Emergent Power-Law Phase in the 2D Heisenberg Windmill Antiferromagnet: A Computational Experiment

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In an extensive computational experiment, we test Polyakov’s conjecture that under certain circumstances an isotropic Heisenberg model can develop algebraic spin correlations. We demonstrate the emergence of a multispin U(1) order parameter in a Heisenberg antiferromagnet on interpenetrating honeycomb and triangular lattices. The correlations of this relative phase angle are observed to decay algebraically at intermediate temperatures in an extended critical phase. Using finite-size scaling we show that both phase transitions are of the Berezinskii-Kosterlitz-Thouless type, and at lower temperatures we find long-range $Z_6$ order.

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In statistical mechanics it is assumed [1,2] that 2D Heisenberg magnets cannot develop algebraic order at finite temperatures since interaction of the Goldstone modes causes the spin-wave stiffness to renormalize to zero. However, in his pioneering work on this subject [3], Polyakov speculated that a 2D Heisenberg magnet might develop algebraic order if the system were to develop a “vacuum degeneracy”; he further suggested that this possibility might be explored experimentally. Recently Orth, Chandra, Coleman, and Schmalian (OCCS) have proposed that frustration can provide a mechanism to realize Polyakov’s conjecture; here fluctuations induce an emergent $XY$ order parameter that decouples from the rotational degrees of freedom [4,5]. However, these arguments were based on a long-wavelength renormalization group analysis, leaving open the possibility that short-wavelength fluctuations could preempt the scenario via unanticipated transitions into different phases [6–8]. In this Letter, we report a computational experiment that detects the development of an emergent $XY$ order parameter in a 2D Heisenberg spin model with power-law correlations, confirming the OCCS mechanism and its realization of the Polyakov conjecture.

The OCCS mechanism relies on the formation of a multispin U(1) order parameter describing the relative orientation of the magnetization between a honeycomb and a triangular lattice. The development of discrete multispin order is well known in systems with competing interactions: an example is the fluctuation-induced $Z_2$ order in the $J_1 - J_2$ Heisenberg model [9]. This mechanism is thought to be responsible for the high temperature nematic phase observed in the iron pnictides [10–13]. In the OCCS mechanism, the emergent U(1) order parameter is subject to a $Z_6$ order-by-disorder potential at short distances. At intermediate temperatures this potential is irrelevant (in the renormalization group sense) and scales to zero at long distances, leading to emergent power-law correlations. Remarkably, the stiffness of the emergent U(1) order parameter remains finite in the infinite system, despite the short-range correlations of the underlying Heisenberg

FIG. 1 (color online). Finite temperature phase diagram of classical windmill Heisenberg antiferromagnet as a function of intersublattice coupling $J_{th}/J$, $J = \sqrt{J_{tt}J_{hh}}$. Below a coplanar crossover temperature $T_{cp}$, emergent $XY$ spins appear and undergo two BKT phase transitions: at $T_>$ from a disordered to a critical phase with algebraic order and then at $T_\times$ into a $Z_6$ symmetry broken phase with discrete long-range order. At zero temperature the system undergoes a first order transition at $J_{th} = J$ from a 120°/Néel ordered windmill phase to a collinear phase.
spins. In this $XY$ manifold the binding of logarithmically interacting defect vortices leads to multistep ordering via two consecutive transitions in the Berezinskii-Kosterlitz-Thouless (BKT) universality class [4,5,14].

The Hamiltonian studied by OCCS is the “Windmill Heisenberg antiferromagnet,” given by $H = J_{tt} + J_{th} + J_{th} + J_{hh}$ with

$$H_{ab} = J_{ab} \sum_{j=1}^{N} \sum_{\{\delta_{ab}\}} S^a_j \cdot S^b_{j+\delta_{ab}},$$

where $S^a_j$ denotes classical Heisenberg spins at Bravais lattice site $j$ and basis site $a \in \{t, A, B\}$. The windmill lattice can be described as interpenetrating and coupled triangular ($t$) and honeycomb ($A, B$) lattices. The indices $\delta_{ab}$ relate nearest neighbors of sublattices $a, b$, counting each bond once. The antiferromagnetic exchange couplings are $J_{tt} = J_{hh} = J_{th}$, and $J_{hh} = J_{AB}$, and we introduce $J = \sqrt{J_{tt} J_{hh}}$.

We employ large-scale parallel tempering classical Monte Carlo simulations to obtain the finite temperature phase diagram shown in Fig. 1. As the emergent order parameter is a multispin object, we had to design a specific nonlocal Monte Carlo updating sequence consisting of three subroutines: (i) a heat bath step [15] in which a randomly chosen spin is aligned within the local exchange field of its neighbors according to a Boltzmann weight; (ii) a standard parallel tempering move [16,17] for which we run parallel simulations at 40 temperature points and switch neighboring configurations according to the Metropolis rule; finally, step (iii) is specifically tailored to our system where the emergent spins, defined below, exhibit a minute $Z_6$ order-by-disorder potential. We select a (global) rotation axis perpendicular to the average plane of the triangular spins, which exhibit (local) 120° order, and rotate all honeycomb spins around this axis by a randomly chosen angle and accept according to the Metropolis rule. This Monte Carlo algorithm was applied at least for $9 \times 10^5$ Monte Carlo steps of which the first half is discarded to account for thermalization.

The emergent phases we are interested in occur for $J_{th} \leq J$, where the zero temperature ground state is characterized by coplanar 120° order of the triangular spins and Néel order of the honeycomb spins (see Fig. 1) [18]. This order has $SO(3) \times O(3)/O(2)$ symmetry and is described by five Euler angles $(\theta, \phi, \psi) \times (\alpha, \beta)$. As shown in the inset of Fig. 2, the angles $(\alpha, \beta)$ describe the orientation of the honeycomb spins relative to the coordinate system $t$, $(\gamma = 1, 2, 3)$ set by the triangular spins. The Euler angles $(\theta, \phi, \psi)$ relate $t$ to a fixed coordinate system.

While the relative orientation can be changed without energy cost at $T = 0$, thermal fluctuations induce order-by-disorder potentials [19–21]. These potentials arise due to the fact that low-energy fluctuations around a given ground state have entropies that depend on $\alpha$ and $\beta$, a dependence that is captured via the free energy. Considering Gaussian thermal fluctuations around the classical ground state, one finds a contribution to the free energy equal to [22,23]

$$F_{\text{pot}} / NT = \cos(2\beta) \left[ 0.131 \frac{J_{th}^2}{J^2} - 10^{-4} \frac{J_{hh}}{J^6} \cos^2(3\alpha) \right].$$

The first term forces the spins to become coplanar ($\beta = \pi/2$) below a coplanarity crossover temperature $T_{\text{cp}}$. More precisely, long-wavelength excitations out of the plane acquire a mass and are gapped out for $T < T_{\text{cp}}$. The second term shows that the remaining $U(1)$ relative angle $\alpha$ is subject to a $\mathbb{Z}_6$ potential.

As shown in Fig. 2, we track this coplanarity crossover within the Monte Carlo simulations by measuring the coplanarity estimator

$$\kappa = 1 - \frac{3}{N} \sum_{j=1}^{N} \langle \cos^2(\beta_j) \rangle,$$

where $\cos \beta_j = S^a_j \cdot (S^a_j \times S^a_{j+\delta_j})$, with $\delta_j$ being a nearest-neighbor vector on the triangular lattice. At high temperatures, where no relative spin configuration is preferred, a straightforward averaging over all orientations of the three spins entering the definition of $\beta_j$, yields the value $\kappa = 1/3$. On the other hand, for a completely coplanar state we have all $\beta_j = \pi/2$ and thus $\kappa = 1$. For local triangular 120° and honeycomb Néel order that is uncorrelated with each other one finds $\kappa = 0$. Our Monte Carlo results show that coplanarity develops as soon as $T \lesssim 0.25J$ and $\kappa$ smoothly approaches unity for lower temperatures. Interestingly, $\kappa$ depends only weakly on $J_{th}$ as long as $J_{th} \gtrsim J/10$. We define the location of the coplanar crossover $T_{\text{cp}}$ shown in Fig. 1 to be the location of the minimum of $\kappa$. Note that

![FIG. 2 (color online). Coplanarity estimator $\kappa$ as a function of temperature for various values of $J_{th}/J$ for system size $L = 60$, $J_t = 1.0$, $J = 1.22$. The inset shows the definition of relative angles $\alpha$ and $\beta$.](image)
down to the lowest temperatures we observe substantial out-of-the-plane fluctuations and $\kappa < 1$. We have identified these to be predominantly of short-wavelength nature.

Below the coplanar crossover temperature $T_{\text{cp}}$, one may define emergent $XY$ spins $m_j$ at all Bravais lattice sites via projecting the honeycomb spin $S^i_j$ (or $S^j_i = -S^i_j$) onto the plane that is spanned by the three nearest-neighbor triangular spins and normalizing

$$m_j = \frac{(S^A_j \cdot t_{1,j}, S^A_j \cdot t_{2,j})}{\| (S^A_j \cdot t_{1,j}, S^A_j \cdot t_{2,j}) \|} = (\cos \alpha_j, \sin \alpha_j). \quad (4)$$

We study the behavior of these emergent spins in the remainder of this Letter. The local triangular triad $t_{r,j}$ is defined as follows: the spins on the triangular lattice are first partitioned into three classes $\{S^X_j, S^Y_j, S^Z_j\}$ as shown in Fig. 2. One then defines $t_{1,j} = S^X_j$ and $t_{2,j}$ to point along the component of $S^Z_j$ that is perpendicular to $t_{1,j}$. Finally, $t_{3,j} = t_{1,j} \times t_{2,j}$ completes the local triad. We show below that although the system exhibits out-of-the-plane fluctuations and $\kappa < 1$, the emergent spins $m_j$ decouple from these fluctuations and behave as U(1) degrees of freedom.

To map out the low temperature phase diagram we analyze the correlations of the emergent spins $m_j$ in the following. First, we define the total magnetization as

$$m = \frac{1}{N} \sum_{j=1}^{N} m_j = |m| (\cos \alpha, \sin \alpha). \quad (5)$$

The magnetization amplitude $|m|$ depends on the (linear) system size $L$, in particular, it vanishes in the absence of long-range order for $L \to \infty$. Performing the Monte Carlo average, we show the dependence of $|m|$ with system size $L$ in Fig. 3(a). While it vanishes faster than algebraic at large temperatures, it exhibits power-law scaling $|m| \propto L^{-\eta(T)/2}$ with $0 < \eta \lesssim 0.3$ for intermediate temperatures, a key signature of a critical phase. At the lowest temperatures, the exponent approaches zero and the magnetization saturates. To directly prove that the system develops (discrete) long-range order, we show the direction of the magnetization vector expressed as $\langle \cos(6\alpha) \rangle$ in Fig. 3(b). Clearly, $\langle \cos(6\alpha) \rangle$ approaches its saturation value of unity at low temperatures and large system sizes. The relative phase vector $m$ points into one of the six directions preferred by the $\mathbb{Z}_6$ potential in Eq. (2). The honeycomb spins are then aligned with one of the triangular spin classes $\{S^X_j, S^Y_j, S^Z_j\}$, in agreement with the general order-from-disorder mechanism that spins tend to align their fluctuation Weiss fields to maximize their coupling [21].

To determine the universality class of the phase transition and the transition temperatures $T_s$ and $T_c$, which partition the regimes of algebraic and long-range ordering, we perform a finite-size scaling analysis of the $XY$ susceptibility and magnetization for various values of $J_{\text{th}}/J$ [24–28]. As shown in Fig. 4 we obtain perfect data collapse using a BKT scaling ansatz. Since the susceptibility diverges when the system enters a critical phase, we can detect the upper transition at $T_s$ by analyzing

$$\chi(T, L) = \frac{N}{T} \langle |m|^2 \rangle = \frac{1}{NT} \left\langle \sum_j m_j^2 \right\rangle \quad (6)$$

for different temperatures $T$ and system sizes $L$. We employ a BKT ansatz for the correlation length $\xi_s = \exp(a_s \sqrt{T_s/T - T_s})$ with $a_s$ being a nonuniversal constant. Since $\chi(T, \infty) \sim \xi_s(T)^{2-\eta_s}$, in the infinite system, it holds that $\chi(T, L) = L^{2-\eta_s} \chi_0(T)/L$ with a universal function $\chi_0(x)$. For $J_{\text{th}} = 0.6J$ we extract the values $T_s = 0.200(4)J$, $a_s = 1.9(3)$, and $\eta_s = 0.25(1)$ from optimizing the collapse. This agrees very well with the theoretically expected value $\eta_s = 1/4$ [14].
Performing the analysis for other values of $J_{th}$ yields data collapse of similar quality with a value $\eta_* = 0.25$ within error bars. This determines $T_{\star\star}$ (scal.) and the upper phase transition line in Fig. 1. As an independent way to determine $T_{\star\star}$, we use the power-law scaling of the magnetization with the system size $L$, which is expected to be $\langle |m| \rangle \propto L^{-\eta_*}$ with $\eta = 1/4$ at the upper transition. This yields $T_{\star\star}(\eta)$ included in Fig. 1. The two temperatures agree within error bars with $T_{\star\star}(\eta)$ being systematically slightly larger. Finally, we note that we have also tried to achieve data collapse using a scaling ansatz corresponding to a second order phase transition, but the resulting collapse is worse in this case, especially for data points close to the phase transition.

To determine the lower transition temperature $T_<$ we perform a finite-size scaling analysis of the magnetization amplitude $\langle |m| (T, L) \rangle$. Since it holds in the infinite system that $\langle |m| (T) \rangle \propto \xi_<(T)^{-\eta_*}$ with correlation length $\xi_\star = \exp(a_\star \sqrt{T_\star} / \sqrt{T_\star - T})$ and nonuniversal factor $a_\star$, it follows for a finite system that $\langle |m| (T, L) \rangle = L^{-\eta_*} Y_m(\xi_\star (T) / L)$, where $Y_m(x)$ is a universal function. In Fig. 4(b) we show the best data collapse for $J_{th} = 0.6 J$ which yields $T_\star = 0.18(1), \eta_\star = 0.11(1), \text{and } a_\star = 5.0(5)$.

This is in good agreement with the theoretically expected value of $\eta_\star = 1/9$ at the lower transition [6,14].

Two independent ways to obtain $T_<$ are (i) to investigate the power-law scaling of $\langle |m| \rangle$ with system size and (ii) to directly look for the symmetry breaking as indicated by the quantity $\langle \cos(6\alpha) \rangle$. Using the first method, we find that our data can be fitted to $\log(\langle |m| \rangle) \propto -\eta(T) / 2 \log L$ with a temperature-dependent slope $\eta(T)$ that is monotonically decreasing over the full range $0 < T < T_\star$. At high temperatures, we find $\eta(T_\star) \approx 0.25$ (as expected) and we define $T_{\star\star}(\eta)$ as the temperature where $\eta(T_\star) = 1/9$. The fact that the system appears to be critical within our simulation even for lower temperatures (with an exponent $\eta < 1/9$) is a simple consequence of the fact that the system size is much smaller than the correlation length [25,28]. If we were able to reach larger system sizes in the simulation, we would eventually see a saturation of $\langle |m| \rangle$ to a finite value.

Next, we discuss detecting $T_<$ via direct observation of symmetry breaking. We see in Fig. 3(b) that $\langle \cos(6\alpha) \rangle$ approaches unity at low temperatures and large system sizes. In a finite-size system, we can observe this ordering only for not too small values of $J_{th} \geq 0.83 J$ because the bare value of the order-from-disorder sixfold potential scales with $(J_{th} / J)^6$ with an additional small numerical prefactor $10^{-4}$ [see Eq. (2)]. While the lower phase transition occurs when this potential becomes relevant at long length scales, independently of the bare value, the finite system size serves as a cutoff of the scaling making an effect of the potential only visible at sufficiently large bare values. To extract the transition temperature $T_\star$ from $\langle \cos(6\alpha) \rangle$ we have to take into account that while at low temperatures the Gaussian order-from-disorder potential predicts free energy minima at $\alpha = 2\pi n / 6$ (in agreement with our simulation), at intermediate temperatures we observe in the finite-size system a tendency of the spins to prefer a relative direction corresponding to a negative value of $\langle \cos(6\alpha) \rangle$ [see inset in Fig. 3(b)]. This is presumably a result of nonlinear spin fluctuations around the classical ground state order, similarly to the effect of quenched disorder [21]. We thus identify the transition temperature $T_\star(\eta)$ as the location of the minimum of $\langle \cos(6\alpha) \rangle(T)$ which yields temperatures that are within error bars in agreement with the ones predicted from scaling.

We note that in the critical phase that develops for $T \in [T_{\star\star}, T_{\star\star}]$, the phase $\alpha$ behaves as a perfect, decoupled $XY$ order parameter. Once the vortices bind at the BKT transition $T_{\star\star}$, the ensemble of thermodynamically accessible states divides up into distinct degenerate subspaces, each defined by a pair of winding numbers $\{n_x, n_y\}$ with

$$n_l = \int_0^L dx_1 \frac{dx}{2\pi} \nabla_l \alpha(x), \quad (l = x, y).$$

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**FIG. 4** (color online). Finite-size scaling of susceptibility $\chi(T, L) = L^{2-\eta_*} Y_\eta(\xi_\star / L)$ as a function of $\xi_\star / L$ and magnetization $\langle |m| (T, L) \rangle = L^{-\eta_*} Y_m(\xi_\star / L)$ as a function of $\xi_\star / L$ for $J_{th} = 0.6 J$, $J_x = 1.0$, and $J_y = 1.22$. The best data collapse is obtained with a BKT scaling ansatz and yields $T_{\star\star}, a_{\star\star}$, and $\eta_{\star\star}$ as given in the text.
where $L$ is the linear size of the system, indicating the presence of an emergent topological phase [29]. The multiple degeneracies of this state confirm the Polyakov hypothesis that a power-law phase is possible with a degenerate vacuum.

In conclusion, employing extensive parallel-tempering Monte Carlo simulations, we have presented conclusive evidence for an emergent critical phase in a 2D isotropic classical Heisenberg spin model at finite temperatures. This realizes the Polyakov conjecture [3] that Heisenberg magnets can develop algebraic order if they exhibit a vacuum degeneracy. Using finite-size scaling we have shown that the transitions are in the Berezinskii-Kosterlitz-Thouless universality class and determined the transition temperatures. At low temperatures, we find direct evidence of long-range order in the relative orientation of the spins via breaking of a discrete sixfold symmetry induced by an order-from-disorder potential. Direct numerical analysis of the spin stiffness tensor, the metric of the associated $SO(3) \times U(1)$ topological manifold, and its Ricci flow will be the topic of future work.

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