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

Bhilahari Jeevanesan,¹ Premala Chandra,² Piers Coleman,^{2,3} and Peter P. Orth^{1,4}

¹*Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany*

²*Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08854, USA*

³*Hubbard Theory Consortium and Department of Physics,*

Royal Holloway, University of London, Egham, Surrey TW20 0EX, UK

⁴*School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA*

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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 multi-spin 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 \mathbb{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 multi-spin U(1) order parameter describing the *relative* orientation of the magnetization between a honeycomb and a triangular lattice. The development of discrete multi-spin order is well known in systems with competing interactions: an example is the fluctuation-induced \mathbb{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 \mathbb{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 spins. In this XY manifold the binding of logarithmically interacting defect vortices leads to multi-step ordering via two consecutive transitions in the Berezinskii-Kosterlitz-Thouless (BKT) uni-

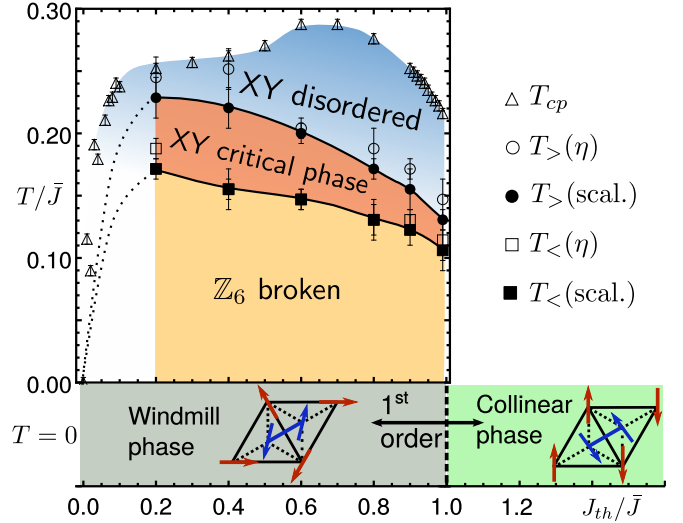


FIG. 1. (color online). Finite temperature phase diagram of classical windmill Heisenberg antiferromagnet as a function of inter-sublattice coupling J_{th}/\bar{J} , $\bar{J} = \sqrt{J_{tt}J_{hh}}$. Below a coplanar crossover temperature T_{cp} , emergent XY spins appear and undergo two BKT phase transitions: at $T_{>}$ from a disordered to a critical phase with algebraic order and then at $T_{<}$ into a \mathbb{Z}_6 symmetry broken phase with discrete long-range order. At zero temperature the system undergoes a first order transition at $J_{th} = \bar{J}$ from a 120° /Néel ordered windmill phase to a collinear phase.

versality class [4, 5, 14].

The Hamiltonian studied by OCCS is the “Windmill Heisenberg antiferromagnet”, given by $H = H_{tt} + H_{AB} + H_{tA} + H_{tB}$ with

$$H_{ab} = J_{ab} \sum_{j=1}^N \sum_{\{\delta_{ab}\}} \mathbf{S}_j^a \cdot \mathbf{S}_{j+\delta_{ab}}^b, \quad (1)$$

where \mathbf{S}_j^a denote 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 δ_{ab} relate nearest-neighbors of sublattices a, b , counting each bond once. The antiferromagnetic exchange couplings are J_{tt} , $J_{th} \equiv J_{tA} = J_{tB}$ and $J_{hh} \equiv J_{AB}$, and we introduce $\bar{J} = \sqrt{J_{tt}J_{hh}}$.

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 multi-spin object, we had to design a specific non-local Monte-Carlo updating sequence consisting of three sub-routines: (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 \mathbb{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 9×10^5 Monte-Carlo steps of which the first half is discarded to account for thermalization.

The emergent phases we are interested in occur for $J_{th} \leq \bar{J}$ 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 $\text{SO}(3) \times \text{O}(3)/\text{O}(2)$ symmetry and is described by five Euler angles $(\theta, \phi, \psi) \times (\alpha, \beta)$. As shown in the inset of Fig. 2, the angles (α, β) describe the orientation of the honeycomb spins relative to the coordinate system \mathbf{t}_γ ($\gamma = 1, 2, 3$) set by the triangular spins. The Euler angles (θ, ϕ, ψ) relate \mathbf{t}_γ 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 α and β , a dependence that is captured via the free-energy. Considering Gaussian thermal fluctuations around the classical ground state, one finds a contribution to the

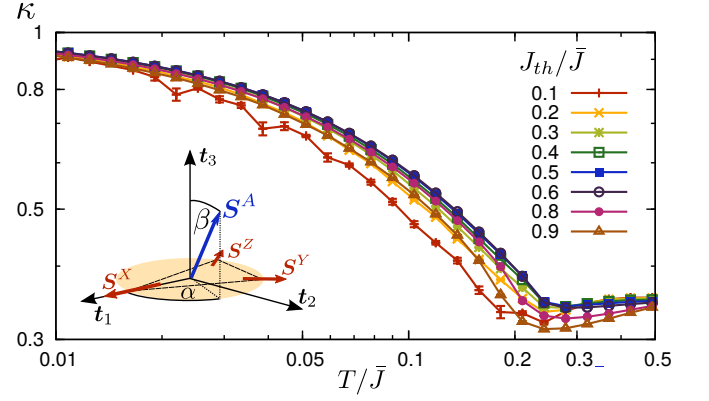


FIG. 2. (Color online) Coplanarity estimator κ as a function of temperature for various values of J_{th}/\bar{J} for system size $L = 60$. Inset shows definition of relative angles α and β .

free energy equal to [22, 23]

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

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

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

where $\cos \beta_j = \mathbf{S}_j^A \cdot (\mathbf{S}_j^t \times \mathbf{S}_{j+\delta_{tt}}^t)$ with δ_{tt} 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 β_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 $T \lesssim 0.25\bar{J}$ and κ smoothly approaches unity for lower temperatures. Interestingly, κ depends only weakly on J_{th} as long as $J_{th} \gtrsim \bar{J}/10$. We define the location of the coplanar crossover T_{cp} shown in Fig. 1 to be the location of the minimum of κ . Note that 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_{cp} one may define emergent XY spins \mathbf{m}_j at all Bravais lattice sites

via projecting the honeycomb spin \mathbf{S}_j^A (or $\mathbf{S}_j^B \simeq -\mathbf{S}_j^A$) onto the plane that is spanned by the three nearest-neighbor triangular spins and normalizing

$$\mathbf{m}_j = \frac{(\mathbf{S}_j^A \cdot \mathbf{t}_{1,j}, \mathbf{S}_j^A \cdot \mathbf{t}_{2,j})}{\|(\mathbf{S}_j^A \cdot \mathbf{t}_{1,j}, \mathbf{S}_j^A \cdot \mathbf{t}_{2,j})\|} = (\cos \alpha_j, \sin \alpha_j). \quad (4)$$

We study the behavior of these emergent spins in the remainder of this paper. The local triangular triad $\mathbf{t}_{\gamma,j}$ is defined as follows: the spins on the triangular lattice are first partitioned into three classes $\{\mathbf{S}_j^{t,X}, \mathbf{S}_j^{t,Y}, \mathbf{S}_j^{t,Z}\}$ as shown in Fig. 2. One then defines $\mathbf{t}_{1,j} = \mathbf{S}_j^{t,X}$ and $\mathbf{t}_{2,j}$ to point along the component of $\mathbf{S}_j^{t,Y}$ that is perpendicular to $\mathbf{t}_{1,j}$. Finally, $\mathbf{t}_{3,j} = \mathbf{t}_{1,j} \times \mathbf{t}_{2,j}$ completes the local triad. We show below that although the system exhibits out-of-the plane fluctuations and $\kappa < 1$, the emergent spins \mathbf{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 \mathbf{m}_j in the following. First, we define the total magnetization as

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

The magnetization amplitude $|\mathbf{m}|$ depends on the (linear) system size L , in particular, it vanishes in the absence of long-range order for $L \rightarrow \infty$. Performing the Monte-Carlo average, we show the dependence of $\langle |\mathbf{m}| \rangle$ with system size L in Fig. 3(a). While it vanishes faster than algebraic at large temperatures, it exhibits power-law scaling $\langle |\mathbf{m}| \rangle \propto L^{-\eta(T)/2}$ 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 \mathbf{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 three triangular spin classes $\{\mathbf{S}^{t,X}, \mathbf{S}^{t,Y}, \mathbf{S}^{t,Z}\}$, 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 $T_>$ and $T_<$, 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_{th}/\bar{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,

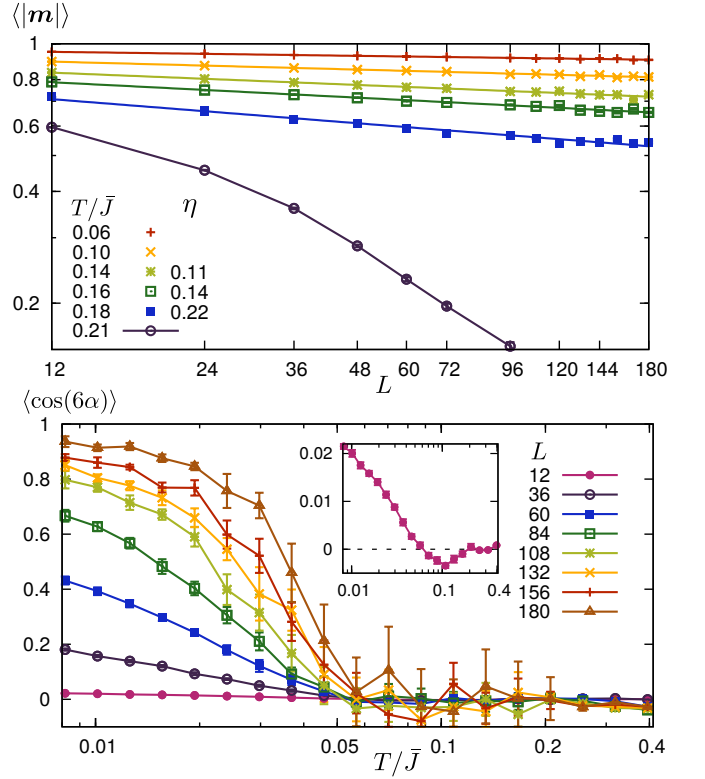


FIG. 3. (color online). (a) XY magnetization amplitude $\langle |\mathbf{m}| \rangle$ as a function of linear system size L for various temperatures T/\bar{J} and fixed $J_{th}/\bar{J} = 0.8$. On a double logarithmic plot it exhibits linear scaling within the critical phase with indicated floating exponent $\eta(T)$. It bends down in the disordered phase. Due to the finite system size we cannot clearly observe a saturation (at a finite value) at low temperatures, but η approaches zero in a linear fit. (b) Direction of the magnetization expressed as $\langle \cos(6\alpha) \rangle$ as a function of T for $J_{th} = 0.9\bar{J}$. A non-zero value signals breaking of the six-fold symmetry at low temperatures $T < T_<$. Inset shows $L = 12$.

we can detect the upper transition at $T_>$ by analyzing

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

for different temperatures T and system sizes L . We employ a BKT ansatz for the correlation length $\xi_> = \exp(a_> \sqrt{T_>}/\sqrt{T - T_>})$ with $a_>$ being a non-universal constant. Since $\chi(T, \infty) \sim \xi_>(T)^{2-\eta_>}$ in the infinite system, it holds that $\chi(T, L) = L^{2-\eta_>} Y_\chi(\xi_>(T)/L)$ with a universal function $Y_\chi(x)$. For $J_{th} = 0.6\bar{J}$ we extract the values $T_> = 0.200(4)\bar{J}$, $a_> = 1.9(3)$ and $\eta_> = 0.25(1)$ from optimizing the collapse. This agrees very well with the theoretically expected value $\eta_> = 1/4$ [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 $T_>(\text{scal.})$ and the upper phase transition line in Fig. 1. As an independent way to determine $T_>$, we use the power-law scaling of the magnetization with the system size L , which is ex-

pected to be $\langle |\mathbf{m}| \rangle \propto L^{-\eta/2}$ with $\eta = 1/4$ at the upper transition. This yields $T_>(\eta)$ included in Fig. 1. The two temperatures agree within error bars with $T_>(\eta)$ 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 $\langle |\mathbf{m}|(T, L) \rangle$. Since it holds in the infinite system that $\langle |\mathbf{m}|(T) \rangle \propto \xi(T)^{-\eta_{<}/2}$ with correlation length $\xi_< = \exp(a_<\sqrt{T_<}/\sqrt{T_< - T})$ and non-universal factor $a_<$, it follows for a finite system that $\langle |\mathbf{m}|(T, L) \rangle = L^{-\eta_{<}/2} Y_m(\xi_<(T)/L)$, where $Y_m(x)$ is a universal function. In Fig. 4(b) we show the best data collapse for $J_{th} = 0.6\bar{J}$ which yields $T_< = 0.18(1)$, $\eta_< = 0.11(1)$ and $a_< = 5.0(5)$. This is in good agreement with the theoretically expected value of $\eta_< = 1/9$ at the lower transition [6, 14].

Two independent ways to obtain $T_<$ are (i) to investigate the power-law scaling of $\langle |\mathbf{m}| \rangle$ 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 $\log \langle |\mathbf{m}| \rangle \propto -\frac{\eta(T)}{2} \log L$ with a temperature-dependent slope $\eta(T)$ that is monotonically decreasing over the full range $0 < T < T_>$. At high temperatures, we find $\eta(T_>) \simeq 0.25$ (as expected) and we define $T_<(\eta)$ as the temperature where $\eta(T_<) = 1/9$. 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 $\langle |\mathbf{m}| \rangle$ to a finite value.

Next we discuss the second method to detect $T_<$, namely 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 $J_{th} \geq 0.8\bar{J}$ because the bare value of the order-from-disorder six-fold potential scales with $(J_{th}/\bar{J})^6$ with an additional small numerical prefactor 10^{-4} (see Eq. (2)). While the lower phase transition occurs when this potential becomes relevant at long lengthscales, independently of the bare value, the finite system size serves as a cut-off of the scaling making an effect of the potential only visible at sufficiently large bare values. To extract the transition temperature $T_<$ 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

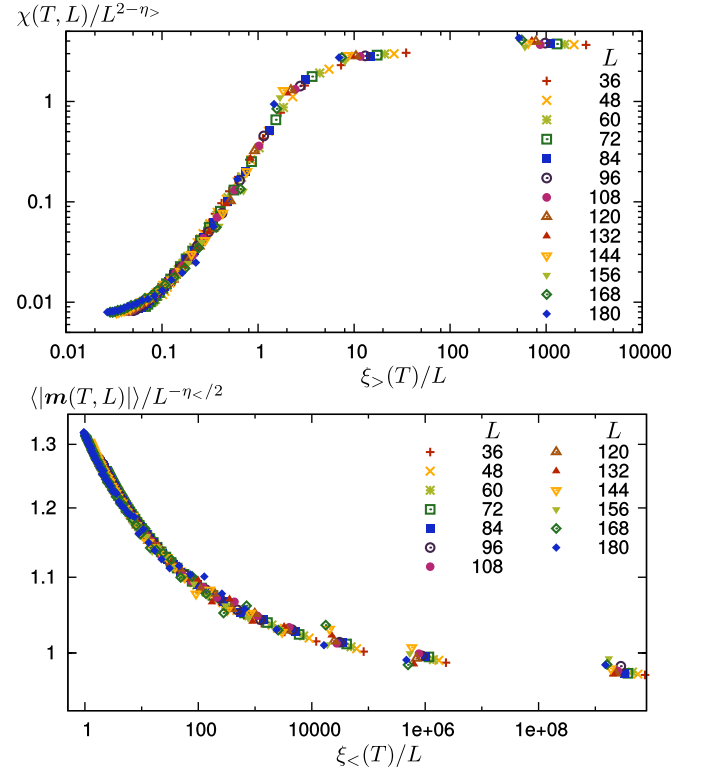


FIG. 4. (Color online) Finite size scaling of susceptibility $\chi(T, L) = L^{2-\eta_>} Y_\chi(\xi_>/L)$ as a function of $\xi_>/L$ and magnetization $\langle |\mathbf{m}|(T, L) \rangle = L^{-\eta_</2} Y_m(\xi_</L)$ as a function of $\xi_</L$ for $J_{th} = 0.6\bar{J}$, $J_{tt} = 1.0$ and $\bar{J} = 1.22$. Best data collapse is obtained with a BKT scaling ansatz and yields $T_{<,>}$, $a_{<,>}$ and $\eta_{<,>}$ as given in the text.

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 $T_<(\mathbb{Z}_6)$ 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 $T \in [T_<, T_>]$, the phase α behaves as a perfect, decoupled XY order parameter. Once the vortices bind at the BKT transition $T_>$, 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

$$n_l = \int_0^L \frac{dx_l}{2\pi} \nabla_l \alpha(x), \quad (l = x, y), \quad (7)$$

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 six-fold 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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