Frustrated magnetism via bold diagrammatic Monte Carlo

Oleg Starykh, University of Utah

collaborators: S. A. Kulagin, N. Prokof'ev, B. Svistunov, and C. N. Varney
(U Mass, Amherst)

International Workshop on the Sign Problem in QCD and beyond,
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Outline

- Geometrically frustrated magnets
  - experiments
  - Field theory vs numerics at finite T
- Popov-Fedotov fermions and bold diagrammatic Monte Carlo
- Quantum-classical correspondence (at intermediate T)
- Physical insight into prolonged “high-T” behavior
- Conclusions
Triangular lattice Ising antiferromagnet

Antiferromagnetism. The Triangular Ising Net

G. H. Wannier
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received February 11, 1950)

In this paper the statistical mechanics of a two-dimensionally infinite set of Ising spins is worked out for the case in which they form either a triangular or a honeycomb arrangement. Results for the honeycomb and the ferromagnetic triangular net differ little from the published ones for the square net (Curie point with logarithmically infinite specific heat). The triangular net with antiferromagnetic interaction is a sample case of antiferromagnetism in a non-fitting lattice. The binding energy comes out to be only one-third of what it is in the ferromagnetic case. The entropy at absolute zero is finite; it equals

\[ S(0) = R \frac{2}{\pi} \int_{0}^{\pi/3} \ln(2 \cos \omega) d\omega = 0.3383 R. \]

The system is disordered at all temperatures and possesses no Curie point.

**Frustration:** pairwise interactions between spins cannot be minimized simultaneously (1/3 of bonds are unhappy)

Ising spins \( S_r = +1 \) or -1 only
Experimental indications

- spin liquid: no broken symmetries, strong correlations

\[ f = \frac{\theta_{cw}}{T_N} > 10 \]

strong frustration

\[ \frac{1}{\chi} \]

\[ T_N \]

\[ -\theta_{cw} \]

\[ T \]

- triangular lattice
- kagome lattice
- pyrochlore lattice

<table>
<thead>
<tr>
<th>Compound</th>
<th>Magnetic lattice</th>
<th>$-\theta_{cw}$ (K)</th>
<th>$T_c$ (K)</th>
<th>$f$</th>
<th>Ordered state</th>
<th>Electronic configuration</th>
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Hyper-Kagome $\text{Na}_4\text{Ir}_3\text{O}_8$ : 3D lattice of corner-sharing triangles

$\theta_{cw} = -650$ K, $T_N < 2$ K

Experimentally very relevant issue: temperature interval from $T \sim J$ to $T << J$ is often the only accessible regime.

And yet we do not have good description of it.
Why triangle-based spin systems are so unusual?

- Classically – strongly **frustrated**
  (unable to satisfy all pairwise interactions simultaneously; finite entropy at $T=0$)

- Number of classical (Ising) ground states ($N$ sites):
  - triangular lattice $= e^{0.323 N}$
  - kagome lattice $= e^{0.502 N}$

- Frustration leads to classical degeneracy

- Quantum fluctuations: can stabilize spin liquid via sampling of all classical degenerate states? $Z_2$ spin liquid in kagome and $J_1$-$J_2$ models [Huse, White 2011]

\[ E = J \sum_{i,j} S_i S_j \]
\[ J > 0, \quad S = +1 \text{ or } -1 \]
Heisenberg (vector) spins relieve frustration

**Classical vector spins:** three-sublattice $120^\circ$ structure

**Spiral magnetic order:** co-planar, non-collinear

$$H = J \sum_{i,j} \vec{S}_i \cdot \vec{S}_j = \frac{J}{2} \sum_{\triangle} \left( \sum_{i \in \triangle} \vec{S}_i \right)^2 + \text{const}$$

Relieve frustration by sharing it with the neighbors: Energy per bond = $S^2 \cos(120^\circ) = -0.5 S^2$

Does it hold for quantum $S=1/2$ spins? **YES**

**Numerical results:** classical $120^\circ$ structure survives (Singh, Huse 1992 ... Chernyshev, White 2007)
Finite $T$ expectations (field theory = nonlinear sigma model)

- $d=2$ and SU(2) symmetric spin system is characterized by exponentially large spin correlation length

$$\xi(T) = 0.021 \left( \frac{c}{\rho_s} \right) \left( \frac{4\pi\rho_s}{T} \right)^{1/2} \exp \left( \frac{4\pi\rho_s}{T} \right)$$

- Static structure factor

$$S(Q) \approx 0.85 \left( \frac{T}{4\pi\rho_s} \right)^4 \xi(T)^2.$$
Finite T: classical triangular AFM

FIG. 3. $T \ln S(Q)$ as a function of temperature $T$. The Monte Carlo data for different system sizes are indicated by the symbols. The solid line is a fit to the low-$T$ RG predictions (Ref. 3) and the dotted lines represent Padé approximants to the function using the high-temperature series coefficients in the table. $[N/M]$ denotes the ratio of a polynomial of order $N$ in the numerator to one of order $M$ in the denominator.

FIG. 4. $T \ln(4T \xi^2)$ as a function of temperature $T$. The notation is the same as that in Fig. 3.

FIG. 2. Square lattice: $T \ln[4S(Q)]$ and $T \ln(4T \xi^2/T_{mf})$ (on the insert) vs $T/T_{mf}$; $u = 1/(T + 0.2)$.

Southern, Young 1993

ordered

spin-$\frac{1}{2}$ square AFM

High-T series expansion

ordered

low entropy

FIG. 4. Square lattice: entropy $S/N$ and susceptibility $4\chi$ vs $T/T_{mf}$; $u = 1/(T + 0.2)$. 10
Finite T: triangular AFM \[ S = \infty \text{ vs } S = 1/2 \]

\[ S = \infty \]
Southern, Young 1993

\[ S = 1/2 \]
spin-1/2 triangular AFM
High-T series expansion

FIG. 1. Triangular lattice: \( T \ln[4S(Q)] \) vs \( T/T_{mf} \). The plots represent \([L,M]\) Padé in the Euler transformed variable \( u = 1/(T+0.08) \). The insert shows results for the correlation length. \( T \ln[4T\xi^2/T_{mf}] \) vs \( T/T_{mf} ; u = 1/(T+0.2) \).

FIG. 3. \( T \ln S(Q) \) as a function of temperature \( T \). The Monte Carlo data for different system sizes are indicated by [26x6 to 791x701].

ordered

\[ T \ln(4T\xi^2) \text{ as a function of temperature } T. \text{ The same as that in Fig. 3.} \]
Popov Fedotov fermions (JETP 1988)

\[ H = J \sum_{\langle R,R' \rangle} \vec{S}_R \cdot \vec{S}_{R'} = \frac{J}{4} \sum_{\langle R,R' \rangle} c_{R,\alpha}^\dagger \bar{\sigma}_{\alpha \beta} c_{R,\beta} \cdot c_{R',\gamma}^\dagger \bar{\sigma}_{\gamma \delta} c_{R',\delta} \]

Spin states \(|\text{phys}\rangle = |\uparrow\rangle, |\downarrow\rangle\)

Fermion states \(|\uparrow\rangle, |\downarrow\rangle, |0\rangle, |2 = \uparrow, \downarrow\rangle\) \(\vec{S}_R |\text{unphys}\rangle = 0\)

|\text{unphys}\rangle

At any finite T, contribution of unphysical states can be removed exactly with the help of single complex chemical potential \(\mu\)

\[ H \rightarrow H_{\text{PF}} = H + \frac{i \pi}{2 \beta} \sum_{s=\uparrow, \downarrow} c_{R,s}^\dagger c_{R,s} \]

\[ \mu = -\frac{i \pi}{2 \beta} \]
Popov Fedotov fermions (JETP 1988)

$$\text{Tr } e^{-\beta H_{PF}} \rightarrow \text{Tr}_\text{the rest} \left( \text{Tr}_{R,\text{phys}} e^{-\beta H_{PF}} + \text{Tr}_{R,\text{unphys}} e^{-\beta H_{PF}} \right)$$

$$\text{Tr}_{R,\text{unphys}} e^{-\beta H_{PF}} = e^{-\beta H_{PF}, \neq R} \left\{ \langle 0 | e^{-i \frac{\pi}{2} \hat{N}_R} | 0 \rangle + \langle 2 | e^{-i \frac{\pi}{2} \hat{N}_R} | 2 \rangle \right\} \rightarrow \{1 + (-1)\} = 0.$$

Obtained standard diagram technique for PF fermions, but with shifted Matsubara frequency

$$G = \frac{1}{i \omega_n + \mu} = \frac{1}{i \omega_n - \frac{i \pi}{2 \beta}} \quad \text{with} \quad \omega_n - \frac{\pi}{2 \beta} = \frac{2\pi}{\beta} (n + \frac{1}{4})$$

Alternatively, fermions with \textbf{semionic} boundary conditions in ‘time’

$$\psi_R(\beta) = i \psi_R(0), \quad \psi_R^\dagger(\beta) = -i \psi_R^\dagger(0)$$

More arguments in Prokof'ev, Svistunov PRB 2011
Standard diagrammatics for interacting fermions starting from the flat band.

\[ \Sigma = \{ \text{diagram 1} \} \]

\[ \Pi = \{ \text{diagram 2} \} \]

\[ G_{\sigma} = G_{\sigma}^{(0)} + G_{\sigma}^{(0)}\Sigma_{\sigma} G_{\sigma} \]

\[ U = J - J\Pi U \]

Main quantity of interest is magnetic susceptibility

\[ \chi = \left\langle S_{0}^{z}(0)S_{j}^{z}(\tau) \right\rangle_{\omega} = \frac{\Pi}{1 - J\Pi} \]

Quantum soup (cooperative paramagnet): not ordered but strongly correlated

\[ \frac{T}{zJ} < 1 \]
Sign-blessing (cancellation of high-order diagrams)

High-temperature series expansions
(sites or clusters,
Rigol, Bryant, Singh 2007)
vs BDMC
Uniform susceptibility \( \chi(q = 0) = \frac{\partial M(h = 0)}{\partial h} \)

Static susceptibility \( \chi(q, \omega_n = 0) \)

measures ordering tendency at momentum \( q \)

[series expansion cannot access finite \( q \) ]
Quantum-to-classical (QCC) correspondence for static response:

Quantum $\chi(q,T)$ is the same as classical $\chi(q,T_{cl})$ for some $T_{cl}(T)$ (relative accuracy of 1%)
(this correspondence also takes place for the square lattice with relative accuracy 0.3% at all $T$)

$$\chi(r, \omega = 0) = \int_0^{1/T} d\tau \langle S_0^z(0) S_r^z(\tau) \rangle$$
QCC, if confirmed, implies (in 2D):

1. If $T_{cl}(T=0) \neq 0$ then the quantum ground state is disordered, i.e. it is a spin liquid

2. If the classical ground state is disordered (macro degeneracy) then the quantum ground state is a spin liquid

Example: Kagome antiferromagnet

Efficient tool in the search for spin liquids

**Triangular lattice:** Naive extrapolation suggests: $T_{cl} = 0.28$ J for $T_q=0$. This coincides with a crossover, at $T_v = 0.285$ J, from high-$T$ $Z_2$-vortex dominated regime to low-$T$ spin-fluctuation dominated regime [“spin-gel” state, Kawamura (2010)].

**Square lattice:** $T_{cl}(T)$ turns around at low $T$ so that $T_{cl} = 0$ for $T_q=0$. Thus both models, classical and quantum, predict ordered magnetic state (as they should).

**Triangular AFM:** Low-$T$ regime is not reached yet
3 spin “chain”: QCC is not the law of nature

\[ \langle S_1 S_3 \rangle_{\omega=0} \]
\[ \langle S_1 S_2 \rangle_{\omega=0} \]

Quantum-Classical correspondence is a result of approximate extended high-T scaling

\[ \langle S_1 S_n \rangle_{\text{classical}} = \left( \coth \left[ \frac{3\beta}{4} \right] - \frac{4}{3\beta} \right)^{n-1} \to (\beta/4)^{n-1} \]

[also, 5σ deviations on a square lattice]
Possible reason for strongly delayed universal (field-theoretical) scaling limit?

- Non-universal “roton” [almost flat band] regime due to non-collinear short-range spin order
- Strong quantum renormalization of the dispersion (specific no non-collinear short-range order) leads to strong enhancement of the density of states at ~ J
- Strong similarity with He II: high-energy rotons (with $\epsilon_{\text{min}} = \Delta = 8.6 \text{ K}$) control thermodynamics down to $T = 1 \text{ K}$ [this is large density of states effect].
The minimal explanation: non-collinear spin structure is the key!

- Rotated basis: order along $S^z$ (via rotation about $S^x$)

$$H = \sum_{ij} -\frac{1}{2}(S^z_i S^z_j + S^y_i S^y_j) + S^x_i S^x_j + \sin(\phi_i - \phi_j)(S^z_i S^y_j - S^y_i S^z_j)$$

$H_{\text{coll}}$: collinear piece: 2, 4, 6...magnons

$H_{\text{non-coll}}$: non-collinear piece: 3, 5, ... magnons

Spin wave expansion: $S >> 1$

$$S^z = S - a^+ a, \quad S^x = \sqrt{\frac{S}{2}}(a^+ + a), \quad S^y = i\sqrt{\frac{S}{2}}(a^+ - a)$$

$H_{\text{non-coll}}$ describes magnon decay ($a a^+ + a^+ a$) and creation/annihilation ($a a a + \text{h.c.}$)

Absent in collinear AFM (where $\phi_i = 0, \pi$)

✓ Similar to anharmonic phonons and He$^4$

- Produces $1/S$ (!) correction to magnon spectrum: renormalization + lifetime

[ Square lattice: corrections only at $1/S^2$ order, numerically small]
Results: 1/S corrections are huge
(shown in 1/4 of the Brillouin zone)

Renormalized dispersion,
with 1/S correction

Semi-quantitative agreement with sophisticated
series expansion technique with no adjustable parameters
(except for S=1/2).
- “rotons” are part of global renormalization (weak local minimum)
- large regions of (almost) flat dispersion;
- finite lifetime [not present in numerics].

OS, Chubukov, Abanov 2006; Numerics (dots) - Zheng et al, 2006
Conclusions

- We need \((k, \omega)\) BDMC results at finite \(T\) for the *retarded* spin susceptibility \(\chi(k, \omega)\).

- Apply to strongly frustrated 3D systems: \(s=\frac{1}{2}\) pyrochlore antiferromagnet disordered classically. quantum model - not known. expect \(\xi \sim 1/T\), hence no slowing down due to incipient ordering
A puzzling coincidence

$\Pi_1(\text{SO}(3)) = \mathbb{Z}_2$

$\mathbb{Z}_2$ vortex binding transition

$T_v = 0.285$ J

(T-derivative of ) vorticity modulus,
Kawamura, Yamamoto, Okubo 2010
Series expansion: **Huge** renormalization of the dispersion for $s = \frac{1}{2}$ antiferromagnet. (Note: cannot probe finite lifetime.)

Agrees in details with the leading $1/S$ spin wave renormalization of the dispersion.
Structurally perfect $S=1/2$ Kagome antiferromagnets: Herbersmithite $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ and spatially anisotropic Volborthite $\text{Cu}_3\text{V}_2\text{O}_7(\text{OH})_2\ 2\text{H}_2\text{O}$

$\theta_{cw}=-300\text{K}, T_N<0.05\text{K}$

$\theta_{cw}=-115\text{K}, T_N<1.8\text{K}$

**LETTER**

Fractionalized excitations in the spin–liquid state of a kagome–lattice antiferromagnet

Shores et al 2005

Hiroi et al 2001

Han et al, Nature 2012