Continuous Easy-Plane Deconfined Phase Transition on the Kagome Lattice

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We use large scale quantum Monte Carlo simulations to study an extended Hubbard model of hard core bosons on the kagome lattice. In the limit of strong nearest-neighbor interactions at 1/3 filling, the interplay between frustration and quantum fluctuations leads to a valence bond solid ground state. The system undergoes a quantum phase transition to a superfluid phase as the interaction strength is decreased. It is still under debate whether the transition is weakly first order or represents an unconventional continuous phase transition. We present a theory in terms of an easy plane noncompact CP^1 gauge theory describing the phase transition at 1/3 filling. Utilizing large scale quantum Monte Carlo simulations with parallel tempering in the canonical ensemble up to 15552 spins, we provide evidence that the phase transition is continuous at exactly 1/3 filling. A careful finite size scaling analysis reveals an unconventional scaling behavior hinting at deconfined quantum criticality.

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Introduction.—Understanding universal and nonuniversal properties of quantum phase transitions in strongly correlated systems is a key topic in modern physics [1]. In many cases, quantum phase transitions can be described by Landau's theory of spontaneous symmetry breaking just like classical ones. On the other hand, there appear to exist exotic quantum phase transitions beyond the Landau's paradigm, such as continuous deconfined phase transitions (DCPs) between phases with different, incompatible symmetry breakings. A well-known example is the transition between a Néel state and a valence bond solid (VBS) [2,3].

Contrary to conventional phase transitions, a deconfined phase transition exhibits fractionalized quasiparticles that couple to emergent gauge fields [2,3]. Deconfined phase transitions are generically described by strongly interacting gauge theories. One example is the noncompact CP^1 (NCCP^1) model with a bosonic CP^1 field z_α (describing spinons with SU(2) flavors $\alpha = 1, 2$), which couples to a noncompact $U(1)$ gauge field a_μ. Depending on the symmetries of the field z_α, the NCCP^1 models are divided into SU(2) NCCP^1 and the easy plane NCCP^1, which describe the Néel to VBS transition in SU(2) or XY magnets [2–4], respectively.

The concept of DCPs leads to several interesting questions: First, to what extent do these emergent gauge fields and fractionalized excitations appear at critical points in concrete model systems? Second, what is the fate of the NCCP^1 model in the infrared (IR) limit? Recent progress in the understanding of dualities of gauge theories has brought new perspectives to deconfined phase transitions [4–13]. It has been conjectured that the bosonic easy plane NCCP^1 theory is dual to a widely studied fermionic $N_f = 2$ QED_3 theory [8–13]. Significant effort has been put into the investigation of the IR fate of QED_3, but it remains an open issue after several decades of study [14–21]. Studying concrete realizations of DCPs helps to deepen the understanding of this long-standing problem.

Numerical work [22–44] has studied both the SU(2) and easy plane DCPs—most of them focused on the J-Q model [22–31,42,43] and classical loop models [32,33,39]. It is still controversially discussed if SU(2) DCPs are continuous [35], and an emergent SO(5) symmetry is observed [33] between Néel and VBS phases. The easy plane case, on the other hand, appears to be a first order transition in all previous numerical studies on various candidate model systems [40–43,45]. The question arises whether the easy plane NCCP^1 is intrinsically first order or if it is specific to the models that have been studied so far.

In this Letter, we provide numerical evidence for the existence of a continuous easy plane DCP using large scale quantum Monte Carlo simulations, and our results are in agreement with a parallel work [44]. Specifically, we study an extended Hubbard model of hard core bosons on the kagome lattice,

$$H = -t\sum_{\langle ij\rangle}(b_i^\dagger b_j + b_j^\dagger b_i) + V\sum_{\langle ij\rangle} n_i n_j, \tag{1}$$

at 1/3 filling with t, $V > 0$. The system is known to form a VBS ground state in the limit $V \gg t$ and a superfluid for

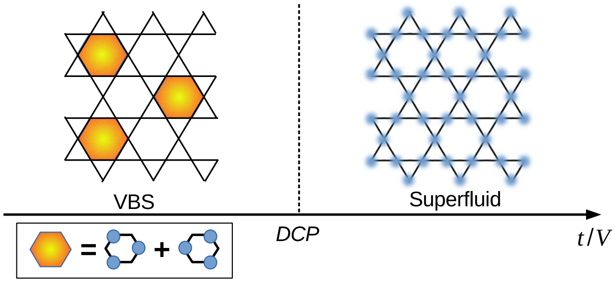

FIG. 1. Phase diagram of Hamiltonian (1) at $1/3$ filling with a DCP separating a VBS and a superfluid phase. In the VBS phase, resonant processes (colored hexagon) spontaneously break translation symmetry. In contrast, in the superfluid phase, the bosons condense and spontaneously break the $U(1)$ symmetry.

$V \ll t$, where both phases are separated by a quantum phase transition [46–49] as indicated in Fig. 1. We first discuss the easy plane NCCP^1 theory [2,3] that describes the superfluid-VBS transition. In particular, we highlight the difference between our system and other systems hosting DCPs (e.g., the J-Q model). By using large scale quantum Monte Carlo methods with parallel tempering (QMC-PT) in the canonical ensemble, we find that the phase transition between VBS to the superfluid is anomalously continuous at exactly $1/3$ filling. Several hallmarks of DCP are found. (i) At the critical point, the superfluid density decays slower than at regular continuous phase transitions. In comparison with different scenarios [27,28,32], we adopt logarithmic corrections to fit this drift. (ii) A direct analysis of two-point correlations reveals that the anomalous critical exponent $\eta \approx 0.3$ is relatively large. (iii) We identify a lattice operator for a conserved charge (i.e., the spinon density) of NCCP^1, and we numerically show that its scaling dimension is close to two, as expected for a $2+1$D conformal field theory (CFT) [50]. (iv) An emergent $U(1)$ symmetry is identified at the critical point.

Effective theory and phases.—Similar to the much studied Néel-VBS transition in antiferromagnets [2,3], the superfluid-VBS transition in our system is also described by the NCCP^1 theory,

$$\mathcal{L} = \sum_{\alpha=1}^{2} [|(\partial_\mu - i a_\mu) z_\alpha|^2 + s|z_\alpha|^2 + u|z_\alpha|^4] + v|z_1|^2|z_2|^2 + \cdots, \tag{2}$$

where the $z_{\alpha=1,2}$ are bosonic (CP^1) fields (or spinon operators) carrying half the charge of the physical bosons, and they are coupled to an emergent dynamical $U(1)$ gauge field a_μ. The mass term $s|z_\alpha|^2$ with $s \approx V/t - 7$ controls the phases: (i) if z_α condenses, a superfluid phase is formed, (ii) if z_α is gapped, a VBS state forms due to the proliferation of monopoles of the gauge field a_μ [51], and (iii) the case of z_α being gapless corresponds to the critical point. The quartic terms with $u \approx O(t^3)$ and $v \approx O(t^3)$ control the putative IR fixed point to which the theory flows under renormalization. When $v = 2u$, there is a SU(2) symmetry between z_1 and z_2, and the theory is called SU(2) NCCP^1. Usually the SU(2) symmetry will be manifest as a global SU(2) symmetry of the spin system. On the other hand, if $v < 2u$, the theory flows to the easy plane NCCP^1 fixed point where the SU(2) symmetry is broken. Our hard core boson model, Eq. (1), naturally falls into the easy plane NCCP^1 class. The same field theory also describes the Néel-VBS transition in other related spin models (e.g., the J-Q model), and the hard core boson model we are studying can be exactly mapped to a spin-1/2 model by $b^\dagger \to S^+$, $n = b^\dagger b \to S^z + 1/2$.

In our system, however, the relation between the continuous field operator and the lattice operators is very different from the usual DCP in spin models. In usual spin models (e.g., the J-Q model), one would have $S^+ \sim z_1^* z_2$, $S^z \sim |z_1|^2 - |z_2|^2$. In our case, the relations are

$$b_i^\dagger \sim z_1^* z_2, \qquad n_i = b_i^\dagger b_i \sim E_i + \mathrm{Re}(e^{i\theta_i}\mathcal{M}_a), \tag{3}$$

$$\sum_{i\in\triangle} n_i \sim z_1^* \partial_t z_1, \qquad \sum_{i\in\nabla} n_i \sim z_2^* \partial_t z_2. \tag{4}$$

Here, E_i represents the electric fields of the dynamical gauge field a_μ, M_a is the monopole operator, while θ_i is a phase factor ($= 0, \pm 2\pi/3$) depending on the sublattice index. $\sum_{i\in\triangle,\nabla} n_i$ refers to the summation of the density of three sites in the up or down triangles of the kagome lattice. The difference originates from the different fractionalization schemes of the spin operator $\vec{S}$ into the CP^1 (spinon) field $\mathbf{z} = (z_1, z_2)$. Usually at DCPs, the spin operator is fractionalized via the CP^1 representation $\vec{S}_i = \mathbf{z}_i^* \vec{\sigma} \mathbf{z}_i^T$ [2,3], and such a spinon operator is argued to capture the low energy physics. In contrast, our kagome model can be faithfully mapped onto a lattice gauge model defined on the medial honeycomb lattice [52,53], in which spinons ($z_{1,2}$) live on honeycomb sites (i.e., center of kagome triangles) and U(1) gauge fields live on the honeycomb links. Then we can straightforwardly take the continuum limit of the lattice gauge model, which precisely gives the easy plane NCCP^1 theory.

The relations in Eqs. (3) and (4) call for a slightly different way of extracting critical exponents. Specifically, the anomalous dimension η_{VBS} of the VBS order parameter should be extracted from the density operator n_i, instead of the dimer operator in the J-Q model. The operators $s_{\triangle,\nabla} = \sum_{i\in\triangle,\nabla} n_i$, correspond to conserved charges of the gauge theory, $z_\alpha^* \partial_t z_\alpha$. For any $2+1$D CFT, such a conserved charge will always have scaling dimension two [50], providing an additional numerical check.

Numerical results.—We use a stochastic cluster series expansion with parallel tempering [54–57] and adopt periodic boundary conditions with $L_x = L_y$. To reach the ground state, we use half million steps of thermalization before producing two million samples for measuring and consider temperatures down to $\beta V/L = 25/3$ ($\beta = 1/T$). We identify the diagonal order in the VBS phase using the structure factor $S(\mathbf{Q}) = \langle |n(\mathbf{Q},\tau)|^2\rangle = \langle|\sum_{k=1}^{N} n_{k,\tau} e^{\mathbf{i}\mathbf{Q}\cdot\mathbf{r}_k}|^2\rangle/N^2$ at $\mathbf{Q} = (4\pi/3, 0)$, where N is the number of sites. For the superfluid phase, we consider the superfluid density $\rho_s = \langle W^2\rangle/\beta t$, where W is the winding number [58] and also the condensate fraction $\rho_0 = \langle\sum_{i,j} b_i^\dagger b_j\rangle/N^2$ to characterize long range off-diagonal correlations.

It turns out that a continuous phase transition only occurs at exactly 1/3 filling where the system has particle-hole symmetry. In previous studies [46,47], a grand canonical ensemble was used for the QMC simulations that made it difficult to fine tune to exactly 1/3 filling. Here, we restrict our simulations to the canonical ensemble by tuning the chemical potential to minimize the deviation from 1/3 filling during the loop-update and then only accept samples with exactly 1/3 filling. From Fig. 2, we find (i) the structure factor $S(\mathbf{Q})$ does not show any discontinuity for sizes up to a linear dimension of $L = 72$ ($N = 15552$ spins), (ii) its Binder cumulant $S(\mathbf{Q})_{b.c.} = 1 - (\langle S(\mathbf{Q})^2\rangle/3\langle S(\mathbf{Q})\rangle^2)$ is always positive and crosses at approximately same point $t_c/V \approx 0.1303$, and (iii) at variance with Ref. [46], at larger size $L = 72$ near the critical point, we do not find any double peak structure in the probability distribution of kinetic energy. Since the parameter $t/V = 0.1283$ in Ref. [46] is actually far from t_c/V, it reflects the weakly first-order phase transition at the upper or lower boundary of the lobe, but not at the tip. These three findings strongly support a continuous phase transition up to system size $L = 72$.

Next we perform finite size scaling (FSS) for different variables to extract the critical behavior. For a continuous phase transition, the scaling function takes the form:

$$A(L,\delta) = L^{-\kappa} f(\delta L^{1/\nu}), \tag{5}$$

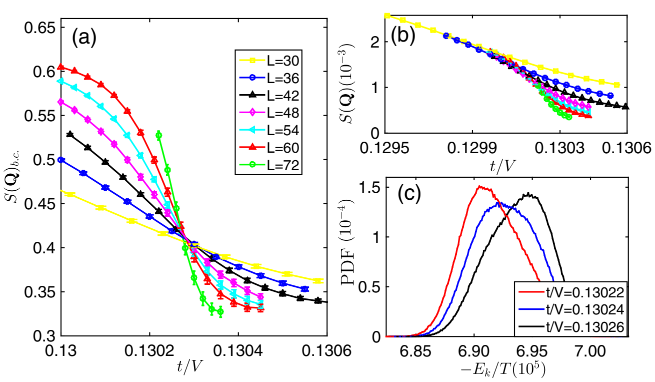

FIG. 2. The structure factor (b) and its Binder cumulant (a) vs t/V at 1/3 filling and $\beta V/L = 25/3$ with different L. (c) The probability density function (PDF) of kinetic energy at $L = 72$ and $\beta V = 600$ near the critical point.

where ν and κ are related to the universality class of the phase transition, and $\delta = t/V - t_c/V$. Because the form of the scaling function f is not known, we choose the proposed method of Kawashima and Ito to do the data collapse [59,60].

An anomalous behavior of FSS of physical quantities has been observed in all previous numerical works on DCP (see examples [22,23,25–28,32–34]). It has been suggested that these anomalous scaling behaviors arise due to finite size effects of dangerously irrelevant operators [32]. For example, the superfluid density ρ_s shows a drift [27,28,32] compared to the scaling of the conventional phase transition, $\rho_s(L,\delta) = L^{-1} f(\delta L^{1/\nu})$. To resolve the drift, two schemes have been proposed: (i) logarithmic corrections (LCs) $\rho_s(L,\delta) = L^{-1}\log(L/L_0) f(\delta L^{1/\nu})$ [26,32] and (ii) two-length scales $\rho_s(L,\delta) = L^{-\nu/\nu'} f(\delta L^{1/\nu})$ [27]. In our work, we use the LCs and find a good data collapse with $1/\nu = 2.37(0.04)$, as shown in Fig. 3(a). Using two length scales also gives a reasonably good collapse [61].

Scaling violations are also observed in the diagonal structure factor $S(\mathbf{Q})$ and condensate fraction ρ_0, whose FSS has previously been used to extract the anomalous dimension η_{VBS} and η_{SF}. The anomalous dimensions $\eta_{\mathrm{VBS}} = 0.015(0.014)$ and $\eta_{\mathrm{SF}} = 0.200(0.006)$ extracted from $S(\mathbf{Q})$ and ρ_0, respectively, strongly deviate from each other [shown in Fig. 3(b) and Fig. 3(c)]. This is not expected for the easy plane NCCP[1] theory as both anomalous exponents are the same due to self-duality [4]. Previous studies [32,62] find a large drift of the critical

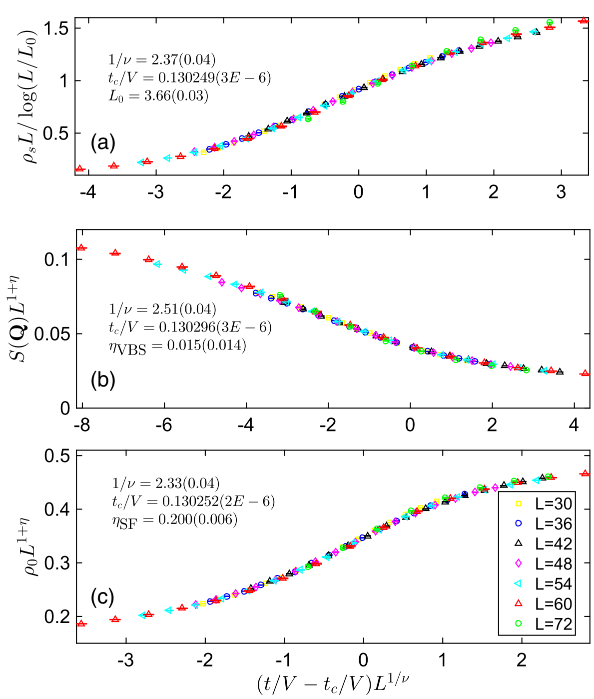

FIG. 3. Data collapse of (a) superfluid density with logarithmic correction, (b) structure factor, and (c) condensate fraction at 1/3 filling and $\beta V/L = 25/3$.

exponent and anomalous dimension due to the $1/L^2$-correction [63]. Therefore, a simple data collapse does not give good results, but by using the two-point correlator, a size-dependent anomalous dimension can be extracted, which shows a systematic convergence to the thermodynamic limit as discussed in the following and in the Supplemental Material [61].

We find two different scaling behaviors as we approach the continuous quantum phase transition from the two neighboring phases. In the disordered phase $C_s(\delta, r) = ar^{-1-\eta}\exp[-r/\xi(\delta)]$ with the correlation length $\xi(\delta) \propto \delta^{-\nu}$, while approaching the critical point from the ordered phase, $C_l(\delta, r) = ar^{-1-\eta} + b(\delta)$ $(b(0) = 0)$ [1]. At the critical point, we then expect a power law decay $C_l = ar^{-1-\eta}$. As shown in Fig. 4(a), the off-diagonal correlation function $\langle b_i^\dagger b_j \rangle$ decays very fast in the VBS phase $(t/V = 0.1)$, which hints at an exponential behavior, while it decays slowly to a constant in the superfluid phase $(t/V = 0.137)$. Near the critical point $(t/V = 0.126)$, it shows a clear power law behavior. To approach the thermodynamic limit (TDL), we calculate the correlation function near the critical point $(t/V = 0.1303)$, and we perform a FSS analysis on the exponent. As shown in Fig. 4(b), we identify a power law decay with increasing system size. The inset of Fig. 4(b) shows strong finite size effects of the anomalous exponent, and these size effects can extremely depress the exponent obtained from the data collapse of the condensate fraction [61]. With second order polynomial fitting, we get $\eta_{\mathrm{SF}} = 0.305(0.020)$ in the TDL. Figure 4(c) shows the density correlation function for different parameters. Contrary to the off-diagonal correlations, the density correlation functions have a density modulation due to translational symmetry breaking in the VBS. We thus subtract its mean value and divide by the density modulation $\cos(\mathbf{Q}r_{i,j})$. While the correlations show strong fluctuations at a short distance, a smooth power law decay emerges at long distances, and we thus neglect the first ten points for the fitting. Comparing to the off-diagonal correlations, the error is larger and the anomalous exponent in the TDL is $\eta_{\mathrm{VBS}} = 0.313(0.057)$.

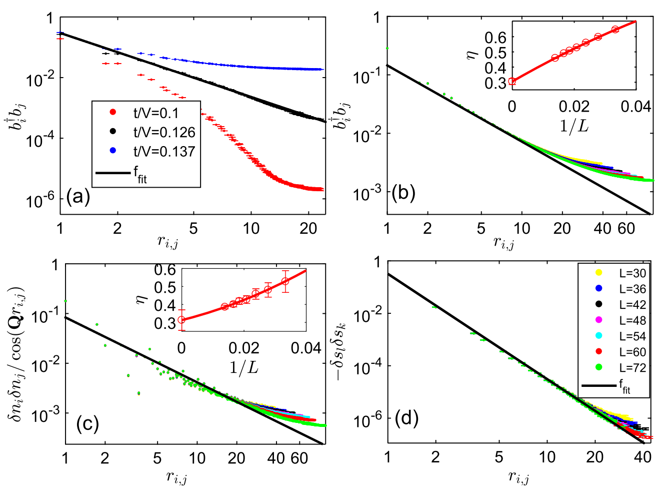

FIG. 4. (a) Off-diagonal correlation function vs distance at $1/3$ filling for $L = 18$, $\beta V = 300$, and different t/V. (b) Off-diagonal and (c) diagonal correlation function vs distance for different system sizes near the critical point at $1/3$ filling, $t/V = 0.1303$ and $\beta V/L = 25/3$. Inset: FSS of the anomalous exponents from fitting to $C_l(\delta, r)$. The extracted critical exponents are $\eta_{\mathrm{SF}} = 0.305(0.020)$ and $\eta_{\mathrm{VBS}} = 0.313(0.057)$. (d) Spinon correlation function vs distance at $1/3$ filling, near the critical point $t/V = 0.1303$ and $\beta V/L = 25/3$ for different system sizes. The black line is a fit to a power law decay $r^{-4.02(0.18)}$.

From Eq. (4), we identify the spinon density $s_{\triangle,\bigtriangledown} = \sum_{i\in\triangle,\bigtriangledown} n_i$ as a conserved charge. Such a conserved charge should have a scaling dimension $\Delta = 2$ for any $2+1$D CFT. As shown in Fig. 4(d), the corresponding correlation function shows a fast power law decay and rather small finite size effects. The extracted exponent is $-4.02(0.18)$, which is relatively close to -2Δ, strongly supporting the scenario that the easy plane-NCCP^1 is a CFT.

A hallmark of DCPs are emergent symmetries [3,12,33]. For example, at the critical point, the lattice Z_3 rotation symmetry will be enlarged to a continuous $U(1)$ rotation symmetry. To check this, we consider the resonant valence bond order parameter $\Xi(\mathbf{Q}_h) = \sum_{k=1}^{N_h} \Xi_k e^{\mathbf{i}\mathbf{Q_h}\cdot\mathbf{r}_k}/\sqrt{N_h}$ with $\mathbf{Q_h} = (2\pi/3, 0)$ where Ξ_k is the density operator of a hexagon of a resonant configuration, and N_h is the number of hexagons. In the VBS phase, the Z_3 degeneracy implies the phases of $\Xi(\mathbf{Q}_h)$ are 0, $2\pi/3$ and $4\pi/3$. We define $\Xi(\mathbf{Q}_h)_x$ $(\Xi(\mathbf{Q}_h)_y)$ as the real (imaginary) part $\mathrm{Re}[\Xi(\mathbf{Q}_h)]$ $(\mathrm{Im}[\Xi(\mathbf{Q}_h)])$ of $\Xi(\mathbf{Q}_h)$. From the histogram shown in Fig. 5 we find that it has three peaks in the VBS phase, indicating Z_3 symmetry, which shrinks to one point in the superfluid phase, reflecting no solid order. Near the critical point, the distribution approaches a uniform circle which reveals

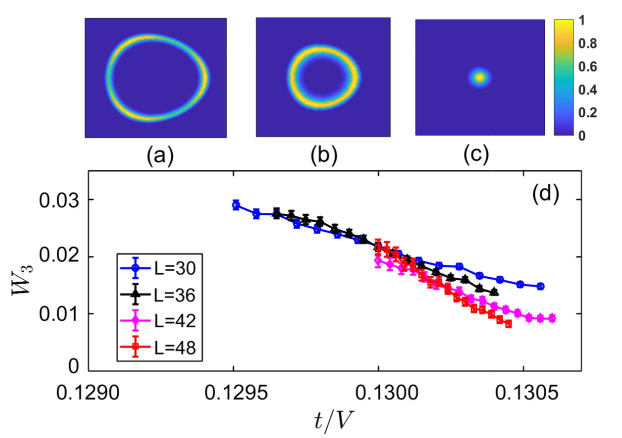

FIG. 5. Histogram of $[\Xi(\mathbf{Q}_h)_x, \Xi(\mathbf{Q}_h)_y]$ in (a) VBS phase $(t/V = 0.124)$, (b) near the critical point $(t/V = 0.129)$, and (c) the superfluid phase $(t/V = 0.131)$ at $1/3$ filling, $L = 30$ and $\beta V = 500$. (d) The Z_3 anisotropy parameter W_3 at $1/3$ filling and $\beta V/L = 25/3$ for different system sizes.

emerging $U(1)$ symmetry. In order to quantitatively check this, we introduce a Z_3 anisotropy parameter $W_3 = \langle \cos(3 \arg[\Xi(\mathbf{Q}_h)]) \rangle$. Figure 5(d) shows this quantity to increase in the VBS phase and to vanish with increasing system size in the superfluid phase.

Conclusions and discussions.—We have studied the easy plane deconfined phase transition of a hard core Bose-Hubbard model using QMC simulation. Finite size simulations of clusters up to $L = 72$ indicate an anomalous critical point separating the VBS and superfluid phase. We estimate that the critical point is at $t_c/V \approx 0.1303$. Following the approach in Ref. [32], we extract the anomalous exponents $\eta_{\rm SF} \approx 0.305$ and $\eta_{\rm VBS} \approx 0.313$ from the two-point correlation functions. In addition, we identify a lattice operator for the conserved charge of $NCCP^1$, and we numerically show its scaling dimension is $\Delta \approx 2$. At last, the emergent $U(1)$ rotation symmetry is found at the critical point.

In comparison with another easy plane $NCCP^1$ model [45], our model can be viewed as a different way to regularize an easy plane $NCCP^1$ continuous field theory on a discrete lattice. For example, in our system there is only one $U(1)$ global symmetry, while in the paper by Kuklov *et al.* there are two $U(1)$ global symmetries. Due to this difference the winding numbers of the two types of spinons are now equal $W_- = W_\triangle - W_\triangledown = 0$, which means no super-counter fluid phase exists. Such a difference may also strongly change the type of phase transition. Altogether, our results strongly support the presence of easy plane deconfined criticality. Similar to previous works, our data show some scaling violation that require further studies.

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