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Long-range order in the classical kagome antiferromagnet: Effective Hamiltonian approach

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Following Huse and Rutenberg [Phys. Rev. B **45**, 7536 (1992)], I argue the classical Heisenberg antiferromagnet on the kagome lattice has long-range spin order of the $\sqrt{3}\times\sqrt{3}$ type in the limit of zero temperature. I start from the effective quartic Hamiltonian for the soft (out of plane) spin-fluctuation modes and treat as a perturbation those terms which depend on the discrete coplanar state. Soft-mode expectations become the coefficients of a discrete effective Hamiltonian, which (after a coarse graining) has the sign favoring a locking transition in the interface representation of the discrete model.

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I. INTRODUCTION

Consider the nearest-neighbor antiferromagnet with classical spins of $n=3$ components on the kagome lattice of corner-sharing triangles,

$$\mathcal{H} = J\sum_{\langle ij\rangle} \mathbf{s}_i \cdot \mathbf{s}_j. \tag{1}$$

This is the prototypical *highly frustrated* system, meaning its ground-state manifold has macroscopically many degrees of freedom, and any spin order or freezing sets in at temperatures $T \ll J$.[1] It is well established that as $T\to 0$, the free energy of spin-mode fluctuations causes ordering into a *coplanar* state, a particular kind of classical ground state in which all spins lie in the same plane of spin space pointing in just three directions (120° apart).[2] These directions—which can be written as colors $c_i \equiv A$, B, or C taken by spins in a three-state Potts model—constitute a 3-coloring (the ground-state constraint implies every triangle has one of each color). The number of such colorings is exponential in the system size. The same is true for three-dimensional lattices of corner-sharing triangles such as the (half) garnet lattice[3] or equivalently hyperkagome lattice[4] and others.[5]

Can the coloring achieve a long-range order? All simulations[2,6–8] indicate the Potts spins are disordered (or algebraically correlated) as in the unweighted coloring (see below). However, following Huse and Rutenberg,[9] I propose this coloring develops long-range order in the $T\to 0$ limit as a consequence of the *unequal* weighting of the discrete states when one takes into account the free energy of fluctuations about each state. Of course, for $d=2$ at $T>0$, the orientation of the spin plane must fluctuate slowly in space; nevertheless the colors or Potts directions may be unambiguously defined throughout the system. But my goal is only the $T\to 0$ limiting ensemble, well defined (and nontrivial) since the obtained effective Hamiltonian [e.g., Eq. (16)] scales as T; whereas the spin-plane correlation length diverges exponentially[10] as $T\to 0$.

The calculation entails a series of mappings and effective Hamiltonians. First I shall review how, starting from the usual spin-deviation expansion, one integrates out most of the fluctuations leaving a *quartic* effective Hamiltonian $\mathcal{Q}$ for the dominant fluctuations.[11] The largest terms of $\mathcal{Q}$ are independent of the discrete Potts configuration, so treating the rest as a perturbation yields an effective Hamiltonian Φ for the Potts spins, purely entropic in that $\Phi \propto T$. Its coefficients may be inferred from simulations or approximated analytically (taking advantage of a "divergence constraint" on the dominant fluctuations). The Potts spins map in turn to a "height model," whence it becomes clear that Φ causes locking into an ordered state.[9] The expected long-range order is too tenuous to see directly in simulations but might be estimated analytically from the height model.

II. EFFECTIVE HAMILTONIAN DERIVATION

The object is to obtain an effective Hamiltonian for any of the discrete coplanar ground states, which absorbs the free energy of the low-temperature (anharmonic) fluctuations about that state. The first step is the "spin-wave" expansion in deviations from a given coplanar state. We parametrize the out-of-plane deviation as σ_i and the other deviation component as θ_i, the spin's in-plane rotation about the plane normal axis. Then the spin-wave expansion (I set $J\equiv 1$) is

$$\mathcal{H}_{\rm sw} \equiv \mathcal{H}^{(2)} + \mathcal{H}^{(3)} + \mathcal{H}^{(4)} + \cdots,$$

$$\mathcal{H}^{(2)} = \sum_{\langle ij\rangle}\left[\frac{1}{4}(\theta_i-\theta_j)^2 + \sigma_i\sigma_j\right] + \sum_i \sigma_i^2, \tag{2a}$$

$$\mathcal{H}^{(3)}_{\rm dom} = \sum_\alpha \eta_\alpha \mathcal{H}^{(3,\alpha)}_{\rm dom}, \tag{2b}$$

$$\mathcal{H}^{(4)}_{\rm dom} = \sum_{\langle ij\rangle}\frac{1}{16}(\sigma_i^2-\sigma_j^2)^2. \tag{2c}$$

In Eq. (2), α indexes the center of each triangle, and

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

From here on, I use "αm" ($m=1,2,3$) to denote the site on triangle α in sublattice m, as an alias for the site index "i;" the index m is taken modulo 3 (in expressions such as "$m+1$") and runs counterclockwise around the triangles whose centers are even sites on the honeycomb lattice of triangle centers. Following Ref. 11, I retained only

"dominant" anharmonic terms $\mathcal{H}^{(3)}_{\rm dom}$ and $\mathcal{H}^{(4)}_{\rm dom}$, being the parts of Eqs. (3) and (2c) containing the highest powers of σ (this will be justified shortly).

The η_α prefactor in $\mathcal{H}^{(3)}$ is the *only* dependence in Eq. (2) on the coloring state; this "chirality" η_α, is defined by $\eta_\alpha \equiv +1(-1)$ when the Potts labels are ordered as *ABC* (*CBA*) as one walks counterclockwise about triangle α. It is convenient to label coplanar states by the configuration $\{\eta_\alpha\}$.[12] Then a discrete Hamiltonian Φ can be defined for colorings, a function of the $\{c_i\}$ implicitly through the η_αs in Eq. (2):

$$e^{-\Phi(\{c_i\})/T} = \mathcal{Z}(\{c_i\}) \equiv \int_{\rm basin} \prod_i (d\theta_i d\sigma_i) e^{-\mathcal{H}_{\rm sw}/T}. \quad (4)$$

As $T \to 0$, the ensemble weight concentrates closer and closer to the coplanar state;[2,13] the integral in Eq. (4) is implicitly limited to the "basin" in configuration space centered on one coplanar state, and $\mathcal{Z}(\{c_i\})$ is the portion of the total partition function assigned to the corresponding coloring. Since $\mathcal{H}^{(2)}$ is independent of which coplanar state we are in, Φ is independent of $\{c_i\}$ at harmonic order.

Before we go on to anharmonic order, let us note the σ part of $\mathcal{H}^{(2)}$ can be written $\mathcal{H}^{(2)}_\sigma = \frac{1}{2}\Sigma_\alpha(\Sigma_m \sigma_{\alpha m})^2$. So there is a well-known whole branch of out-of-plane (σ) modes, called "soft modes," having *zero* cost at harmonic order; the soft-mode subspace is defined by the constraint

$$\sum_{m=1}^{3} \sigma_{\alpha m} = 0 \quad \text{(soft)} \quad (5)$$

being satisfied on every triangle α. (Two more out-of-plane branches, as well as all θ branches, are called ordinary modes.) Being limited only by higher-order terms, soft modes have large mean-square fluctuations, of $O(\sqrt{T})$, compared to $O(T)$ for ordinary modes;[2,11] this explains why factors containing soft modes were "dominant" in Eq. (2). The σ_is in dominant terms are limited to the "soft" subspace satisfying Eq. (5).

The next step is to do the Gaussian integral over all θ_i modes[2] as worked out in Ref. 11, obtaining a quartic effective Hamiltonian $\mathcal{Q}$ for only soft modes:

$$\mathcal{Q} = \mathcal{H}^{(4)}_{\rm dom} - \sum_{\alpha,\beta} \eta_\alpha \eta_\beta \mathcal{Q}'_{\alpha\beta}, \quad (6)$$

with[14]

$$\mathcal{Q}'_{\alpha,\beta} \equiv \sum_{m,n=1}^{3} \left(\frac{\sqrt{3}}{4}\right)^2 G_{\alpha m,\beta n} \sigma^2_{\alpha m} \sigma^2_{\beta n}. \quad (7)$$

The Green's function of the θ modes was defined by

$$TG_{\alpha m,\beta n} \equiv \langle (\theta_{\alpha,m+1} - \theta_{\alpha,m-1})(\theta_{\beta,n+1} - \theta_{\beta,n-1}) \rangle_\theta, \quad (8)$$

where "$\langle \ldots \rangle_\theta$" means taken in the (Gaussian) ensemble of $\mathcal{H}^{(2)}_\theta$ ($\equiv$ the θ part of $\mathcal{H}^{(2)}$). As G_{ij} decays with distance, the largest terms are state independent: $\mathcal{Q}'_{\alpha\alpha} = (3/16)[G_0 \Sigma^3_{m=1} \sigma^4_{\alpha m} + 2G_1 \Sigma_{m<n} \sigma^2_{\alpha m} \sigma^2_{\alpha n}]$, where G_0 and G_1 are the on site and first neighbor G_{ij}. Trivially $2G_1 = -G_0$, and $G_0 \equiv 1$ (due to equipartition, which implies $\langle \mathcal{H}^{(2)}_\theta \rangle = 3T/4$ per triangle). Also, given Eq. (5), $\Sigma_{m<n} \sigma^2_{\alpha_m} \sigma^2_{\alpha n} \to \frac{1}{2}\Sigma_m \sigma^4_{\alpha m}$ in $\mathcal{Q}'_{\alpha\alpha}$ and similarly in Eq. (2c) $\mathcal{H}^{(4)}_{\rm dom} \to (1/16)\Sigma_i \sigma^4_i$. Finally we can regroup Eq. (6) as

$$\mathcal{Q} = \mathcal{Q}_0 - \sum_{\alpha \neq \beta} \eta_\alpha \eta_\beta \mathcal{Q}'_{\alpha,\beta}, \quad \mathcal{Q}_0 = B_0 \sum_i \sigma^4_i, \quad (9)$$

with $B_0 = 13/16$ from both $\mathcal{H}^{(4)}_{\rm dom}$ and $\mathcal{Q}'_{\alpha\alpha}$ terms.

Now I turn to the perturbation expansion: the key step in our whole derivation is to expand Eq. (4) treating the $\{\eta_\alpha\}$ as if they were small quantities. (In fact $|\eta_\alpha| = 1$, so a perturbative treatment might appear questionable, but quantitatively $\mathcal{Q}_0$ has a much larger coefficient than the terms in $\mathcal{Q}'$, owing to the decay of G_{ij} with separation.) The resulting (and final) effective Hamiltonian is, to lowest order,

$$\Phi = -\frac{1}{2} \sum_{\alpha \neq \beta} \mathcal{J}_{\alpha\beta} \eta_\alpha \eta_\beta, \quad (10)$$

with

$$\mathcal{J}_{\alpha\beta} \equiv \langle \mathcal{Q}'_{\alpha,\beta} \rangle_0 = \sum_{m,n=1}^{3} \left(\frac{\sqrt{3}}{4}\right)^2 G_{\alpha m,\beta n} \langle \sigma^2_{\alpha m} \sigma^2_{\beta n} \rangle_0, \quad (11)$$

where the expectation is taken in the ensemble of $\mathcal{Q}_0$. Notice that since $\mathcal{Q}$ is homogeneous in $\{\sigma_i\}$, it follows that the partial partition function $\mathcal{Z}(\{c_i\})$ in Eq. (4)—and consequently Φ/T—is *temperature independent* as $T \to 0$, apart from a configuration-independent power of T.

A corollary of my assumption that $\mathcal{Q}'_{\alpha,\beta}$ is "small" is that expectations $\langle \ldots \rangle_{\rm sw}$ of polynomials in $\{\sigma_i\}$, measured under the *full* spin-wave Hamiltonian $\mathcal{H}_{\rm sw}$, should be practically independent of the coloring configuration $\{\eta_\alpha\}$.[15] That can be checked in Monte Carlo or molecular dynamics simulations[16] of the Heisenberg model. The needed correlations can be measured even if the system is confined to the basin of one coplanar state: there is no need to equilibrate the relative occupation of different basins. Those same simulations would numerically evaluate the quartic expectations.

III. SELF-CONSISTENT APPROXIMATION FOR COUPLINGS AND ASYMPTOTIC BEHAVIOR

An alternative to simulation is to analytically evaluate the quartic expectations in Eq. (11) using a self-consistent decoupling. That is, Eq. (9) is replaced by

$$F_{\rm var} \equiv \frac{1}{2} B \sum_i \sigma^2_i, \quad (12)$$

defining a Gaussian variational approximation to the soft-mode ensemble; here

$$B \equiv 6B_0 \langle \sigma^2_i \rangle_{\rm var}, \quad (13)$$

with "$\langle \ldots \rangle_{\rm var}$" taken in the ensemble of Eq. (12). Now let Γ_{ij} (also written $\Gamma_{\alpha m,\beta n}$) be the Green's function for σ_i modes:

$$\langle \sigma_i \sigma_j \rangle_{\rm var} = T\Gamma_{ij}/B \quad (14)$$

(this definition makes Γ_{ij} independent of B and T), and let $\Gamma_{ii} \equiv \Gamma_0 = 1/3$. Combining Eqs. (13) and (14), I get the self-consistency condition $B = (6B_0\Gamma_0 T)^{1/2} = (13T/8)^{1/2}$. Next, the

expectations in Eq. (11) are evaluated in the variational approximation, decoupling by Wick's theorem as

$$\langle \sigma_i^2 \sigma_j^2 \rangle_{\rm var} = \langle \sigma_i^2 \rangle_{\rm var} \langle \sigma_j^2 \rangle_{\rm var} + 2\langle \sigma_i \sigma_j \rangle_{\rm var}^2 = \left(\frac{T}{B}\right)^2 [\Gamma_0^2 + 2\Gamma_{ij}^2]. \tag{15}$$

Substituting Eq. (15) into Eq. (11) gives my central result for the effective Hamiltonian,

$$\frac{\mathcal{J}_{\alpha\beta}}{T} \approx \frac{3}{13} \sum_{m,n=1}^{3} G_{\alpha m,\beta n} \Gamma_{\alpha m,\beta n}^2 \tag{16}$$

[Γ_0^2 from Eq. (15) always cancels in the m,n sum].

Equation (16) gives $\mathcal{J}_1/T \approx -1.88 \times 10^{-3}$ and $\mathcal{J}_2/T \approx -4.3 \times 10^{-4}$. Assuming these two dominate, the state with the lowest Φ value is the "$\sqrt{3} \times \sqrt{3}$" pattern, the "antiferromagnetic" arrangement of chiralities η_α, but other coloring configurations are only slightly less likely. The long-range order suggested by Ref. 9 is a subtle crossover of correlation functions at large (but not diverging) scales, best expressed in terms of a "height model," as will be developed in Sec. IV.

Before that, in order to check that more distant couplings $\mathcal{J}_{\alpha\beta}$ can be neglected, I will work out how they scale at large R. We need both kinds of Green's function in Eq. (16), tackling the θ_i fluctuations first. In Eqs. (2a) and (8), $(\theta_{m+1} - \theta_{m-1}) \approx -a\epsilon_\alpha \hat{\mathbf{e}}_m^\perp \cdot \nabla\theta$, where a is the nearest-neighbor distance, and $\epsilon_\alpha = +1(-1)$ when α labels an even (odd) triangle. The unit vector $\hat{\mathbf{e}}_m \equiv (\cos\psi_m, \sin\psi_m)$, is defined to point from the center of any even triangle to its m corner, and $\hat{\mathbf{e}}_m^\perp \equiv \hat{\mathbf{z}} \times \hat{\mathbf{e}}_m$. At long wavelengths,

$$\mathcal{H}_\theta^{(2)} \approx \frac{1}{2}\rho_\theta \int d^2\mathbf{r} |\nabla\theta(\mathbf{r})|^2, \tag{17}$$

where $\rho_\theta = \sqrt{3}/2$. Asymptotically the Green's function of Eq. (17) is pseudodipolar:

$$G_{\alpha m,\beta n} \approx \frac{a^2}{2\pi\rho_\theta R^2} \epsilon_\alpha \epsilon_\beta \cos(\psi_m + \psi_n - 2\psi_R). \tag{18}$$

Here (R, ψ_R) are the polar coordinates of the vector between triangle centers α and β.

The σ_i fluctuations are handled similarly. The soft-mode constraint [Eq. (5)] is implemented by writing σ_i as a discrete gradient, $\sigma_i \equiv \phi_\nu - \phi_\mu$, analogous to the "height" model constructions.[17] Here $\{\phi_\mu\}$ is defined on the hexagon centers, and $\mu \to \nu$ is oriented counterclockwise around even kagome triangles. The discrete gradient defining σ_i can be converted into a continuous one, $\sigma_{\alpha m} \approx 2a\hat{\mathbf{e}}_m^\perp \cdot \nabla\phi$. Then the long-wavelength limit of Eq. (12) looks like Eq. (17), with $\rho_\theta \to \rho_\phi = 2\sqrt{3}B$. That implies that for large separations R, $\Gamma_{\alpha m,\beta n}$ looks like Eq. (18) with $\rho_\theta \to \rho_\phi/4$. Inserting both Green's-function behaviors into Eq. (16), I get the asymptotic behavior of the couplings:

$$\frac{\mathcal{J}_{\alpha\beta}}{T} \approx \frac{A}{(R/a)^6} \epsilon_\alpha \epsilon_\beta \cos 6\psi_R \tag{19}$$

for large R with $A = 6\sqrt{3}/13^2\pi^3 \approx 2.0 \times 10^{-3}$. Equation (19) shows the interaction decays rapidly with distance and oscillates as a function of angle.

IV. HEIGHT MODEL AND LONG-RANGE ORDER

The *discrete* ensemble in which every 3-coloring c_i is equally likely is known to have power-law correlations, which may be understood via a mapping of the Potts microstates to a two component "height" variable $\mathbf{h}(\mathbf{r})$.[9,18] At coarse-grained scales, the ensemble weight of $\{\mathbf{h}(\mathbf{r})\}$ is described by a free energy

$$F_{\mathbf{h}} = \int d_{\mathbf{r}}^2 \frac{1}{2} K |\nabla\mathbf{h}|^2, \tag{20}$$

handled by standard Coulomb-gas techniques.[19]

Reference 9 pointed out the equal-weighted coloring has a height stiffness $K = K_c$ exactly, where K_c is the critical value for the roughening transition. Any increase in K must cause $\mathbf{h}(\mathbf{r})$ to lock to a uniform mean value.[9,19,20] That corresponds to long-range order of the colors (=Potts spins), into the pattern of with the flattest $\mathbf{h}(\mathbf{r})$, namely, the "$\sqrt{3} \times \sqrt{3}$" state. Since (as shown above) Φ favors that flat state, the coloring ensemble with the Φ weighting is coarse-grained to a height ensemble with a slightly larger K, and therefore we get long-range order, as claimed.[9]

The couplings $\mathcal{J}_{\alpha\beta}$ as approximated analytically or obtained from a simulation may be used as a Hamiltonian in discrete simulations of the coloring model. These are far faster than simulations of the Heisenberg spins, but I still doubt such simulations will see long-range order directly, in the accessible system sizes. But the height stiffness K can be accurately measured (using Fourier transforms[21]). With that, by iteration of renormalization-group equations,[20] it should be possible to semianalytically estimate the length scale ξ at which the color correlations cross over from power-law decay to long-range order and the size of the order parameter.

What happens to this whole story in $d=3$, for the Heisenberg antiferromagnet on triangle-sharing lattices[3–5]? A minor difference is that in $d=3$ the spin plane orientation has *true* long-range coplanar order at some $T>0$ as do the three spin directions within the plane.[7] The derivation and result for the effective Hamiltonian (16) extend to $d=3$; there is also the unimportant difference that, in deriving the asymptotic behavior of $\mathcal{J}_{\alpha\beta}$, a "Coulomb phase"[22,23] rather than a "height function" viewpoint must be used for coarse graining σ, but Γ_{ij} still has a pseudodipolar form,[22,23] and the final asymptotic form is analogous to Eq. (19) ($\mathcal{J}_{\alpha\beta} \propto 1/R^9$ with an oscillating angular dependence).

The crucial difference in $d=3$ is that the discrete (Potts) variables also have a "Coulomb phase" in place of the "height representation" used by Ref. 9. There exists a coarse-grained "flux field" analogous to $\nabla\mathbf{h}$, but the analog of $\mathbf{h}$ itself is a vector potential and is not uniquely defined. The Hamiltonian Φ, I conjecture, tends to favor states with zero

coarse-grained flux, which means it tends to increase the flux stiffness K of the three-dimensional model. But, in contrast to two dimensions, in the absence of Φ the system is *not* sitting at a critical K; therefore, the tiny increase in K due to the transverse spin fluctuations cannot drive us into a new phase. Thus, no long-range order of the colorings is expected in $d=3$, merely the pseudodipolar correlations inherent to the Coulomb phase.

V. CONCLUSION

A path has been shown to the elusive long-range order of the classical kagome antiferromagnet, through a string of mappings or elimination of degrees of freedom: ground states to colorings to chiralities to discrete $\mathbf{h}_\mu$ height representation and finally its coarse-grained continuum version. Other maps go from all spin deviations, to soft modes σ_i, to their height field ϕ_μ or $\phi(\mathbf{r})$. The boldest approximations were (i) the perturbation expansion [Eq. (11)] of the effective quartic Hamiltonian (6); this had no controllable small parameter, but it was argued the terms were numerically small (ii) the variational or decoupling handling of the quartic ensemble $\{\sigma_i\}$.

The philosophy followed here[24] is to obtain an effective Hamiltonian defined for *arbitrary* spin arrangements, not just especially symmetric ones (even if that necessitates cruder approximations). I have previously used the trick of turning the spin configuration into a set of coefficients or matrix entries and then expanding in them for several systems.[25–27] In particular, a related expansion in $\mathcal{H}^{(3)}$ to obtain a Hamiltonian of form (10) was carried out for the large-S *quantum* Heisenberg antiferromagnet in Ref. 27.

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