Dipolar order by disorder in the classical Heisenberg antiferromagnet on the kagome lattice

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Ever since the experiments which founded the field of highly frustrated magnetism, the kagome Heisenberg antiferromagnet has been the archetype setting for the study of fluctuation induced exotic ordering. To this day the nature of its classical low-temperature state has remained a mystery: the non-linear nature of the fluctuations around the exponentially numerous harmonically degenerate ground states has not permitted a controlled theory, while its complex energy landscape has precluded numerical simulations at low temperature, $T$. Here we present an efficient Monte Carlo algorithm which removes the latter obstacle. Our simulations detect a low-temperature regime in which correlations asymptote to a remarkably small value as $T \to 0$. Feeding these results into an effective model and analyzing the results in the framework of an appropriate field theory implies the presence of long-range dipolar spin order with a doubled unit cell.

The first experiments on the ‘kagome bilayer’ SCGO \cite{1,2} triggered a wave of interest in kagome antiferromagnets in particular, and frustrated systems in general. A cluster of early seminal theoretical papers \cite{3-7} established kagome magnets as model systems for novel ordering phenomena, discussing in particular spin liquidity, partial order, disorder-free glassiness and order by disorder. The excitement persists, not least in the quantum realm \cite{8}, where there has been much recent progress in understanding the nature of low-temperature phase has not been established, despite the deceptive simplicity of its Hamiltonian, encoding only nearest-neighbour interactions of strength $J > 0$ between classical unit-length spins $S_i$: $H = J \sum_{\langle ij \rangle} S_i \cdot S_j$. This happens because classical Heisenberg spins do not lend themselves at all to the numerical methods applied to $S = 1/2$ (e.g. \cite{9-11}), while classical Monte Carlo (e.g. \cite{3,5,12,13}) has not been able to sample the different local free energy minima separated by entropic barriers – for the best effort yet, see Ref. \cite{14}. At the same time, analytical approaches have managed to develop different possible scenarios, described below, without being able to choose between them \cite{3,15}.

Here, we present a Monte Carlo algorithm which enables us to simulate systems containing over 2000 spins down to a low-temperature regime, where we find that correlations no longer change as $T$ is lowered further. We use the results to determine the best parameters in effective models, a stiffness in a height model, an effective field theory; as well as a further-neighbour coupling in an extended Potts model. In particular the latter can then be simulated for over $10^6$ spins, which enables us to verify the critical behavior encapsulated by the height model. Thus we identify which ordering scenario applies: we obtain spin ordering with a remarkably small ordered moment, which we estimate to be about an order of magnitude below fully developed order. In the remainder of this manuscript, we give an account of our analysis, starting with a review of the unusual behaviour of the kagome magnet as the temperature is lowered.

**Complex energy landscape:** As the kagome magnet is cooled from high temperatures, it develops short-range order like any other magnet. Upon cooling further, its frustrated nature asserts itself: at the Curie temperature, $J$, there is no sign of any ordering predicted by mean-field theory, despite the fact that the spins in each triangle firmly point at $120^\circ$ to one another. Instead, it is not until much lower $T \lesssim 10^{-3}J$...
that all spins adopt a common plane

This coplanar ordering is described mathematically by two order parameters [14]: a quadrupolar (also known as nematic or coplanar) one for the direction normal to the plane; and an octupolar one as follows. If one denotes the angle the spins make in the plane with respect to a reference spin by $\theta$, it is $\exp(3i\theta)$ which orders. Crucially, the existence of dipolar (spin) order, in $\exp(i\theta)$, remains an open question.

It should be noted that since the Kagome lattice is two-dimensional, di-, quadru- and octupolar orders in fact only set in algebraically, being cut off on a lengthscale $\xi_{MW}$ for $T > 0$, below which scale our analysis applies. Crucially, however, $\xi_{MW}$ diverges exponentially as the temperature is lowered, so that the ordered regimes are still well-defined in practice even at small but nonzero $T$.

As the ground state is continuously degenerate, the energy landscape has many zero-energy directions (flat valleys). However, at non-zero temperature, in the free energy landscape there are many zero-energy directions (flat valleys). No algorithm has so far managed to take into account that the different coplanar states acquire different free energies. Here we present an algorithm which achieves this as follows.

**Numerical algorithm:** At low temperature, fluctuations around an ideal coplanar (Potts) state are small. We can thus identify a Potts configuration nearest to the state of the system. We then rotate spins on an alternating loop of spins of two colours so that these two colours are interchanged. Crucially, we have found a way of mapping configurations into each other which are equivalent as far as the linearised equations of motion are concerned – whether or not to accept a move thus depends only on precisely the anharmonic terms responsible for the low-temperature state selection. Our algorithm implements the semiclassical dynamical symmetry identified in Ref. [17].

Firstly, we construct the Potts configuration by assigning color R to all spins with a positive projection onto a randomly chosen initial spin. Then, the other spins along the resulting loops are alternatingly colored G–B. Next, for each loop, we evaluate the average orientations $\mathbf{Y}_\alpha$ of spins colored $\alpha = R$, G or B. Finally, we attempt a move consisting of rotating spins G (B) by the angle $\varangle (\mathbf{Y}_B, \mathbf{Y}_G)$ in opposite directions in the nematic plane of the loop; this move is accepted by a standard Metropolis condition. To see how the dynamical symmetry is implemented, write a spin $S_{\alpha,i} = Y_\alpha + s_{\alpha,i}$ so that the total spin of a triangle $i$, $\ell_i = \sum_\alpha S_{\alpha,i} = \sum_\alpha Y_\alpha + \sum_\alpha s_{\alpha,i}$. At the lowest temperatures, $\sum_\alpha Y_\alpha = 0$ (the ground state condition), and the rotation operation $R_B Y_B = Y_B$, $R_B Y_B = Y_G$ and $R_G Y_G = Y_B$ as $\varangle (Y_B, Y_G) = \frac{\pi}{6}$. Now, $R_B s_{B,i} + R_G s_{G,i} = (\ell_i^r, \ell_i^q, -\ell_i^z)$. The linear equations of motion are invariant under this change [17]. We can thus fully equilibrate systems with, depending on boundary conditions, up to 2025 spins at temperatures down to $T = 10^{-6} J$. Lower temperatures are achievable but, as we discuss next, this is not necessary. In all the data we show here, we have imposed a stringent condition for equilibration, namely that memory of the starting configuration be lost, even for initialisation in maximally topologically distinct sectors — $q = 0$ and $q = \sqrt{3} \times \sqrt{3}$ [18].

**Correlations at low temperature:** There is a limiting low-temperature regime where the correlations cease to change as $T$ is lowered further below $T \sim 10^{-3} J$. This is shown in Fig. 2 for spin-correlations in real space for a system of $N = 2025$ spins with open boundary conditions. This implies that the effective weights differentiating between different coplanar states become temperature independent, as follows. The fluctuations selecting an ordered state are subdominant compared to those which select the nematic order: the modes which cost no energy are dressed by the finite-energy
and does not appear to reach a limiting value, signaling not shown in Fig. 4(a). This quantity is clearly bigger than one, by the two hexagons \cite{18}. The ratio of the stiffnesses is given

\[ \frac{m_{\sqrt{3}}}{} \]

\( \equiv \langle |h_{\text{heisenberg}}(q)|^2 \rangle / \langle |h_{\text{potts}}(q)|^2 \rangle \), as shown in Fig. 4(a). This quantity is clearly bigger than one, and does not appear to reach a limiting value, signaling not only enhanced correlations but indeed the onset of ordering. The nature of the ordering is indicated by the histogram of the height vector, which is a periodic variable and hence best

\[ \Theta(q^2) \]

\[ 0 \leq q \leq \infty \]

\[ \lim_{q \to 0} \Theta(q^2) \]

\[ = \frac{\langle |h_{\text{potts}}(q)|^2 \rangle}{\langle |h_{\text{heisenberg}}(q)|^2 \rangle} \]

\[ \geq 1 \]

\[ \frac{m_{\sqrt{3}}}{} \]

\[ \equiv \langle |h_{\text{heisenberg}}(q)|^2 \rangle / \langle |h_{\text{potts}}(q)|^2 \rangle \]

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\[ \geq 1 \]
Fig. 3(b) displays the size of the model to get a better handle on very large system sizes. A ratio \( \Theta(q) > 1 \) for \( q^2 \to 0 \) reflects the increased stiffness of the Heisenberg model compared to the Potts model, and the resultant ordering at low temperature. Of course, there may be small additional terms which we cannot directly detect in an unambiguous fashion, we can use information from the exact solution, which leads us to expect a transition at \( J_2 = 0 \). Assuming a scaling form, \( F \), appropriate for a Kosterlitz-Thouless transition, we obtain data collapse for \( m_\sqrt{3} \). The maxima correspond to \( \sqrt{3} \times \sqrt{2} \) order.

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