Spin order of the classical Kagome antiferromagnet: via effective Hamiltonians

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The kagome lattice
The Hamiltonian

\[ H = J \sum_{\langle ij \rangle} s_i \cdot s_j. \]  \hspace{1cm} (1)

“Highly frustrated”: ground state manifold has \textbf{macroscopically many} degrees of freedom characterized by ("frustration parameter")

\[ T_f / T_{MF} \ll 1 \]  \hspace{1cm} (2)
Coplanar ground states

Coplanar ground state: all spins in just 3 directions (120° apart).

View as 3-coloring of triangle vertices
[colors \((A, B, C) = 3\)-state Potts model spins]

Number of colorings is

\[ O\left(e^{\text{const}N}\right). \]
Coplanar states and colorings

Ground state of one triangle: \( \sum S_i = 0 \)

i.e. 120 state... we can do this on all triangles

subclass of "coplanar" states

\[ \begin{array}{c}
\text{discrete 3–state Potts spins}
\end{array} \]
Simplest periodic states

"3 x 3" state

"Q=0" state
Irregular state
Chiralities $\eta_\alpha$:

Ising variable $\eta_\alpha \equiv +1(-1)$ when the Potts labels go as ABC (CBA) as one walks c.c.w. about triangle $\alpha$.

(We shall use these later.)

Mapping 1-to-1?

A valid configuration $\{\eta_\alpha\}$ does map to a unique coloring $\{c_i\}$ (modulo color permutations).

But some Ising configurations don’t come from any coloring.
how chiralities defined on each triangle

$\eta_\alpha = +1$

turn through +360

[Potts spins $A, B, C$]

$\eta_\alpha = -1$

turn through −360

[Potts spins $A, C, B$]
periodic states in terms of chiralities

"\sqrt{3} \times \sqrt{3}\)"

...is "antiferromagnetic"

...is "ferromagnetic"

...in terms of chiralities
Coplanar ordering

Well-known: [Chalker, Holdsworth, & Shender, PRL 1992] as $T \to 0$, 3-component spins order into coplanar states,

[Moessner & Chalker 1998 called “order due to disorder, ensemble weight is concentrated near singular points at $T \to 0$.]

[You can see which state is favored by an effective Hamiltonian – not featured in this talk – from integrating out all harmonic-order fluctuations. Whether that suffices to cause order requires counting degrees of freedom. What kind of order is not provided.]
I ask: does coloring achieve LRO?

Of course, in $d = 2$ with spins of $> 2$ components at $T > 0$, orientation of the spin plane fluctuates slowly in space. (Its correl. length scales as $\xi_{\text{plane}} \sim \exp(\text{const}/\sqrt{T})$ – I think!)

Nevertheless we can define the colors/Potts variables unambiguously, by working our way from one reference triangle. (Technically a “hidden” or “string” order parameter?)

More pertinent:
just take $\lim_{T \to 0} C(R)$ for whatever correlation $C(R)$:

$$\xi_{\text{plane}} \to \infty$$

as $T \to 0$, whereas the coloring ensemble (see results below!) goes to a fixed limit.
Beyond coplanar order

Random 3-coloring (Potts \( \{c_i\} \) with equal weights [Huse & Rutenberg 1992]:

Potts spins \( C_c(R) \sim 1/R^{4/3} \).

chiralities \( C_\eta(R) \sim 1/R^4 \). [Baxter, 1971.]

All simulations see:

Potts spins \( C_c(R) \sim 1/R^x, x \approx 4/3 \).

chiralities \( C_\eta(R) \) fast decay (exponential?)

I say [with Huse & Rutenberg 1992]:

all correlations have LRO, \( C(R) \sim \text{const.} \)

... due to the unequal weighting of different Potts states, taking into account the fluctuations about each.
Philosophy:

obtain an effective Hamiltonian defined for arbitrary spin arrangements, not just specially symmetric ones. (with cruder approximations!)

A technical theme: turn the spin configuration into a set of coefficients/matrix entries – then perturb blithely in them

[CLH 1987 fcc type I]
[E. P. Chan and CLH 1995, kagome quantum large S]
[CLH and U. Hizi, PRL/PRB 2006, pyrochlore quantum large S]
Prehistory: review “order by disorder”

NON highly frustrated (just one global degeneracy parameter $\psi$)
resolve degeneracy by (harmonic) zero-point $E$.

Define effective Hamiltonian

$$V_{\text{eff}}(\psi) = \frac{1}{2} \sum \hbar \omega^{(a)}(k)$$

same classical energy ($O J(S^2)$)
different harmonic spinwave spectra

favors collinear

disfavors noncollinear
Mappings to 5 eff. Hamiltonians (preview)

A series of mappings // reduced degrees of freedom // effective Hamiltonians.

1. $\mathcal{H}(\{s_i\})$: Full Heisenberg model
   \[ \downarrow \]
2. $\mathcal{H}_{sw}(\{\theta_i, z_i\})$: Coplanar states with all spin deviations
   \[ \downarrow \]
3. $Q(\{z_i\})$: Coplanar states with soft $z$ deviations.
   \[ \downarrow \]
4. $\Phi(\{c_i\})$: Colorings (Potts). [equivalently, chiralities]
   \[ \downarrow \]
5. $F_h(\{h(r)\})$: free energy in terms of coarse-grained height field

Goal: effective Hamiltonian for any of the discrete coplanar ground states, which absorbs the free energy of the low-$T$ anharmonic fluctuations about that state.
Three Gaussian fields appearing (preview)

... or treated as such; gradient-squared free energies.

[When you transform the correlations back into real space, you get (at the least) pseudo-dipolar correlations]

(a) . in-plane spin rotations $\theta_i$

$$\mathcal{H}_{sw}^{(2)} \theta \approx \frac{1}{2} \rho \int d^2r |\nabla \theta(r)|^2$$

(b) . out-of-plane spin deviations: potential $\phi$ s.t. $z_i = \Delta \phi$.

$$F_{\text{var}} = \frac{1}{2} B \sum_{\mu\nu} |\phi_{\mu} - \phi_{\nu}|^2 \approx \frac{1}{2} \rho \int d^2r |\nabla \phi(r)|^2 \quad \text{(variational $\rho\phi$)}.$$  

(c) . 2-component height field $h_{\mu}$: s.t. $s_i^{(0)} = \Delta h_{\mu}$

(for coplanar ground state of the spins).

$$F_h = \int d^2r \frac{1}{2} K |\nabla h|^2,$$
where we are ...

(1) $\mathcal{H}(\{s_i\})$: Full Heisenberg model
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1 → 2: Spin wave expansion

Use triad of spin axes at each site

\( \hat{x}_i \) – spin’s classical direction

\( \hat{z}_i \) – normal to plane of coplanarity.

\( \hat{y}_i \equiv \hat{z}_i \times \hat{x}_i \)

Spin deviations

\( \delta s_i^z \rightarrow z_i \)

\( \delta s_i^y \) (in-plane) → parametrize as small rotation \( \theta_i \)

Spin-wave expansion (\( J \equiv 1 \)):

\[ \mathcal{H}_{\text{sw}} \equiv \mathcal{H}_{\text{sw}}^{(2)} + \mathcal{H}_{\text{sw}}^{(3)} + \mathcal{H}_{\text{sw}}^{(4)} + \ldots, \]  

with:
\[ \mathcal{H}_{sw}^{(2)} = \sum_{\langle ij \rangle} \left[ \frac{1}{4} (\theta_i - \theta_j)^2 + z_i z_j \right] + \sum_i z_i^2 \]

\[ \mathcal{H}_{sw}^{(3)}_{dom} = \sum_{\alpha} \eta_{\alpha} \mathcal{H}^{(3, \alpha)}_{dom} \]

\[ \mathcal{H}_{sw}^{(4)}_{dom} = \sum_{\langle ij \rangle} \frac{1}{16} (z_i^2 - z_j^2)^2. \]

\( \alpha \) indexes triangle centers, \( \eta_{\alpha} = \) chirality.

\[ \mathcal{H}^{(3, \alpha)}_{dom} \equiv \frac{\sqrt{3}}{4} \sum_{m=1}^{3} [z_{\alpha m}^2 (\theta_{\alpha, m+1} - \theta_{\alpha, m-1})]. \]

“dominant” anharmonic terms in \( \mathcal{H}_{sw}^{(3)}_{dom} \) and \( \mathcal{H}_{sw}^{(4)}_{dom} \): parts containing the \textbf{highest} powers of \( z_i \).

Notice: in \( \mathcal{H}_{sw}^{(3)} \):
\( \eta_{\alpha} \) prefactor is \textbf{only} dependence on coloring state \( \{c_i\} \).
**Soft (zero) modes**

The $z$ part of $\mathcal{H}_{\text{sw}}^{(2)}$:

$$\mathcal{H}_{\text{sw}}^{(2)} z = \frac{1}{2} \sum_{\alpha} \left( \sum_{i \in \alpha} z_i \right)^2$$

Soft mode subspace defined by constraint

$$\sum_{i \in \alpha} z_i = 0 \quad \text{(soft)}$$

on every triangle.

Soft modes cost zero at harmonic order – limited by higher order.

$\Rightarrow$ big mean-square fluctuations $O(\sqrt{T})$,

versus $O(T)$ for ordinary modes [Chalker et al 1992].

$\Rightarrow$ factors w/soft modes were “dominant” in spin-wave exp. $\mathcal{H}_{\text{sw}}$.)
where we are ...

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(5) $F_h(\{h(r)\})$: free energy in terms of coarse-grained height field
2 $\rightarrow$ 3: Quartic eff. Ham. for soft $z$ modes

[Following Shender & Holdsworth JPCM 1996.]

— do (Gaussian) integral over all $\theta_i$

— get

$$Q = \mathcal{H}_{sw}^{(4)}_{dom} - \sum_{\alpha, \beta} \eta_{\alpha} \eta_{\beta} Q'_{\alpha, \beta}$$

here

$$Q'_{\alpha, \beta} \equiv \sum_{i \in \alpha, j \in \beta} \left( \frac{\sqrt{3}}{4} \right)^2 G_{ij} z_i^2 z_j^2$$

where $G_{ij}$ is the Green’s function of the $\theta$ modes.
Regroup as

\[ Q = Q_0 - \sum_{\alpha \neq \beta} \eta_\alpha \eta_\beta Q'_{\alpha\beta} \]

absorbing \( \mathcal{H}_{sw}^{(4)}_{\text{dom}} \) + the \((\alpha = \beta)\) terms into \( Q_0 \).
(Those were the largest terms.)

Notice: **not** invariant under \( z_i \to -z_i \): must satisfy soft-mode constraint (reminder: \( \sum_{i \in \alpha} z_i = 0 \) on each triangle).

Using that constraint, can simplify to \( Q_0 = B_0 \sum_i z_i^4 \),
with \( B_0 \equiv \frac{1}{4} (1 + \frac{9}{4} G_0) = \frac{13}{16} \).
Asymptotic behavior of Greens function
(an aside for later use)

At long wavelengths,

\[ \mathcal{H}_{sw}^{(2)} \approx \frac{1}{2} \rho \int d^2r |\nabla \theta(r)|^2 \]

so the Greens function is pseudo-dipolar:

\[ G_{\alpha m, \beta n} \approx \frac{a^2}{2\pi \rho \epsilon R^2} \epsilon_{\alpha \epsilon} \epsilon_{\beta} \cos(\psi_m + \psi_n - 2\psi_R). \]

where \( R = \) distance between triangle centers \( \alpha \) and \( \beta \); angle \( \psi_R \) is orientation of that vector.
where we are ...

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$3 \rightarrow 4$ Discrete eff. Ham. $\Phi(\{c_i\})$

$$e^{-\Phi(\{c_i\})/T} = \mathcal{Z}(\{c_i\}) \equiv \int_{\text{basin}} \prod_i (d\theta_i \, dz_i) e^{-\mathcal{H}_{sw}/T}$$

$$\equiv \int_{\text{basin}} \prod_i (dz_i) e^{-Q/T}$$

$\mathcal{Z}(\{c_i\}) \equiv$ portion of total $\mathcal{Z}$ assigned to “basin” of this coloring.

Note: $\mathcal{H}_{sw}^{(2)}$ indep. of which $\{c_i\}$

$\Rightarrow \Phi$ was indep. of $\{c_i\}$ at harmonic order.
Perturbation expansion

Key step: expand partition function formula to 1st order in $\eta_{\alpha}$’s, (as if they were small), get

$$\Phi = -\frac{1}{2} \sum_{\alpha \neq \beta} \mathcal{J}_{\alpha\beta} \eta_{\alpha} \eta_{\beta}$$

with $(\langle \ldots \rangle_0$ means “in $Q_0$ ensemble ”)

$$\mathcal{J}_{\alpha\beta} \equiv \langle Q'_{\alpha\beta} \rangle_0 = \sum_{i \in \alpha, j \in \beta} \left( \frac{\sqrt{3}}{4} \right)^2 G_{ij} \langle z_i^2 z_j^2 \rangle_0$$

Since $Q$ is homogeneous in $\{z_i\}$, partial part. function $Z(\{c_i\})$ – and hence $\Phi/T$ – temperature independent as $T \to 0$. 
Perturbation justified???

Well, since $G_{ij} \propto 1/R_{ij}^2$, we’ll see

$$\frac{Q'\text{coeff}}{Q_0\text{coeff}} < O(1/10).$$
**Self-consistent approx’n for \{\mathcal{J}_{\alpha\beta}\}**

Need: expectations in order \(Q_0\) (quartic) ensemble, subject to soft-mode constraint.

**Ideas**

(1) Try a self-consistent decoupling (Gaussian variational ensemble):

\[ F_{\text{var}} \equiv \frac{1}{2}B \sum_i z_i^2, \]

(2) Express the constraint via a potential like \(h_\mu\) (living on hexagon centers), \(z_i \equiv \Delta \phi_\mu\)

(Note for specialists: \((h, \phi)\) combined are the **origami field** of [Shender et al PRL 1993])

Thus

\[ \langle z_i z_j \rangle_{\text{var}} = T \frac{\Gamma_{ij}}{B} \]

where \(\Gamma_{ij}\) is the Green’s function of \(F_{\text{var}}\).
We needed
\[
\langle z_i^2 z_j^2 \rangle_{\text{var}} = \langle z_i^2 \rangle_{\text{var}} \langle z_j^2 \rangle_{\text{var}} + 2 \langle z_i z_j \rangle_{\text{var}}^2 = \left( \frac{T}{B} \right)^2 \left[ \Gamma_0^2 + 2 \Gamma_{ij}^2 \right]
\]
using Wick’s theorem.

Result:
\[
\frac{J_{\alpha\beta}}{T} \approx \frac{3}{13} \sum_{m,n=1}^{3} G_{\alpha m,\beta n} \Gamma_{\alpha m,\beta n}^2
\]
(The 3/13 came from combining various known stiffness prefactors and values of Green’s function at nearest-neighbor lattice sites.)
Limiting behavior of eff. couplings (aside)

Long range

Greens functions $G_{\ldots}$ and $\Gamma_{\ldots}$ have the same angular and $R$ dependences. Plug in, get $(1/R^2)^{1+2}$

$$\frac{\mathcal{J}_{\alpha\beta}}{T} \approx \frac{A}{(R/a)^6} \epsilon_\alpha \epsilon_\beta \cos 6\psi_R$$

for large $R$. where $A = 6\sqrt{3}/13^2\pi^3$ after combining all the factors.

Short range. Self-consistent formula gives (small!)

$$\mathcal{J}_1/T \approx -1.88 \times 10^{-3}$$

$$\mathcal{J}_2/T \approx -4.3 \times 10^{-4}.$$  

This favors the "$\sqrt{3} \times \sqrt{3}$" pattern slightly

$\Rightarrow$ will increase the height stiffness $K$.  


**where we are ...**

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4 → 5: Height model and locking

Why the random 3-colorings ensemble has power-law correlations: which may be understood via

Map Potts microstates → 2-component “height” variable $h_\mu$:

s.t. $s_i^{(0)} = \Delta h_\mu$ (\(\mu\) labels hexagon centers)

$\Rightarrow h(\mathbf{r})$ parametrizes fluctuating interface [Huse, CLH]

Coarse-grained ensemble weight

$$F_h = \int d^2 \mathbf{r} \frac{1}{2} K |\nabla h|^2,$$

Kosterlitz-Thouless (“Coulomb-gas”) techniques yield power laws

$$C(R) \sim \exp(-\text{const}(\ln R)).$$

[not used in this talk]
Incidentally: vortices, if any, are unbound.

Locking

Equal-weighted coloring has a height stiffness $K = K_c$, right at interface’s roughening transition.

Increase in $K \Rightarrow h(r)$ locks to LRO
$\Rightarrow$ LRO of colors $\{c_i\}$ in “$\sqrt{3} \times \sqrt{3}$” state.
[Huse & Rutenberg 1992].

QED.
Discussion: uses of discrete eff. Hamiltonian

(1) Use $\mathcal{J}_{\alpha\beta}$ as a Hamiltonian in discrete simulations of coloring model. Measure the modified height stiffness $K$

- Faster than Heisenberg simulation
- System still too small to see predicted LRO directly?

(2) Analytic: iterate RG equations semi-analytically. Estimate correlation length $\xi$ and order parameter

($\xi$: where correlations $C(R)$ cross over $q/R^x \to \text{LRO}$)
Test: $z$ fluctuations indep. of coloring

If valid, $\langle z_i z_j \rangle_{sw}$ (in spin-wave approx) are $\sim$ indep. of which coloring $\{c_i\}$.

Can check it in Monte Carlo or molecular dynamics

(Can obtain even if system is confined to one “basis” of one coplanar state = one coloring: no need to equilibrate over the entropy barriers between basins.)

Also: numerically evaluate quartic $\langle zzzz \rangle$ xexpectations; check variational predictions for dependence on separation $(R, \psi)$. 
Discussion: extending to $d=3$?

3D lattices of corner-sharing triangles:

(1) (half) garnet lattice [Petrenko & Paul, PRB 2000]
$\equiv$ hyperkagomé lattice [Hopkinson PRL 2007]

(2) other depleted pyrochlore lattices

A minor difference in $d = 3$:
spin plane orientation has true long-range coplanar order

In $d = 3$ we get the same formula for effective Ising couplings $J_{\alpha\beta}$.
(now it gives a $1/R^9$ envelope). Can coarse-grain discrete variables,
but merely get “Coulomb phase” in place of “height field” – no
potential, just vector pot. w/gauge freedom.

The stiffness for $\Phi$ is modified, but insufficient to drive a phase
transition: LRO is not expected in $d = 3$. 