Frustrated spin systems

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Scope

- Competing interactions and degeneracy
- Classical ground-state correlations
- Order by disorder
- Spin liquids
  - RVB spin liquids
  - Algebraic spin liquids
  - Chiral spin liquids
  - Spin nematics
- Conclusions
The basic models

- **Ising**

\[ H = \sum_{(i,j)} J_{ij} S_i S_j, \quad S_i, S_j = \pm 1 \text{ or } \uparrow, \downarrow \]

- **Heisenberg model**

\[ H = \sum_{(i,j)} J_{ij} \vec{S}_i \cdot \vec{S}_j \]

\[
[S_i^\alpha, S_i^\beta] = i\epsilon^{\alpha\beta\gamma} S_i^\gamma, \text{ and } \vec{S}_i^2 = S(S+1)
\]

Classical limit

\[ \vec{S}_i \text{ are unit vectors} \]
Geometrical frustration

Not frustrated

Antiferromagnetic coupling + odd loops

Frustrated

Competition between exchange paths = frustration
Ising on triangular lattice

- At least one unsatisfied bond per triangle
- **Infinite number of ways** to achieve only one unsatisfied bond on each triangle

At least $2^{N/3}$ GS

Residual entropy

$S/N > (1/3) \ln 2 = 0.210...$
Entropy of triangular Ising model

- Wannier (1950): $S/N = 0.3230...$
- Alternative: dimer problem on dual lattice

$\#\text{ GS} = 2 \times \#\text{ dimer coverings on honeycomb lattice}$
Kasteleyn matrix

Bonds oriented with odd number of clockwise arrows on even plaquettes

\[
a(i, j) = \begin{cases} 
1 & \text{if } i, j \text{ adjacent and } i \rightarrow j \\
-1 & \text{if } i, j \text{ adjacent and } i \leftarrow j \\
0 & \text{otherwise.}
\end{cases}
\]

\[
Z = \sqrt{\det a}
\]

\[
\frac{1}{N_{hc}} \ln Z = \frac{1}{4} \int_0^1 dx \int_0^1 dy \ln |3 + 2 \cos(2\pi y) - 2 \cos(2\pi (x + y)) - 2 \cos(2\pi x)| \simeq 0.1615
\]
Spin Ice

- Dy$_2$Ti$_2$O$_6$, Ho$_2$Ti$_2$O$_6$
- Pyrochlore lattice
- Ferromagnetic exchange interactions
- Strong anisotropy: spins ‘in’ or ‘out’

Ground state:
2 spins in, 2 spins out

Residual entropy:
the ‘ice problem’
Pyrochlore lattice
Residual entropy

Spin ice  Ice

‘Exact’: $S/k_B \approx 0.20501$
(Nagle, 1966)

Pauling (1945): $S/k_B \approx \frac{1}{2} \ln \left(\frac{3}{2}\right) = 0.202732$

Ramirez et al, 1999
Heisenberg model

- Bravais lattice: helical order
  \[ \text{pitch vector} = \text{minimum of } J(q), \text{ FT of } J_{ij} \]

- Triangular lattice: 3-sublattice order
  \[ \text{Sum of spins} = 0 \text{ on each triangle} \]
Infinite degeneracy

- $J_1$-$J_2$ model on square lattice

Classical energy independent of $\theta$
Kagome

- Coplanar ground states: sum of spins = 0 on each triangle → degeneracy of 3-state Potts model
- Non-coplanar ground states

Rotate a chain of blue and red spins around green direction
Classical GS correlations (Ising)

- Correlations = average over all GS
- Triangular lattice (Stephenson, 1964)

$$\langle \sigma(\vec{r})\sigma(\vec{0}) \rangle \propto 1/r^{1/2}$$

- Simple argument: Kasteleyn matrix on honeycomb gapless (Dirac points at 0)
- Physical interpretation: the maximally flippable configuration dominates the sum
Maximally flippable state

All red spins flippable (2/3)
Mapping on height model

on up triangles, height $z(r)$:
increases by $+2$ clockwise if dimer decreases by $1$ otherwise
Coarse graining

\[ h(\vec{x}) = \frac{1}{3} [z(\vec{r}_1) + z(\vec{r}_2) + z(\vec{r}_3)] \]

Maximally flippable state = flat surface (h=0)

\[ F \{h(\vec{x})\} = \int d\vec{x} \frac{K}{2} \left| \nabla h(\vec{x}) \right|^2 \]

\[ \langle \sigma(\vec{r})\sigma(\vec{0}) \rangle \propto \left( \frac{\pi r}{a} \right) - \frac{2\pi}{36K} \]

Consistent with \(1/ r^{1/2}\) if

\[ K = \frac{\pi}{9} \]

Rough phase
Pyrochlore

- 2 in - 2 out on each tetrahedron
- Continuum limit: magnetic field

\[ \text{div } \vec{B} = 0 \]

\[ S(\vec{B}(\vec{x})) = \exp \left[ -\frac{K}{2} \int d^3\vec{r} \vec{B}(\vec{r})^2 \right] \]

\[ \left\langle S_\alpha(\vec{r}) S_\beta(\vec{0}) \right\rangle = \frac{1}{4\pi K} \frac{3(\hat{e}_\alpha \cdot \vec{r})(\hat{e}_\beta \cdot \vec{r}) - (\hat{e}_\alpha \cdot \hat{e}_\beta) r^2}{r^5} \]

Dipolar correlations
Pinch points in Ho$_2$Ti$_2$O$_7$

Experiment

Theory

T. Fennel et al., 2009
Quantum fluctuations

Holstein-Primakoff

\[ S_{i}^{z} = S - a_{i}^\dagger a_{i} \]
\[ S_{i}^{+} = \sqrt{2S - a_{i}^\dagger a_{i} a_{i}} \]
\[ S_{i}^{-} = a_{i}^\dagger \sqrt{2S - a_{i}^\dagger a_{i}} \]

1/S expansion + Fourier transform

\[ H = E_{\text{classical}} + \sum_{\vec{k}} \left[ B_{\vec{k}} a_{\vec{k}}^\dagger a_{-\vec{k}} + \frac{1}{2} A_{\vec{k}} \left( a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger + a_{\vec{k}} a_{-\vec{k}} \right) \right] \]
Zero-point energy

Bogoliubov rotation

\[ \alpha_{\vec{k}} = u_{\vec{k}} a_{\vec{k}} + v_{\vec{k}} a_{-\vec{k}}^\dagger \]

\[ \mathcal{H} = E_0 + \sum_{\vec{k}} \omega_{\vec{k}} \left( \alpha_{\vec{k}}^\dagger \alpha_{\vec{k}} + \frac{1}{2} \right) \]

Zero-point energy

\[ E(\theta) = E_0 + \frac{1}{2} \sum_{\vec{k}} \omega_{\vec{k}}(\theta) \]
Order by disorder

- Even if the GS is degenerate, the spectrum depends on GS

→ selection by zero-point energy

$\theta = 0$

$\theta = \pi$

$J_1 - J_2$
Ising transition

2 collinear states → Ising degree of freedom

Ising transition for any S
Chandra, Coleman, Larkin, PRL’ 89

MC: Ising transition for classical spins

C. Weber, L. Capriotti, G. Misguich, F. Becca, M. Elhajal, FM, PRL’ 03
Thermal fluctuations

In general, minimize

Exception: zero (harmonic) modes

Selection of the state(s) with maximal number of zero modes
Spin liquids

- Quantum correction to local magnetization

$$\delta_m \equiv S - \langle S^z_i \rangle = \frac{1}{N} \sum_k \langle a^+_k a_k \rangle$$

$$\langle a^+_k a_k \rangle = \frac{v^2}{k} \propto \frac{1}{\omega_k}$$

- Frustration
  - soft spectrum
  - strong (often diverging) correction
  - no magnetic long-range order
Spin gap

$J_1$-$J_2$ chain

Majumdar-Ghosh point: $J_2/J_1 = 1/2$

2 exactly dimerized ground states

$$|\psi_{\text{even}}\rangle = \prod_{i \text{ even}} |S(i, i + 1)\rangle$$

$$|\psi_{\text{odd}}\rangle = \prod_{i \text{ odd}} |S(i, i + 1)\rangle$$

$$|S(i, i + 1)\rangle = \text{singlet}$$
Shastry-Sutherland

Product of singlets on red bonds:
→ always an eigenstate
→ GS if inter-dimer coupling not too large

- Spin gap
- Magnetization plateaux
Incomplete Devil’s Staircase in the Magnetization Curve of SrCu$_2$(BO$_3$)$_2$

M. Takigawa, M. Horvatić, T. Waki, S. Krämer, C. Berthier, F. Lévy-Bertrand, I. Sheikin, H. Kageyama, Y. Ueda, and F. Mila

1/8, 2/15, 1/6, 1/4,...
Magnetization of SrCu$_2$(BO$_3$)$_2$ in Ultrahigh Magnetic Fields up to 118 T

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...1/3, 1/2
RVB spin liquids

- Anderson, 1973: restore translational symmetry by a superposition of dimer coverings

→ Resonating Valence Bond spin liquid

\[ |\text{GS} > = + + \cdots \]

Not realized on triangular lattice (3-sublattice LRO)
Quantum dimer model

\[ \mathcal{H} = \sum_{\text{Plaquette}} \left[ -J \left( \langle \uparrow \downarrow \rangle \langle \downarrow \uparrow \rangle + \text{H.c.} \right) + V \left( \langle \uparrow \uparrow \rangle \langle \downarrow \downarrow \rangle + \langle \downarrow \uparrow \rangle \langle \uparrow \downarrow \rangle \right) \right] \]

Rokhsar-Kivelson 1988

- RK point: \( V/J = 1 \) \( \rightarrow \) \( \text{GS} = \text{sum of all configurations} \)
- Correlations: algebraic (Kasteleyn matrix gapless) \( \rightarrow \) Isolated point, no RVB phase
QDM on triangular lattice

Moessner and Sondhi, PRL 2001

RK point $V/J=1$ $\rightarrow$ Kasteleyn matrix gapped
$\rightarrow$ exponentially decaying correlations
$\rightarrow$ RVB phase
Topological sectors

Number of dimers cutting a given line

Parity conserved $\rightarrow$ 2 topological sectors $(N \text{ even or } N \text{ odd})$
Torus: four topological sectors (two cuts)
RVB phase in Heisenberg model?

- Spin-1/2 kagome antiferromagnet
  - DMRG simulations
    - Han, Huse, White, 2011
  - Effective QDM
    - Rousochatzakis, Wan, Tchernyshov, FM, 2014

- Experimental realization?
  - Problematic (residual interactions, DM,...)
Algebraic spin liquids

- Spin-1/2 chain: algebraic correlations (Bethe ansatz, bosonisation)
- Extension in 2D?

\[ H = \frac{1}{2} \sum_{i,j} J_{ij} \left( \frac{1}{2} \left( c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} + \text{h.c.} \right) + \frac{1}{4} \left( c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow} \right) \left( c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow} \right) \right) \]

Abrikosov fermions
Mean-field decoupling

\[ \chi_{ij} = c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow} \]

\[ \chi_{ij}^0 = \chi_0 e^{i\theta_{ij}} \]

\[ \theta_{ij} = \pi / 4 \]

Affleck-Marston 1988

\[ E = \pm J \chi_0 \sqrt{\cos^2 k_x + \cos^2 k_y} \]

Dirac points

\[ k_x, k_y = \pm \pi / 2 \]

→ Algebraic correlations
Variational approach

- Gutzwiller projection:

\[ P_G = \prod_i (1 - n_i \uparrow n_i \downarrow) \]

- Variational wave-functions:

\[ P_G \left| \psi_{\text{fermion}} \right\rangle \]

Good variational energy for spin-1/2 kagome

Ran, Hermele, Lee, Wen, 2007
Chiral spin liquids

- The order parameter breaks P and T, but not PT
- Example: $\vec{S}_1 \cdot (\vec{S}_2 \times \vec{S}_3)$
- Simple approach: Gutzwiller projected wave functions with fractional fluxes
- Best candidate: a small parameter range in the $J_1$-$J_2$-$J_3$ model on kagome

Gong, Zhu, Sheng 2014
Nematic order

- Order parameter: 2-spin operator
- p-nematic: $\vec{S}_i \times \vec{S}_j$
- n-nematic: rank-2 tensor with 5 components

$$\vec{Q}_{ij} = \begin{pmatrix} S_i^x S_j^x - S_i^y S_j^y \\ \frac{1}{\sqrt{3}} \left( 3 S_i^z S_j^z - \vec{S}_i \cdot \vec{S}_j \right) \\ S_i^x S_j^y + S_i^y S_j^x \\ S_i^y S_j^z + S_i^z S_j^y \\ S_i^z S_j^x + S_i^x S_j^z \end{pmatrix}$$
Simple example: $S=1$

Consider

$$|S^z = 0\rangle$$

$$\langle S^\alpha \rangle = 0 \quad \langle (S^z)^2 \rangle = 0 \quad \langle (S^x,y)^2 \rangle \neq 0$$

True for any $\alpha$

Broken SU(2) symmetry

Not magnetic
Quadrupole states and directors

\[ |Q(\zeta, \phi)\rangle = i \frac{\sin \zeta}{\sqrt{2}} \left( e^{-i\phi} |1\rangle - e^{i\phi} |\bar{1}\rangle \right) - i \cos \zeta |0\rangle \]

Rotation of \( l \) \( S_z=0 \rangle \)

\[ \mathbf{d} = (\sin \zeta \cos \phi, \sin \zeta \sin \phi, \cos \zeta) \]

« director »
S=1 with biquadratic interaction

\[ H = J \sum_{i,j} \left[ \cos \vartheta S_i S_j + \sin \vartheta (S_i S_j)^2 \right] - h \sum_i S_i^z \]

\[ \hat{Q}_i = \begin{pmatrix} \hat{Q}_i^{x^2-y^2} \\ \hat{Q}_i^{3z^2-r^2} \\ \hat{Q}_i^{xy} \\ \hat{Q}_i^{yz} \\ \hat{Q}_i^{xz} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{3}} \left[ (S_i^x)^2 - (S_i^y)^2 \right] \\ \frac{1}{\sqrt{3}} \left[ 2(S_i^z)^2 - (S_i^x)^2 - (S_i^y)^2 \right] \\ S_i^x S_i^y + S_i^y S_i^x \\ S_i^y S_i^z + S_i^z S_i^y \\ S_i^x S_i^z + S_i^z S_i^x \end{pmatrix} \]

\[ \hat{Q}_i \hat{Q}_j = 2 \left( \hat{S}_i \hat{S}_j \right)^2 + \hat{S}_i \hat{S}_j - 8/3 \]
S=1 on triangular lattice

Directors mutually perpendicular on 3 sublattices

(see also Tsunetsugu-Arikawa, ’06)

Antiferroquadrupolar

Directors mutually perpendicular on 3 sublattices

Ferroquadrupolar

Parallel directors

Conclusions

- A lot of exotic phases have been predicted
- Only a few of them have been found in realistic models or in actual compounds
  → room for important discoveries

Further reading:

Introduction to Frustrated Magnetism
Eds C. Lacroix, P. Mendels, and F. Mila