order $\langle 2n_i - 1 \rangle$ while arrows denote superfluid order $\langle b_i^\dagger \rangle$, for (a): Frustrated hopping ($t <$ ...
Phase Diagram of the Frustrated Hopping Model

- Include information of \( \frac{t}{J_z} = -\frac{1}{2} \) Heisenberg point with 120° order. Can be connected smoothly with \( \frac{t}{J_z} = 0 \) supersolid phase.
- Extended supersolid phase in frustrated model: \( |\frac{J_z}{t}| > 2 \). (vs. unfrustrated \( \frac{J_z}{t} > 10 \)).
- Realization in cold atom systems by molecular pair hopping.
Frustration
Can Lead to Rare and Complex Orders