Deconfined Criticality: Generic First-Order Transition in the SU(2) Symmetry Case

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Monte Carlo simulations of the SU(2)-symmetric deconfined critical point action reveal strong violations of scale invariance for the deconfinement transition. We find compelling evidence that the generic runaway renormalization flow of the gauge coupling is to a weak first-order transition, similar to the case of U(1) × U(1) symmetry. Our results imply that recent numeric studies of the Nèel antiferromagnet to valence bond solid quantum phase transition in SU(2)-symmetric models were not accurate enough in determining the nature of the transition.

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Within the standard Ginzburg-Landau-Wilson description of critical phenomena, a direct transition between states which break different symmetries is expected to be of first order. The existence of a generic line of deconfined critical points (DCPs) proposed in Refs. [1–3]—an exotic second-order phase transition between two competing orders—remains one of the most intriguing and controversial topics in the modern theory of phase transitions. In particular, the DCP theory makes the prediction that certain types of superfluid to solid and the Nèel antiferromagnet to valence bond solid (VBS) quantum phase transitions in 2D lattice systems can be continuous. The new criticality is in the same universality class as a 3D system of $N = 2$ identical complex-valued classical fields coupled to a gauge vector field. This makes the DCP theory relevant also for the superfluid to normal liquid transition in symmetric two-component superconductors [4].

An intrinsic difficulty in understanding properties of the N-component DCP action is its runaway renormalization flow to strong coupling at large scales and the absence of perturbative fixed points for realistic N [5,6]. One may only speculate that the value of N might be of little importance since the possibility of the continuous transition for $N = 1$ is guaranteed by the exact duality mapping between the inverted-XY and XY-universality classes [7], and for $N \to \infty$ it follows from the large-N expansion for N of the order of a hundred. However, there are no exact analytic results either showing that in a two-component system there exists a generic line of second-order phase transitions or proving that the second-order phase transition is fundamentally impossible. The problem of deconfined criticality for the most interesting case of $N = 2$ thus has to be resolved by numerical simulations.

The initial effort was focused on models of the superfluid to solid quantum phase transitions and U(1) × U(1)-symmetric DCP actions [1,8]. The first claims of deconfined criticality were confronted with the observation of weak first-order transitions in other models [9]. While presenting a particular model featuring a first-order phase transition does not prove the impossibility of a continuous DCP yet, it does raise a warning flag. One needs to pay special attention to any signatures of violation of the scale invariance which may be indicative of a runaway flow to a first-order transition even when all other quantities appear to change continuously due to limited system sizes available in simulations [10]. The flowgram method [11] was developed as a generic tool for monitoring such runaways flow to strong coupling and was used to prove the generic first-order nature of the deconfinement transition in the U(1) × U(1)-symmetric DCP action. A subsequent refined analysis resulted in the reconsideration of the original claims in favor of a discontinuous transition for all known models [12,13].

Recently, the SU(2)-symmetric case has been studied in a series of papers [14–16], and an exciting observation of a continuous DCP point was reported. However, the story seems to repeat itself since renormalization flows for the J-Q model studied in Refs. [14,15] were shown to be in violation of scale invariance and, possibly, indicative of the first-order transition [17]. Here we show that a runaway flow to strong coupling and a first-order transition is a generic feature of all SU(2)-symmetric DCP models analogous to the U(1) × U(1) case [18].

We consider the lattice version of the SU(2)-symmetric NCCP^1 model [2,3] and map it onto the two-component J-current model. The DCP action for two spinon fields z_a, $a = 1, 2$, on a three-dimensional simple cubic lattice is

$$S = -\sum_{\langle ij\rangle,a} t(z^*_{ai} z_{aj} e^{iA_{\langle ij\rangle}} + \text{c.c.}) + \frac{1}{8g}\sum_{\square}(\nabla\times A)^2;$$

$$\sum_a |z_{ai}|^2 = 1, \tag{1}$$

where $\langle ij\rangle$ runs over the nearest neighbor pair of sites i and

j, the gauge field $A_{\langle ij\rangle}$ is defined on the bonds, and $\nabla \times A$ is the lattice curl operator. The mapping to the J-current model starts from the partition function $Z = \int DzDz^*DA \exp(-S)$ and a Taylor expansion of the exponentials $\exp\{tz^*_{ai}z_{aj}e^{iA_{\langle ij\rangle}}\}$ and $\exp\{tz^*_{aj}z_{ai}e^{-iA_{\langle ij\rangle}}\}$ on all bonds. One can then perform an explicit integration over $A_{\langle ij\rangle}$, z_{ai} and arrive at a formulation in terms of integer nonnegative bond currents $J^{(a)}_{i,\mu}$. We use $\mu = \pm 1, \pm 2, \pm 3$ to label the directions of bonds going out of a given site, and the corresponding unit vectors are denoted by $\hat{\mu}$. These J currents obey the conservation laws:

$$\sum_{\mu} I^{(a)}_{i,\mu} = 0, \quad \text{with} \quad I^{(a)}_{i,\mu} \equiv J^{(a)}_{i,\mu} - J^{(a)}_{i+\hat{\mu},-\mu}. \tag{2}$$

The final expression for the partition function reads

$$Z = \sum_{\{J\}} \mathcal{Q}_{\text{site}} \mathcal{Q}_{\text{bond}} \exp(-H_J), \tag{3}$$

where

$$H_J = \frac{g}{2} \sum_{i,j;a,b;\mu=1,2,3} I^{(a)}_{i,\mu} V_{ij} I^{(b)}_{j,\mu},$$

$$\mathcal{Q}_{\text{site}} = \prod_i \frac{\mathcal{N}^{(1)}_i!\,\mathcal{N}^{(2)}_i!}{(1+\mathcal{N}^{(1)}_i + \mathcal{N}^{(2)}_i)!}, \quad \mathcal{N}^{(a)}_i = \frac{1}{2}\sum_{\mu} J^{(a)}_{i,\mu}, \tag{4}$$

$$\mathcal{Q}_{\text{bond}} = \prod_{i,a,\mu} \frac{t^{J^{(a)}_{i,\mu}}}{J^{(a)}_{i,\mu}!}.$$

The long-range interaction V_{ij} depends on the distance r_{ij} between the sites i and j. Its Fourier transform is given by $V_{\mathbf{q}} = 1/\sum_{\mu=1,2,3}\sin^2(q_\mu/2)$ and implies an asymptotic behavior $V \sim 1/r_{ij}$ at large distances.

This formulation allows efficient Monte Carlo simulations using a worm algorithm for the two-component system [11]. Assuming periodic boundary conditions, we introduce the winding numbers, which are nothing but instant values of corresponding total currents in a given direction: $W_{a,\mu} = \sum_j J^{(a)}_{j,\mu}/L$, with L being the sample linear size. The mean square fluctuations of the winding numbers provide superfluid stiffnesses [19]: $\rho_\pm = \sum_\mu \langle (W_{1,\mu} \pm W_{2,\mu})^2\rangle/L \equiv \langle (W^2_\pm)\rangle/L$. In particular, we focused on the gauge-invariant superfluid stiffness, ρ_- measuring the response to a twist of the phase of the product $z^*_1 z_2$.

Similar to the U(1) × U(1) case [11], the NCCP^1 model features three phases (Fig. 1) characterized by the following order parameters: VBS: an insulator with $\langle z_{ai}\rangle = 0$ and, accordingly, $\langle\rho_+\rangle = \langle\rho_-\rangle = 0$; 2SF: two-component superfluid (2SF) with $\langle z_{ai}\rangle \neq 0$, $\langle\rho_+\rangle \neq 0$, and $\langle\rho_-\rangle \neq 0$; SFS: supersolid (a paired phase [20]) with $\langle z_{ai}\rangle = 0$, $\langle z^*_{1i}z_{2j}\rangle \neq 0$, $\rho_+ = 0$, and $\rho_- \neq 0$. The point $g = 0$ and $t \approx 0.468$ features a continuous transition in the O(4) universality class. The relevant part of the phase diagram is the region of small g close to this O(4) point, far away

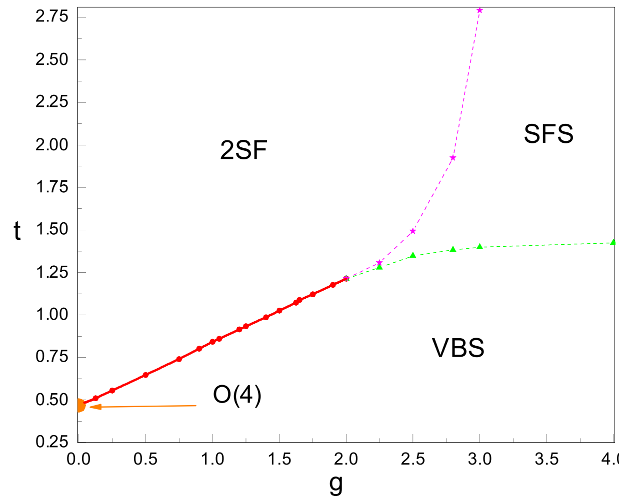

FIG. 1 (color online). Phase diagram of the SU(2)-symmetric DCP action (1). First-order transitions VBS-2SF are shown as a solid red line up to the bicritical point $g_{bc} \approx 2.0$.

from the bicritical point $g_{bc} \approx 2.0$ above which the SFS phase intervenes between the VBS and 2SF phases. The corresponding direct VBS-2SF transition has been proposed to be a deconfined critical line (DCP line) [2,3].

The key idea of the flowgram method [11] is to demonstrate that the universal large-scale behavior at $g \to 0$ is identical to that at some finite coupling $g = g_{\text{coll}}$ where the nature of the transition can be easily revealed. The procedure is as follows: (i) Introduce a definition of the critical point for finite L consistent with the thermodynamic limit and insensitive to the order of the transition. In our model, we used the same definition as in Ref. [11]. Specifically, for any given g and L, we adjusted t so that the ratio of statistical weights of configurations with and without windings was equal to 7.5. (ii) At the transition point, calculate a quantity $R(L, g)$ that is supposed to be scale-invariant for a continuous phase transition in question, vanish in one of the phases, and diverge in the other. Here we consider $R(L, g) = \langle W^2_-\rangle$. (iii) Perform a data collapse for flowgrams of $R(L, g)$, by rescaling the linear system size $L \to C(g)L$, where $C(g)$ is a smooth and monotonically increasing function of the coupling constant g. In the present case, we have $C(g \to 0) \propto g$ [5].

A collapse of the rescaled flows within an interval $g \in [0, g_{\text{coll}}]$ implies that the type of transition within the interval remains the same and thus can be inferred by dealing with the $g = g_{\text{coll}}$ point only. Since the $g \to 0$ limit implies large spatial scales and, therefore, a model-independent runaway renormalization flow pattern, the conclusions are universal.

To have a reference comparison, we first simulated a short-range analog of the NCCP^1 model (4) with $V_{ij} = g\delta_{ij}$. The short-range model has a similar phase diagram but with a second-order phase transition for small g and a first-order one at large g. Figure 2 clearly shows that the corresponding flowgram cannot be collapsed on a single

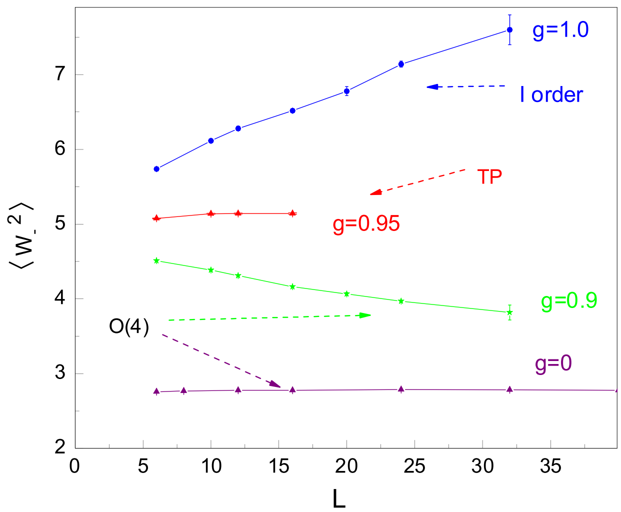

FIG. 2 (color online). Flowgrams for the short-range model. The lower horizontal line features the O(4) universality scaling behavior, so that for $g < g_c \approx 0.95$ all flows are attracted to this line. The upper horizontal line is the tricritical separatrix (marked as TP). Above it, flows diverge due to the first-order transition detected by the bimodal distribution of energy.

master curve by rescaling the length (shifting the lines horizontally in logarithmical scale), and the separatrix at the tricritical point (TP) at $g \approx 0.95$ is clearly visible.

Contrary to the short-range model, we find no such separatrix for the DCP action. As shown in Fig. 3, the flows feature a fan of lines diverging with the system size and with the slope increasing with g without any sign of a TP separatrix.

One can notice that the NCCP^1 flows exhibit a slope change [see Fig. 3 (also observed in Ref. [17] for the J-Q model)] that might be interpreted as a sign of the evolution towards a scale-invariant behavior $\langle W_-^2 \rangle = \text{const}$, possibly achieved at a large enough L. The same feature has been observed recently in Ref. [16] and caused the authors to speculate that the NCCP^1 model features a line of continuous transitions for $g < 1.25$ [21]. The crucial test, then, is to see if the fan of the NCCP^1 lines can be collapsed on a single master curve $\langle W_-^2 \rangle = F(C(g)L)$, where $C(g)$ describes the length-scale renormalization set by the coupling constant g. As it turns out, the NCCP^1 flows collapse perfectly [22] in the whole region $0.125 \leq g < 1.65$ below the bicritical point g_{bc} (see Fig. 4). The rescaling function $C(g)$ exhibits a linear behavior $C(g) \propto g$ at small g consistent with the runaway flow in the lowest-order renormalization group analysis [5]. This behavior all but rules out the existence of the TP on the VBS-2SF line.

Though our conclusions directly contradict claims made in Refs. [14–16], the primary data are in agreement. A data collapse of the flowgram presented in the lower panel of Fig. 13 in Ref. [16] shows the same qualitative behavior as our Fig. 4 [23]. We are also consistent with the conclusion reached in Ref. [17] that the slope change is an intermediate-scale phenomenon and the Nèel antiferromagnet to VBS transition in the J-Q model violates the scale invariance hypothesis as observed by the divergent flow of $\langle W_-^2 \rangle$.

The flow collapse within an interval $g \in [0, g_{\text{coll}}]$ does not yet imply a first-order transition. What appears to be a diverging behavior in Fig. 3 might be just a reconstruction of the flow from the O(4) universality (at $g = 0$) to a novel DCP universality at strong coupling. To complete the proof, we have to determine the nature of the transition for $g = g_{\text{coll}}$. In this parameter range, the standard technique of detecting discontinuous transitions by the bimodal energy distribution becomes feasible. As shown in Fig. 5, a clear bimodal distribution develops at $g = 1.65$, which is below the bicritical point g_{bc} and within the data collapse interval $[0, g_{\text{coll}}]$.

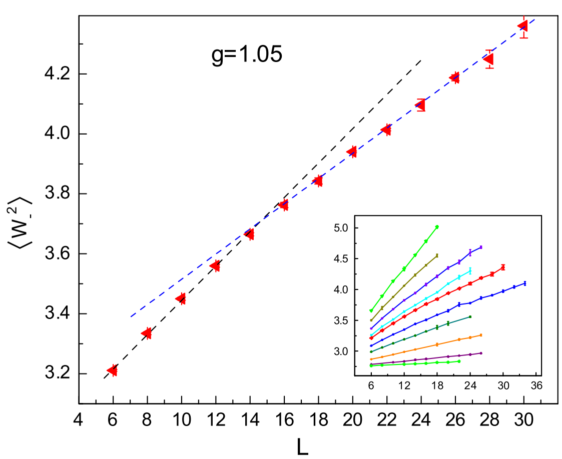

FIG. 3 (color online). A typical flowgram of the gauge-invariant superfluid stiffness in the NCCP^1 model. The inset shows a fan of diverging flows for $0.125 < g < 1.4$.

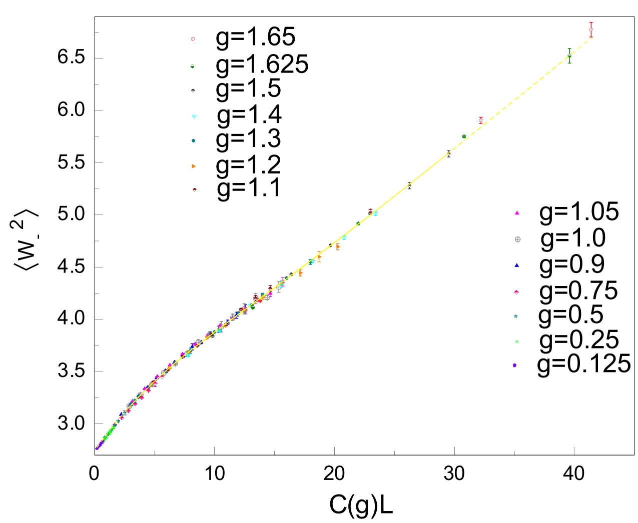

FIG. 4 (color online). Data collapse for the NCCP^1 flows. The yellow line is a fit representing the master curve. The horizontal axis is the scale-reduced variable $C(g)L$, with $C(g) = [\exp(bg) - 1]/[\exp(bg_1) - 1]$, $b = 2.28 \pm 0.02$, and $g_1 = 1.3$. Error bars are shown for all data points.

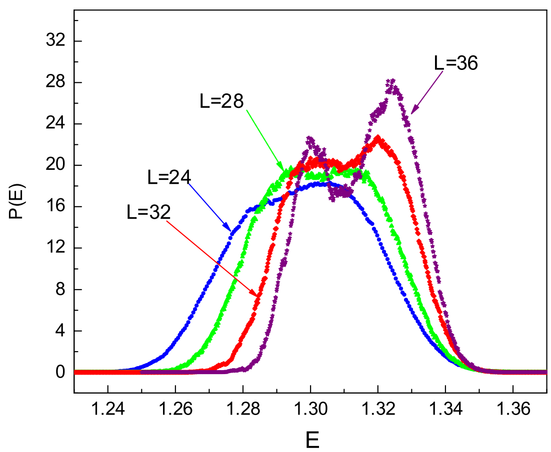

FIG. 5 (color online). Evolution towards the bimodal energy distribution with increasing system size indicative of the first-order deconfinement transition ($g = 1.65$).

This leaves us with the clear conclusion that the whole phase transition line for small g features a generic weak first-order transition identical to the one observed in the $U(1) \times U(1)$ case. Driven by long-range interactions, this behavior develops on length scales $\propto 1/g \rightarrow \infty$ for small g and thus is universal. It cannot be affected by microscopic variations of the $NCCP^1$ model suggested in Ref. [16] to suppress the paired (molecular) phase. With this failure of the paradigmatic DCP action, the only possibility for the DCP should be associated with some hypothetical models featuring a continuous phase transition in the middle of the first-order line—essentially at *finite* couplings g.

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[22] A flow collapse is meaningful even when the collapsing lines $R(L)$ are relatively short and reminiscent of straight lines: A straight line is described by two independent parameters, while the rescaling procedure has only one degree of freedom of shifting the line horizontally in logarithmical scale. The master curve may significantly deviate from a straight line and prove indispensable for understanding the global character of the flow and difficulties with the finite-size scaling in specific models.
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