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Classical antiferromagnets on the Kagomé lattice

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We examine the classical antiferromagnet on the Kagomé lattice with nearest-neighbor interactions and n-component vector spins. Each case $n=1,2,3$ and $n>3$ has its own special behavior. The Ising model ($n=1$) is disordered at all temperatures. The XY model ($n=2$) in the zero-temperature ($T\rightarrow 0$) limit reduces to the three-state Potts model, which in turn can be mapped onto a solid-on-solid model that is *at* its roughening transition. Exact critical exponents are derived for this system. The spins in the Heisenberg model ($n=3$) become coplanar and more ordered than the XY model as $T\rightarrow 0$. Thus we argue that the Heisenberg model has long-range antiferromagnetic order in the limit $T\rightarrow 0$. For $n>3$ the system appears to remain disordered for $T\rightarrow 0$.

An antiferromagnet with only nearest-neighbor interactions on an ideal Kagomé lattice [Fig. 1(a)] is a highly frustrated system. Physically, this system may be approximately realized in[1-3] $SrCr_{8-x}Ga_{4+x}O_{19}$ and in the proposed $\sqrt{7}\times\sqrt{7}$ phase of the second layer of ^{3}He on graphite.[4] The *classical* antiferromagnetic spin Hamiltonian we consider here is

$$H=\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{1}$$

where the sum is over all nearest-neighbor pairs on the Kagomé lattice and we consider unit-length n-component vector spins and also three-state Potts spins. Here we describe our main results; a more detailed report is in preparation.[5]

For Ising spins on a Kagomé lattice, the correlation functions may be exactly mapped onto those of the honeycomb lattice Ising model via star-triangle and decimation transformations.[6] The entire antiferromagnetic range, $T\geq 0$, on the Kagomé lattice maps onto $T\geq 2/\ln 2$ on the honeycomb lattice, which is well within the disordered phase. In fact, the largest eigenvalue of the susceptibility matrix $\chi(\mathbf{q})$ is strictly independent of the momentum $\mathbf{q}$ at *all* T,[5] as was noted to order $1/T^8$ in the high-temperature expansion for Ising spins by Harris, Kallin, and Berlinsky.[7]

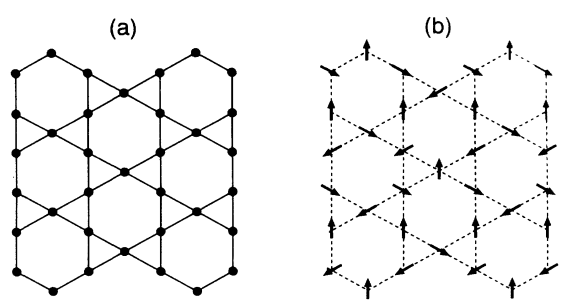

FIG. 1. (a) A section of the Kagomé lattice. (b) Spins on the Kagomé lattice fully ordered in the so-called $\sqrt{3}\times\sqrt{3}$ pattern.

For fixed length XY spins, the Hamiltonian (1) may be written as

$$H=\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j)\,. \tag{2}$$

Up to a global spin rotation, every spin in a ground state of (2) has $\theta_j=0$, or $\pm 2\pi/3$—these are the three states of the corresponding three-state Potts model. The energy of fluctuations, $\theta_i=\theta_i^0+\delta_i$, about a ground-state configuration $\{\theta_i^0\}$ is

$$H=\sum_{\langle ij\rangle}[-\tfrac{1}{2}+\tfrac{1}{4}(\delta_i-\delta_j)^2]+O(\delta^3) \tag{3}$$

for every ground state. The free energies of each ground state plus its fluctuations differ at order T^2 in the $T\rightarrow 0$ limit, so every ground state is given the same Boltzmann weight in this limit. Thus, $T\rightarrow 0$ correlation functions of the XY model are identical to those of the three-state Potts model.

The ground states of the XY model (2) have long-range order in $w_j\equiv\exp(i3\theta_j)$. Since the system is two dimensional this long-range order does not survive for $T>0$. However, a Kosterlitz-Thouless (KT) critical phase with power-law correlations, $\langle w_i^* w_j\rangle\sim r_{ij}^{-\eta_w(T)}$, is stable at low temperatures, with $\eta_w(T)$ increasing continuously with T. The KT phase transition should occur when $\eta_w(T)$ reaches $\frac{1}{4}$ and the vortices of w unbind,[8] unless it is preempted by a first-order phase transition at a lower temperature. Upon encircling a vortex of w the angle θ [mod$(2\pi/3)$] winds once. Thus one may call them $\frac{1}{3}$ vortices of $\mathbf{S}$. Note that the KT phase transition is not to an antiferromagnetic phase, but to a less obvious sort of order; quasi-long-range order in $\exp(i3\theta)$.

At $T=0$, the XY model has the same properties as the three-state Potts model and thus has an entropy of[9] $S\simeq 0.126k_B$ per site. In any ground state of the Potts model the three Potts states are all represented on every triangular plaquette of the lattice. There is an exact mapping of each Potts ground state onto a configuration of a solid-on-solid (SOS) or roughening model.[10] This SOS model has a "height" variable z_h located at the center of

each hexagonal plaquette, h, of the Kagomé lattice. The height variables $\mathbf{z}_h$ are points on a triangular lattice in a two-dimensional height space. (Note the height is thus the position of a two-dimensional surface on a four-dimensional lattice.) Height variables on adjacent hexagons of the Kagomé lattice are restricted to be adjacent points of the triangular lattice in height space. The mapping from the SOS to the Potts model is given by considering two height variables on adjacent hexagons separated by a given Potts spin on the Kagomé lattice. The three possible orientations of the height-space bond connecting the pair of heights map onto the three Potts spin states. This gives a unique mapping of each allowed height state onto a Potts ground state. To make the reverse mapping unique we need only fix the heights on one pair of adjacent hexagons.

Now consider the long-distance correlations of the SOS model and a corresponding coarse-grained height $\mathbf{z}$. For a rough two-dimensional surface the mean-square height difference grows logarithmically:[11] $\langle[\mathbf{z}(\mathbf{r}_i)-\mathbf{z}(\mathbf{r}_j)]^2\rangle \approx \sigma \ln r_{ij}$, where $r_{ij}\equiv|\mathbf{r}_i-\mathbf{r}_j|$. Also consider operators (or order parameters) that are periodic in height space, such as $\psi_{\mathbf{Q}}\equiv e^{i\mathbf{Q}\cdot\mathbf{z}}$. If the surface is rough we have

$$\langle\psi_{\mathbf{Q}}^*(\mathbf{r}_i)\psi_{\mathbf{Q}}(\mathbf{r}_j)\rangle \approx \exp\{-\tfrac{1}{2}|\mathbf{Q}|^2\langle[z_{\mathbf{Q}}(\mathbf{r}_i)-z_{\mathbf{Q}}(\mathbf{r}_j)]^2\rangle\} \sim r_{ij}^{-\eta_{\mathbf{Q}}}, \tag{4}$$

where $z_{\mathbf{Q}}\equiv\mathbf{z}\cdot\mathbf{Q}/|\mathbf{Q}|$ and $\eta_{\mathbf{Q}}=\sigma|\mathbf{Q}|^2/4$. For an operator consisting of more than one $\psi_{\mathbf{Q}}$, the smallest $|\mathbf{Q}|$ determines the long-distance decay exponent η. Three physical operators that are linear combinations of $\psi_{\mathbf{Q}}$'s are (i) the restriction of the heights $\mathbf{z}_h$ to lie on the triangular lattice, (ii) the staggered chirality, and (iii) the staggered magnetization in the $\sqrt{3}\times\sqrt{3}$ pattern illustrated in Fig. 1(b).

Each triangle of the Kagomé lattice Potts antiferromagnet has two types of local ground state: one in which the spins rotate clockwise going around the triangle clockwise, and one in which the spins rotate counterclockwise. These two types have positive and negative chirality, respectively. The total staggered chirality is the chirality of the right-pointing triangles [see Fig. 1(a)] minus that of the left-pointing triangles.

Baxter[9] put on a field conjugate to the total staggered chirality, calculated the free energy of the Potts ground states, and found an essential singularity in the free energy at zero field. Interpreted in standard scaling terms,[12] this means that the staggered chirality is a marginal operator, with correlation exponent $\eta_c=4$. The local staggered chirality is a periodic function in height space that is of one sign in the interior of right-pointing triangles (in height space) and of the other sign in left-pointing triangles, so it has the same periodicity and the same smallest $|\mathbf{Q}|$ as the height space lattice itself. Since the restriction of height to the lattice has the same smallest $|\mathbf{Q}|$ as the staggered chirality, it is a marginal operator also. Thus our SOS model is *at* its roughening transition.

In order to check this picture we have measured the correlations in the three-state Potts model at $T=0$. We use a path-flipping algorithm[5,13] to equilibrate the system. The algorithm finds a continuous path of nearest-neighbor bonds in the Kagomé lattice along which only two Potts states are present, alternating along the path. All spins adjacent to the path are necessarily in the third state. The path is then "flipped" by interchanging the two states along the path. Paths of all lengths are found.

The staggered magnetization in the $\sqrt{3}\times\sqrt{3}$ pattern of Fig. 1(b) is periodic in height space with a unit cell that contains three sites of the triangular lattice; since its smallest $|\mathbf{Q}|^2$ is 3 times smaller than that of the staggered chirality, its correlation exponent should be $\eta_m=\frac{4}{3}=\eta_c/3$. The simplest measurement of η_m seems to be the finite-size scaling of the mean-square staggered magnetization density, $\langle|\mathbf{m}^\dagger|^2\rangle$, as measured in simulations by Broholm *et al.*,[3] who estimated $\eta_m=1.4\pm0.3$. With the path-flipping algorithm, we can obtain more accurate data. The results for linear sizes up to $L=384$ ($192\times192\times3$ spins) are shown in Fig. 2. Significant deviations from the naive expectation $\langle|\mathbf{m}^\dagger|^2\rangle\sim L^{-4/3}$ are seen. Since we believe we are *at* the ordering (roughening) transition there should be logarithmic corrections due to the marginal operator present (i.e., the discreteness of the height lattice). Thus we have fit to the forms

$$\langle|\mathbf{m}^\dagger|^2\rangle \approx AL^{-4/3}(\ln L/a)^b, \approx \tilde{A}L^{-4/3}[1+\tilde{b}/(\ln L/\tilde{a})], \tag{5}$$

which both fit quite well, as illustrated in Fig. 2. We have also measured chirality correlations, but their spatial decay is so rapid that a useful measurement of η_c did not seem feasible.

For Heisenberg spins our simulation results agree qualitatively with Chalker, Holdsworth, and Shender,[14] indicating that coplanar ground states are selected as $T\to0$. Consider the five spins on two adjacent triangles of the Kagomé lattice as shown and numbered in the inset in Fig. 3. At low temperatures, the three spins on each triangle are, nearly, all in one plane in spin space and at mutual angles of $2\pi/3$. Thus a measure of the deviation from

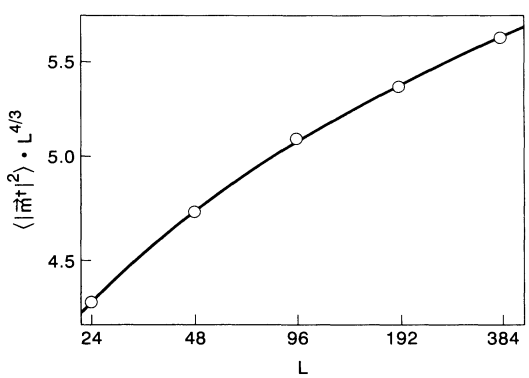

FIG. 2. The mean-square staggered magnetization density with the expected power-law dependence $L^{-4/3}$ removed vs linear system size L for the three-state Potts model at $T=0$. Both scales are logarithmic. The (indistinguishable) fits to (5) are shown. For this figure only, mixed boundary conditions that are periodic in one direction and free in the other were used to facilitate equilibration at $T=0$; fully periodic boundary conditions were used in Figs. 3–5. Where not shown in Figs. 2–5, the error bars are smaller than the points.

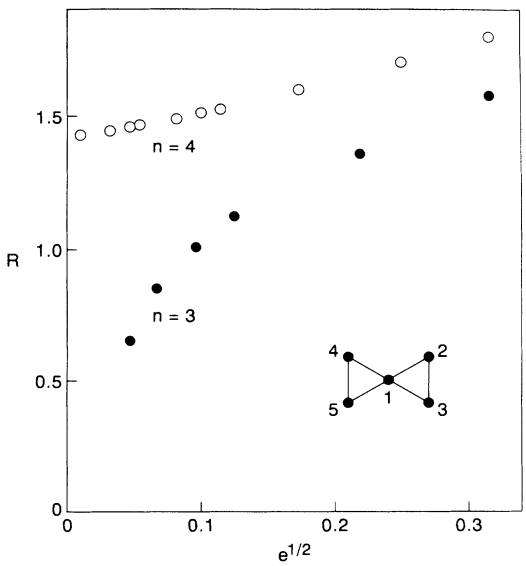

FIG. 3. For n-component spins, the deviation from coplanarity, R, as defined in (6). The excess energy per bond over the ground state e is proportional to the temperature T for $e \to 0$. Inset: Two adjacent triangles of the Kagomé lattice illustrating the site numbering used in Eq. (6).

coplanarity is

$$R \equiv 3 - \langle |(\mathbf{S}_2 - \mathbf{S}_3)\cdot(\mathbf{S}_4 - \mathbf{S}_5)| \rangle . \tag{6}$$

Our results (Fig. 3) for $n=3$ are consistent with the expectation[14] that $R \sim e^{1/2}$ for $e \to 0$, where e is the excess energy per bond over the gound state. This implies that for $n=3$ coplanar ground states are selected for $T \to 0$.

The theoretical arguments[14–16] that suggest that for $n=3$ coplanar ground states are selected for $T \to 0$ have not addressed $n > 3$. We have investigated this issue by measuring R for $n=4$, 5, and 9. We find the equilibration times are much faster than $n=3$, and that even adjacent triangles do not appear to be going coplanar in the $T \to 0$ ($e \to 0$) limit, as is shown for $n=4$ in Fig. 3. Thus the mechanism that selects the coplanar states is for some reason only operative in the $n=3$ system.

For Heisenberg systems with periodic boundary conditions we measured the correlations of the spins in heat-bath Monte Carlo simulations. Equilibration times grow very rapidly as $T \to 0$, so we used an extrapolation technique to estimate the $T=0$ correlations. In addition to the usual unclipped correlations $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$, we have measured "clipped" correlation functions, $\langle f(\mathbf{S}_i \cdot \mathbf{S}_j) \rangle$, with $f(x) = -\frac{1}{2}$ for $x < C$ and $f(x) = 1$ for $x > C$. This treatment is based on the assumption that at $T=0$ the spin configurations are coplanar, so $\mathbf{S}_i \cdot \mathbf{S}_j$ can only take the values $-\frac{1}{2}$ and 1, as in the XY and Potts models. For $T \to 0$ we thus expect the clipped and unclipped correlation functions to agree. We plotted the correlation functions versus the fraction of $\mathbf{S}_i \cdot \mathbf{S}_j$ between 0 and 0.5 (this fraction is a measure of the number of noncoplanar spins and should vanish for $T \to 0$) and extrapolated from the two lowest temperatures (typically $\beta \equiv 1/T = 100$ and 200) to $T=0$. An example for distance $r_{ij}=4$ along a nearest-neighbor direction is shown in Fig. 4, along with the value

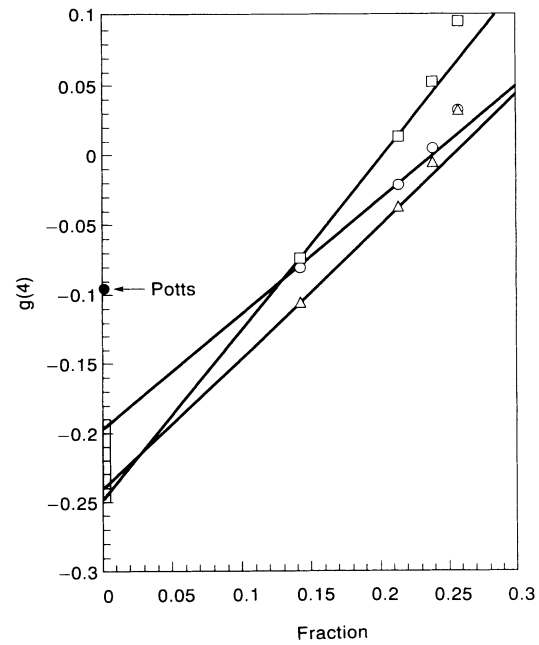

FIG. 4. Spin correlations for Heisenberg spins on a size $L=24$ Kagomé lattice. Plotted are the results for distance $r_{ij}=4$ vs fraction of $\mathbf{S}_i \cdot \mathbf{S}_j$ between 0 and 0.5. The solid dot on the axis is the $T=0$ Potts result, open circles are unclipped spin correlations, triangles are clipped at $C=\frac{1}{3}$, squares are clipped at $C=\frac{1}{4}$ (see text). The shaded region on the axis indicates the naive range of extrapolations of the correlations to $T=0$, where the fraction is zero.

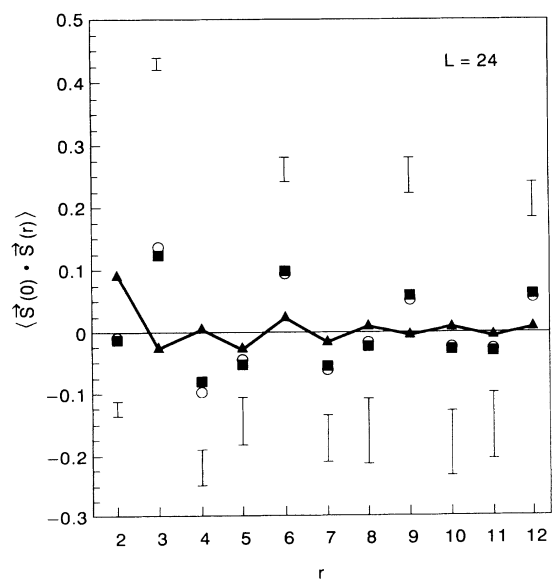

FIG. 5. Spin correlations on a size $L=24$ Kagomé lattice vs distance r in a straight line along a nearest-neighbor direction. The open circles are three-state Potts at $T=0$, solid triangles are $\beta=50$ Heisenberg, solid squares are $\beta=200$ Heisenberg, and the error bars indicate the range for Heisenberg correlations at $T=0$ obtained by the extrapolation method illustrated in Fig. 4.

for the $T=0$ Potts system of the same size.

In Fig. 5 we show some of our results for unclipped spin correlations in a size $L=24$ (432 spins) system. One can still see the high-temperature pattern at the rather low temperature of $\beta=50$, with the correlation function alternating with a period of 2 sites. By $\beta=200$ the low-temperature pattern [with a period of 3 sites; see Fig. 1(b)] is established, with correlations quite similar to the three-state Potts model at $T=0$. The extrapolated correlations of the $T=0$ Heisenberg model clearly exceed the $T=0$ Potts results. While there must be systematic corrections to our simple extrapolations, we find that at every distance (at this lattice size) at least one of the unclipped or the two clipped correlations at $\beta=200$ exceeds in magnitude the corresponding Potts value, and is monotonic at low temperatures, indicating that the extrapolated correlations are qualitatively correct. Results from other system sizes from $L=12$ to 84 support this conclusion. Thus we find that the low-temperature Heisenberg model shows significantly stronger short-range order than the three-state Potts or XY models.

The coplanar ground states of the Heisenberg system that are apparently selected for $T\rightarrow 0$ are equivalent to three-state Potts model ground states. But, unlike in the XY case, the coplanar Potts ground states are not all given the same Boltzmann weight. The relative Boltzmann weight is determined by the nonlinear interactions between the soft modes of the Heisenberg model,[7,14–16] which are different for each inequivalent Potts ground state. In the $T=0$ Potts model where all the states are weighted equally, the system is *at* its ordering (roughening) transition. Since the weighting of the states is changed in a direction that enhances the order, the system should have long-range order. (Note in a more ordered state the surface in the SOS representation is less rough.) Because of this we argue that in the $T\rightarrow 0$ limit the Heisenberg antiferromagnet on the Kagomé lattice has true long-range antiferromagnetic order in the $\sqrt{3}\times\sqrt{3}$ pattern of Fig. 1(b). More extensive simulations to further test this proposal and perhaps obtain a quantitative estimate of the staggered magnetization are in progress.[5]

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