Emergence and spontaneous breaking of approximate $O(4)$ symmetry at a weakly first-order deconfined phase transition

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We investigate approximate emergent nonabelian symmetry in a class of weakly first order ‘deconfined’ phase transitions using Monte Carlo simulations. We study a transition in a 3D classical loop model that is analogous to a deconfined 2+1D quantum phase transition in a magnet with reduced lattice symmetry. The transition is between the Néel phase and a twofold degenerate valence bond solid (lattice-symmetry-breaking) phase. The combined order parameter at the transition is effectively a four-component superspin. It has been argued that in some weakly first order ‘pseudo-critical’ deconfined phase transitions, the renormalization group flow can take the system very close to the ordered fixed point of the symmetric $O(N)$ sigma model, where $N$ is the total number of ‘soft’ order parameter components, despite the fact that $O(N)$ is not a microscopic symmetry. This yields a first order transition with unconventional phenomenology. We argue that this occurs in the present model, with $N = 4$. This means that there is a regime of lengthscales in which the transition resembles a ‘spin-flop’ transition in the ordered $O(4)$ sigma model. We give numerical evidence for (i) the first order nature of the transition, (ii) the emergence of $O(4)$ symmetry to an accurate approximation, and (iii) the existence of a regime in which the emergent $O(4)$ is ‘spontaneously broken’, with distinctive features in the order parameter probability distribution. These results may be relevant for other models studied in the literature, including 2+1D QED with two flavours, the ‘easy-plane’ deconfined critical point, and the Néel–VBS transition on the rectangular lattice.

CONTENTS

I. Introduction 1
II. RG picture 3
III. Model 6
IV. Numerical results 8
  A. Evidence for first order nature of transition 8
  B. Evidence for approximate $O(4)$ symmetry 9
  C. Evidence for $O(4)$–ordered regime 10
V. Outlook 12
Acknowledgments 13
A. Comparison of two VBS components 13
References 14

I. INTRODUCTION

The phenomenology of deconfined criticality [1, 2] in models with small ‘$N$’ — for example spin-1/2 magnets with various symmetries in 2+1D [3–17], and related classical models [18–21] — has turned out to be more interesting and more subtle than could have been guessed from simple large $N$ approximations. Many phenomena have been invoked in order to explain perplexing numerical results: we are gradually elucidating which are only mirages, and which are the crucial features of the problem. Here we demonstrate a remarkable weakly first-order ‘deconfined’ phase transition, with unusual phenomenology, in a model with two competing order parameters. This phase transition combines the ingredient of emergent symmetry with that of ‘quasiuniversality’ [18, 22] at weakly first order deconfined transitions.

Emergent nonabelian symmetries, which unite distinct order parameters, are a key concept for understanding deconfined criticality in small ‘$N$’ models [19, 22–24]. At the Néel to valence-bond-solid (Néel–VBS) transition in square lattice spin-1/2 magnets, with full spin rotation symmetry, five order parameter components become ‘soft’ at the transition. These are the three components of the Néel vector $\mathbf{N}$ and the two components of the VBS order parameter $\phi$. Numerics show a very accurate $SO(5)$ symmetry unifying these five components at the transition [19, 20, 25]. We may write them as a superspin,

$$\mathbf{n} = (N_x, N_y, N_z, \phi_x, \phi_y).$$  (1)

At currently accessible system sizes, the $SO(5)$ symmetry for $\mathbf{n}$ looks like exact symmetry of the infra-red theory, which becomes increasingly accurate at longer lengthscales. At asymptotically long lengthscales it may well only be an approximate symmetry (see [20, 22, 26] for discussions), but it seems to be a robust feature of models described by the noncompact $\mathbb{CP}^1$ field theory (NCCP$^1$)
originally proposed for the Neél-VBS transition. For example, \( SO(5) \) also emerges [20] in a classical dimer model that has very different microscopic symmetries to the Neél-VBS models [27–30]. Emergent \( SO(5) \) is equivalent to an IR self-duality of the NCCP\(^4 \) field theory [22].

A different class of putative ‘deconfined’ phase transitions are those involving only four soft order parameter components. The best-studied is the ‘easy-plane’ Neél-VBS transition, with two Neél and two VBS components [11, 15–17, 31, 32]

\[
n = (N_x, N_y, \phi_x, \phi_y).
\] (2)

It was suggested that this transition, if continuous, may have emergent \( O(4) \) symmetry [16, 22]. There are models where the transition is clearly first order [11, 15, 29, 31, 32], but it has recently been claimed that the transition is continuous in other models [16, 17]. It was also pointed out recently [33] that the same \( O(4) \)-invariant long-distance theory may well apply to another set of transitions with full spin rotation symmetry, but with only a one-component VBS order parameter [23]:

\[
n = (N_x, N_y, N_z, \varphi).
\] (3)

In this last set of examples there is, loosely speaking, a semi-microscopic \( SO(3) \times Z_2 \) symmetry, where the \( Z_2 \) really refers to lattice symmetries (e.g. translation) that change the sign of the VBS order parameter \( \varphi \). One example is the Neél-VBS transition with rectangular anisotropy, which suppresses one direction for the columnar VBS order parameter. Another is a transition [33] for spin-1 Is on the square lattice, between the Neél phase and a VBS phase [34, 35] with a twofold degenerate ground state. The 3D classical transition we study below is analogous to a 2+1D Neél-VBS transition for spin-1/2 Is on the square lattice with reduced lattice symmetry, and also has a four-component order parameter of the form in Eq. 3, with \( SO(3) \times Z_2 \) symmetry.

It is worth noting that the relation between these various models is highly non-obvious in the usual NCCP\(^1 \) language, where easy-plane anisotropy and, say, rectangular anisotropy [33] correspond to perturbations of very different types that reduce the symmetry of the NCCP\(^1 \) model in different ways. However if \( O(4) \) symmetry emerges there is the possibility that these various models converge under RG flow. Even more strikingly, the easy-plane model has been conjectured to be dual to two-flavour quantum electrodynamics \( (N_f = 2 \) QED) [22, 36], and this theory may also acquire \( O(4) \) in the infrared. A conjectured self-duality of \( N_f = 2 \) QED [36–39] would imply \( O(4) \) in that theory (which may also be argued for heuristically by a mapping to the \( O(4) \) sigma model at \( \theta = \pi \) [23], and which has some support from simulations [40]).

A second useful concept is that of pseudocriticality. This is a regime of ‘slow’ renormalization group (RG) flow, associated with a more or less well-defined line in coupling constant space that attracts nearby flow lines, leading to ‘quasiuniversal’ behaviour that is only weakly dependent on the bare parameters. This phenomenon can be made precise in various field theories with a parameter that does not flow under the RG, and was proposed as an explanation for various puzzling phenomena at deconfined phase transitions in [18, 22]. A classic example of this phenomenon is the Potts model, where as the number of states \( Q \) is increased the continuous transition gives way to a first-order one at a universal critical value [41–45]. This is due to the annihilation of a critical and a tricritical fixed point. (Fixed point annihilation has also been discussed in QCD and QED, among other models [46–51].) For \( Q \) slightly larger than the critical value, there is a first order transition with a parametrically large correlation length and quasiuniversal properties that depend only parametrically weakly [22] on the bare couplings. (See [45] for a recent numerical study of the Potts case.)

In models that show a pseudocritical regime, the simplest possibility is that at the very longest lengthscales the RG flow is to a discontinuity fixed point, i.e. a first order transition. However things can be more interesting if an (approximate) emergent symmetry is established during the quasiuniversal RG flow associated with pseudocriticality, i.e. if the attractive flow line has the higher symmetry [22]. In this case the emergent symmetry persists even into the coexistence regime — i.e. the regime of lengthscales where the order parameters no longer appear to be scaling to zero with system size (as at a critical point) but have instead saturated to a finite value. This gives an unconventional first-order transition which resembles a spin-flop transition in an ordered sigma model with the higher symmetry. We review this RG picture below.

It is plausible that the above scenario is what ultimately happens in the models that show an emergent \( SO(5) \) symmetry. But if so, the lengthscales required to see it seems to be inaccessible at present: we can access the ‘pseudocritical’ regime but not the ‘spin flop’ regime at larger scales. (It is also conceivable that the ultimate fate of the models with \( SO(5) \) symmetry is something else, though this is constrained by conformal bootstrap [26, 52, 53].)

By contrast, we show here that the phenomenon of a weakly first order transition with emergent approximate \( O(4) \) symmetry can be seen in models for deconfined criticality with four order parameter components, or rather in at least one such model. In the model we study the lengthscales associated with the first order transition is long enough to allow \( O(4) \) to emerge with good accuracy (we demonstrate this directly using the order parameter distribution) and short enough that we can convincingly demonstrate that the transition is first order.

The resulting first order transition has an interesting phenomenology, because the two competing phases, which coexist at the critical coupling, are related by an effective continuous symmetry in the appropriate range of lengthscales. This has characteristic signatures in the
probability distribution of the order parameters, which
takes a simple universal form, and of quantities like the
energy, which do not have the double peaked shape fa-
miliar in conventional first order transitions. The model
we study is a classical 3D loop model [18] that is closely
related to a deconfined critical point for 2+1D square
lattice magnets, but with reduced lattice symmetry (the
loop model can be viewed as a deformation of the par-
tition function of a quantum magnet to impose isotropy
in the three ’spacetime’ dimensions, making the model
more convenient for simulations). We argue that this
model shows the basic features of the RG scenario out-
lined above.

Work on field theoretic dualities has recently revealed
unexpected connections between 2+1D field theories, and
the present results may be relevant to a variety of other
models. Various examples of deconfined criticality with
four order-parameter components have been discussed in
the literature, and as mentioned above the easy-plane
transition has been argued to be dual to 2+1D quantum
electrodynamics with \( N_f = 2 \). It would be worth look-
ing for the phenomena we discuss in those models. (The
status of duality webs relating different theories, in cases
where the emergent symmetry implied by the dualities
is approximate rather than exact, is discussed in [22].)
Recent numerics has however argued for a continuous
easy-plane transition rather than a weakly first-order one
[16, 17] (see [32, 39] for discussions of relations between
different easy-plane models), and for scale invariance in
\( N_f = 2 \) QED [54]. In the light of the relationships ex-
pected between the various field theories this difference
with what we find here is slightly surprising and would
be worth examining further.

II. RG PICTURE

Before describing a particular model, in this section we
review the scenario of [22] for a weakly first order
decomposed phase transition with approximate emergent
symmetry. For concreteness, we focus on the scenario
with a four-component order parameter which will be
relevant to us below. For a simplified picture, it is use-
ful to think of the nonlinear sigma model as the effective
field theory for this order parameter [23]. This theory
is not precisely defined, since the sigma model is a non-
renormalizable effective field theory whose definition is
regularization dependent, but this will not matter for the
following qualitative discussion of the RG flows (see [22]
for a more careful discussion).

The sigma model for the four-component field \( \mathbf{n} \), with
\( n^2 = 1 \), is
\[
\mathcal{L} = \frac{1}{2g} (\partial \mathbf{n})^2 + \frac{i \pi e_{abcd}}{\text{Area}(S^4)} n_a \partial_x n_b \partial_x n_c \partial_x n_d + \ldots
\]
(4)
The second term is the topological \( \Theta \) term whose pres-
ence was argued for in [23] (see also [24] for a related
discussion of the 5-component case). The ‘\ldots’ include
perturbations that reduce the symmetry to the micro-
scopic symmetry of the lattice model of interest.

These perturbations can be classified into representa-
tions of \( O(4) \) symmetry. We assume that the ones which
are important for us in the pseudocritical regime (de-
scribed below) — i.e. the most relevant allowed perturba-
tions — are two- and four-index symmetric traceless
\( O(4) \) tensors \( X^{(2)}_{ab} \) and \( X^{(4)}_{abcd} \) [19, 22]. We assume that
the former is effectively \textit{relevant} in the pseudocritical regime
and the latter is effectively irrelevant. At the level of sym-
metry \( X^{(2)}_{ab} \sim n_a n_b - \frac{1}{2} \delta_{ab} \) and \( X^{(4)}_{abcd} \sim n_a n_b n_c n_d - \ldots \).

In the loop model we study below, a microscopic \( SO(3) \)
symmetry acts on \( (n_1, n_2, n_3) = (N_x, N_y, N_z) \). There is no
microscopic continuous symmetry acting on \( n_4 = \varphi \),
but this field changes sign under lattice symmetries, for
example appropriate lattice translations. In the contin-
uing we will refer loosely to the model as having \( SO(3) \times \mathbb{Z}_2 \)
symmetry. This is analogous to the case of the Néel-VBS
transition on a rectangular lattice [33] (though with some
differences, see Sec. III).

In these models the microscopic symmetries allow the
following perturbations built from the above operators.
The first is the strongly \textit{relevant} anisotropy between Néel
and VBS that drives the transition:
\[
\delta \mathcal{L} = -g_R X^{(2)}_{44} , \quad g_R \propto (J - J_c) .
\]
(5)
(Here \( J \) is the coupling that tunes the transition in the
microscopic model.) The second is a higher order
anisotropy between Néel and VBS that is assumed to be
effectively \textit{irrelevant} in the pseudocritical regime:
\[
\delta \mathcal{L} = g_I X^{(4)}_{4444} .
\]
(6)
A key point is that \( \mathbb{Z}_2 \times SO(3) \) allows only one (effec-
tively) relevant coupling at the transition [33].

A similar picture applies at the easy-plane Néel–VBS
transition, despite the rather different microscopic sym-
metry. In easy-plane models on the square lattice there is
a relevant perturbation \( \sum_{a=1,2} X^{(2)}_{aa} \) driving the transi-
tion and typically two leading irrelevant perturbations
allowed by the (different) microscopic symmetry [22].
These are a higher-order anisotropy between Néel and
VBS, and fourfold symmetry breaking for the VBS:
\[
\delta \mathcal{L} = g_{1}^{(2)} \sum_{a,b=1,2} X_{ab} + g_{2}^{(2)} \sum_{a=3,4} X_{aaa} .
\]
(7)

The \( O(4) \) pseudocritical regime described below may
also arise in \( N_f = 2 \) QED. An important difference in
that context is that perturbations built from \( X^{(2)} \) and
\( X^{(4)} \) are forbidden by microscopic \( SU(2) \) flavour sym-
metry [22, 23], indicating that \( O(4) \) is even more robust
at long length scales than in the cases we discuss here.

Now let us consider how the renormalization group
flows of a theory with a higher symmetry \( G \) (here

\[
\mathcal{L}_{\mathcal{G}} = \frac{1}{2g_{\mathcal{G}}} (\partial \mathbf{g})^2 + \frac{i \pi e_{abcd}}{\text{Area}(S^4)} g_a \partial_x g_b \partial_x g_c \partial_x g_d + \ldots
\]
(8)
\(G = O(4)\) may allow for an unconventional first order transition in a microscopic model without \(G\) symmetry [22]. We assume there is a flow-line in the \(G\)-symmetric parameter space along which the RG flow becomes very slow. Let us parameterize the flow line by \(\lambda\), with \(\lambda\) decreasing under the flow, and with the slow region of RG flows being close to \(\lambda = 0\). For a heuristic picture, we can imagine that this represents the flow of the coupling constant in the nonlinear sigma model above, with \(\lambda > 0\) corresponding to the region of small stiffness (large \(g\)) and \(\lambda \to -\infty\) corresponding to the ordered fixed point at large stiffness (\(g = 0\)).

'Slow' is a qualitative rather than a precise statement in the present context: its usefulness will ultimately be determined by comparing the following results with numerics. However the idea of pseudocriticality due to slow RG flows can be made precise in cases where we have a tuning parameter that controls the slowness of the RG flows. One example is the \(Q\)-state Potts model for small \(\Delta^2 \equiv Q - Q_c(d)\), where \(Q_c(d)\) is the largest value of \(Q\) for which the transition is continuous in \(d\) dimensions [41-45]. Another is the NCCP\(^{n-1}\) model for small \(\Delta^2 \equiv d - d_c(n)\), where \(d_c(n)\) is the largest value of \(d\) for which the transition is continuous at a given \(n\) [18]. In these examples the RG equations can be expanded systematically in \(\Delta^2\) for small \(\Delta^2\). When \(\Delta^2 \leq 0\) the transition is continuous. \(\Delta^2 \geq 0\) is the 'pseudocritical' regime of interest, with a correlation length that is exponentially large in \(1/\Delta\).

Here we do not have a controlled \(\Delta^2 = 0\) limit that preserves \(O(4)\) symmetry, but to simplify the discussion, let us imagine that such a limit could be found in an appropriately deformed field theory.\(^1\) This limit yields several well-defined regimes of RG flow, giving the simplest illustration of the mechanism of interest. The physical model we study is not in the controllable limit of parametrically small \(\Delta\) (regardless of whether an appropriate deformation of the field theory can be found). Therefore, rather than giving quantitative information about the RG flows in the physical model, the following discussion motivates a conjecture for the qualitative features of those flows. We will see below that the expectations from this conjecture appear to be borne out in simulations.

As discussed in [22, 44], for small \(\Delta\) and \(\lambda\) and in the vicinity of the flow line we have

\[\frac{d\lambda}{d \ln L} = -\lambda^2 - a^2 \Delta^2 + \cdots\]  \(8\)

\[\frac{dg_R}{d \ln L} = +(y_R + c' \lambda) g_R + \cdots\]  \(9\)

\[\frac{dg_I}{d \ln L} = -(y_I + c \lambda) g_I + \cdots\]  \(10\)

Here, in addition to \(\lambda\), we have included the most relevant\(^2\) coupling \(g_R\) and the leading irrelevant one \(g_I\) arising from \(X^{(4)}\) (for simplicity we consider only one \(g_I\)). We have extracted a sign so that \(y_R\) and \(y_I\) are both positive, although \(g_I\) is irrelevant.

\(^1\) See [22] for speculations about such deformations in the 5-component case.

\(^2\) More correctly, these couplings can be classified as relevant/irrelevant at the hypothetical \(\Delta = 0\) fixed point.
First consider the case \( g_R = g_I = 0 \). Integrating the above equation shows that for small \( \Delta \) the lengthscale required for \( \lambda \) to flow from a positive order 1 value to a negative order 1 value scales as

\[
\xi_{\text{order}} \sim e^{\pi/a\Delta}.
\]  

(11)

We make the assumption that for large scales \( \ln L \gg \ln \xi_{\text{order}} \) the flow is to the ordered fixed point of the sigma model in Eq. 4. This is consistent with the existence of a topological term in the sigma model since the topological term is irrelevant by power counting in the ordered phase. This flow is indicated by the flow line marked \( \mathbf{A} \) in Fig. 1. The purple blur indicates the ‘slow’ regime close to \( \lambda = 0 \).

Next consider the case \( g_I \neq 0, g_R = 0 \). This is the flow line marked \( \mathbf{B} \) in Fig. 1. Note that this corresponds to the microscopic model precisely at \( J_\ast \). The perturbation \( g_I \) is the leading effect of \( O(4) \)-breaking perturbations that are present in the microscopic model even at \( J_\ast \).

The key point is that the \( O(4) \)-breaking perturbation \( g_I \) decreases during the period of RG flow close to \( \lambda = 0 \) (Eq. 10). Since the coupling is effectively irrelevant \( (g_I > 0) \), and since \( \xi_{\text{order}} \) is exponentially large in \( \Delta \), by the time \( \lambda \) is negative and of order one, the irrelevant coupling \( g_I \) has become exponentially small: \( g_I^* \sim e^{-\pi y_I/a\Delta} \) [22].

Therefore the flow \( \mathbf{B} \) comes very close to the ordered fixed point of the NLSM. However, the anisotropy encoded in \( g_I \) is relevant at this ordered fixed point. In the next stage of the RG flow the flow line \( \mathbf{B} \) diverges from the ordered fixed point (Fig. 1).\(^3\) This is similar to phenomena in symmetry-breaking transitions with dangerously irrelevant anisotropies [55].

Let us use the rescaled length coordinate \( \tilde{x} = x/\xi_{\text{order}} \). Then an effective action in this regime is

\[
\mathcal{S} = \int d^3\tilde{x} \left[ \frac{1}{2\delta_{\text{eff}}} (\tilde{\eta}_n)^2 + g_I^* \tilde{O}_I \right],
\]

(12)

where \( \tilde{O}_I \) is an anisotropy in the sigma model with the appropriate symmetry. Roughly speaking, the coupling \( g_{\text{eff}} \) is of order one at the scale \( \xi_{\text{order}} \), but grows rapidly under RG. Above, \( n^2 = 1 \), but the lattice order parameters are related to this sigma model field by a power of \( \xi_{\text{order}} \), since the magnitude of the order parameter decreases roughly like a power of \( L \) in the pseudocritical regime.

In fact there are two separate lengthscales associated with the \( O(4) \) breaking perturbation \( g_I^* \), depending on whether we consider the probability distribution of the ordered moment (the zero mode of the field) or the Goldstone modes. The probability distribution for the zero mode becomes asymmetric at a scale

\[
\xi_{\text{zero mode}} \sim \xi_{\text{order}} \times (g_I^*)^{-\frac{1}{2}} \sim e^{\pi(1+y_I/3)}
\]

(13)

(at which point the contribution to the action from the zero mode becomes of order 1). The correlation functions of the Goldstone modes cross over from power law to exponential on a different scale that is in principle longer,

\[
\xi_{\text{Goldstone}} \sim \xi_{\text{order}} \times (g_I^*)^{-\frac{1}{2}} \sim e^{\pi(1+y_I/2)}
\]

(14)

(To see this note that in the rescaled coordinates \( \tilde{x} \) the squared mass is simply proportional to \( g_I^* \), since it is obtained by expanding Eq. 12 to quadratic order around one of the minima of the potential \( O_I \).)

Finally, consider briefly the case where the microscopic model is perturbed away from the transition by \( \delta J = J - J_\ast \). There are three different regimes, depending on the size of \( \delta J \), that are illustrated in Fig. 2. The coupling \( g_R \), which is initially small and proportional to \( \delta J \), is growing at all stages of the RG flow. How small its initial value is will determine which fixed points in the \( g_R = 0 \) plane the flow approaches before being driven away to one of the ordered phases at large (positive or negative) \( g_R \), which here represent the Néel and VBS phases.

The above discussion is all in the idealized limit of small \( \Delta \). In this limit there is a clean separation of scales between \( \xi_{\text{order}} \) and \( \xi_{\text{zero mode}} \) corresponding to the regime ‘close’ to the ordered fixed point of the symmetric sigma model (assuming we are sensitive to the probability distribution of the zero mode).

In the physical models, we do not expect this clean separation of scales, and we do not expect the detailed formulae in Eq. 10 to be accurate. Roughly speaking, the lengthscales relevant to us below are on the scales of, say, 10 to 100 so the relevant RG times are only of order one, because of the logarithmic relationship between length and RG time. So we are certainly not in the above limit where the flow of the coupling becomes extremely slow. But conversely, the exponential dependence of irrelevant variables on RG time means that accurate \( O(4) \) can still emerge on these scales.

We will give evidence that the RG flows in the model we study have the basic qualitative features described above: an initial regime in which approximate \( O(4) \) arises, with \( O(4) \) ‘order’ at larger scales. (At present we cannot access large enough scales to see the subsequent flow away from the symmetric sigma model at \( J_\ast \), although this may be possible.)

Before continuing, we note one caveat. The advantage of the present scenario, as an explanation for the following numerical results, is that it does not assume any fine-tuning of the microscopic parameters of the model beyond tuning of \( J \) to \( J_\ast \): the phenomenon is insensitive to the bare values of the irrelevant couplings \( g_I \). But in principle an alternative way to flow close to the ordered \( O(4) \) fixed point would be to fine-tune the bare parameters to be close to a tricritical [16, 39] fixed point.

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\(^3\) In the case of QED the leading symmetry-breaking terms in the sigma model involve two derivatives and four powers of the field and will have a much weaker effect [22, 29].
with two unstable directions, if an appropriate such fixed point, with $O(4)$ symmetry, happened to exist. Since this requires fine-tuning, we believe it is a less plausible explanation for our numerics than the scenario above.

III. MODEL

The model we study is a simple modification of the loop model in [18], so we summarise it briefly. This modification was initially proposed by [56] as a way to perturb the deconfined critical point to reach a first order transition. The model is an isotropic classical lattice model in three dimensions with cubic symmetry.

The relation to 2+1D deconfined criticality can be seen either from a transfer matrix construction or from an effective field theory [18, 51]. The model has an exact $SO(3)$ spin symmetry which becomes manifest in a dual representation (with a local Néel vector $N = (N_x, N_y, N_z)$ that is defined on each link of the lattice model). Heuristically, the loops can be thought of as wordlines of spinons in a spin-1/2 magnet, with two colours associated with the two spin directions.

The configuration \( \{ \phi_r \} \) determines the geometry of the loops. Each loop can also take one of two colours, which are summed over in the partition function:

\[
Z = \sum_{\{ \phi \}} \sum_{\text{loop colours}} e^{-E}. \tag{15}
\]

Next we specify the energy $E$. The lattice is bipartite and each vertex $r$ is a member of either the $A$ or $B$ sublattice (blue and black in Fig. 3). There are interactions between nearest nodes on the same sublattice. In [18] these interactions were the same for the $A$ and $B$ lattices: we will refer to this here as the ‘symmetric’ model. The modification here is to have a different interaction for the $A$ and $B$ sublattices:

\[
E = -J_A \sum_{(r, r') \in A} \phi_r \phi_{r'} - J_B \sum_{(r, r') \in B} \phi_r \phi_{r'}. \tag{16}
\]

The two components of the VBS order parameter are

\[
(\phi_x, \phi_y) = (1, 1) \quad \text{and} \quad (\phi_x, \phi_y) = (1, -1).
\]

FIG. 4. Two of the four equivalent configurations with minimal length loops (colours are only a guide to the eye). The configuration on the left may be taken as the reference configuration for the $\phi$ variables. In both configurations shown, the $A$ nodes have $\phi_x = 1$. The $B$ nodes have $\phi_y = 1$ in the Left figure and $\phi_y = -1$ in the Right figure. We are interested in a phase transition at which $\phi \equiv \phi_x$ orders while $\phi_y$ remains disordered. The sign of $\phi_x$ can be viewed as picking out a sublattice of cubes for the loops to ‘resonate’ around, see Fig. 5.
At the transition of the model with critical point, is shown in Fig. 6. The full phase diagram for the model, close to the symmetric Ising transition which we will not be interested in. The transition at which loops live on the cubes with centres at $2(a, b, c)$ with $a + b + c = \text{even}$, such as the cube shown centred at the origin. For $\phi_x = -1$, the loops live on cubes with centres at $2(a, b, c)$ with $a + b + c = \text{odd}$ (the length of one link is taken to be 1).

defined by $\phi_r$ for $r \in A$ and $r \in B$ respectively. The overall magnitude of the order parameter is

$$\langle \phi_x, \phi_y \rangle = \frac{\sqrt{2}}{\text{no. sites}} \left( \sum_{r \in A} \phi_r + \sum_{r \in B} \phi_r \right).$$

In the four extreme VBS states above (which are related by lattice symmetry) we have

$$\langle \phi_x, \phi_y \rangle = \frac{1}{\sqrt{2}} (\pm 1, \pm 1).$$

In the symmetric model the transition from Néel to VBS is at $J_A = J_B = 0.088501(3)$. In this work we will fix $J_B$ to zero, to be far away from the symmetric critical point (to avoid crossover effects), and we vary $J_A$ to access the phase transition between the Néel and VBS phases:

$$J_A \equiv J \quad J_B = 0.$$

We take $J > 0$. Therefore $\phi_x$ is more strongly coupled than $\phi_y$. As $J$ is increased, there is a phase transition at which Néel order disappears, and $\phi_x$ orders. At this Néel-VBS phase transition, $\phi_y$ remains disordered (massive). This is the transition that we will study. The sign of the order parameter $\langle \phi_x \rangle$ can be viewed as picking out one of two sublattices of cubes for the loops to ‘resonate’ around, see Fig. 5 for a cartoon.

If, starting in the VBS phase with $\langle \phi_x \rangle \neq 0$, we then increase $J_B$ sufficiently, we encounter another phase transition at which $\phi_y$ also orders. This is a conventional Ising transition which we will not be interested in. The full phase diagram for the model, close to the symmetric critical point, is shown in Fig. 6.

In Appendix A we show data for both components of $\phi$ at the transition of the model with $J_B = 0$. This confirms that $\phi_y$ is a massive field with a short correlation length, and that for these parameters the model is ‘far’ from the symmetric critical point in the model with $J_A = J_B$: i.e. there is a strong asymmetry between $\phi_x$ and $\phi_y$ even at short scales. It is important to check this, because the critical point in the symmetric model is known to have a very accurate $SO(5)$ symmetry. If we studied a very weakly asymmetric model that was too close to this symmetric critical point, there would be an intermediate range of scales with approximate $SO(5)$, and $O(4)$ would be a trivial consequence of this higher symmetry. This is not the case here.

The order parameters that are involved in the phase transition of interest (indicated by the pink arrow in Fig. 6) are $\phi_x$ and $N$. To minimize subscripts we will write

$$\varphi \equiv \phi_x.$$  

The order parameters can be arranged in a superspin $n$, Eq. 3. Since the normalization of the lattice order parameters is arbitrary, $\varphi$ must be rescaled by a fixed but nonuniversal constant in order for $n$ to have a chance of being invariant under $O(4)$ rotations.

Before turning to numerical results, we briefly clarify our notation for the VBS order parameter, and contrast the present model with a square lattice quantum magnet with rectangular anisotropy in the couplings [23, 33].

Our convention for $\phi$ is such that the VBS-ordered states in the symmetric model ($J_A = J_B > J_{\text{critical}}$) are at $\phi \propto (\pm 1, \pm 1)$. If we temporarily redefine the order parameter by $\phi^\prime = \frac{1}{\sqrt{2}} (\phi_x + \phi_y, \phi_x - \phi_y)$, the ordered states are instead at $\phi^\prime \propto (\pm 1, 0), (0, \pm 1)$. This now matches the usual convention for columnar VBS ordered states in square lattice quantum magnets.
different perturbation of the Lagrangian, \((\phi')^2 - (\phi')^2\), which preserves symmetries under reflections across the lines \(\phi'_x = \pm \phi'_y\). If we start in the VBS-ordered phase of the symmetric model and turn this perturbation on weakly, these symmetries ensure that there are still four degenerate ground states: this corresponds to the upper right quadrant of Fig. 6.

This should be contrasted with rectangular anisotropy in the square lattice magnet, which is analogous to rectangular anisotropy in a square lattice quantum magnet at the Néel to columnar VBS transition, see text.

In this language, making \(J_A\) slightly different from \(J_B\), as above, introduces the term \(\phi_x^2 - \phi_y^2 \propto \phi_x \phi_y\), which preserves symmetries under reflections across the lines \(\phi'_x = 0\) and \(\phi'_y = 0\). In the VBS ordered phase, turning this perturbation on immediately reduces the ground state degeneracy from four to two. The phase diagram for a model with rectangular anisotropy, perturbed away from the symmetric critical point by \(\delta L = \delta J_x (\phi'_x)^2 + \delta J_y (\phi'_y)^2\), is shown in Fig. 7. The diagonal line is the four-fold degenerate VBS-ordered phase of the symmetric model.

Despite the different topologies of Figs. 6, 7, if there is indeed a quasuniversal O(4) regime that is accessible via an RG flow from the SO(5) point, then we would expect to be able to access it in both models (at least close enough to the symmetric critical point) on the phase transition lines marked ‘O(4)?’ in Figs. 6, 7.

As discussed above, simulations of the phase transition close to the symmetric point would be complicated by additional crossover effects, so here we study a point on the phase transition line that is relatively far from the line \(J_A = J_B\).

IV. NUMERICAL RESULTS

In Fig. 8 we show the Binder cumulants for the two order parameters close to the critical coupling,

\[ J_c = 0.0993911(14) \]  

(our method for estimating \(J_c\) is described below). At first glance these data for the Binder cumulants appear to show a continuous transition between phases with Néel and VBS order. Note the absence, on these scales, of the diverging positive peaks that would be expected for a conventional first order transition. We will argue that the transition is ultimately first order, but has a broad regime of lengthscales where it resembles an O(4) spin flop transition. On this range of lengthscales, the Néel and VBS states are effectively related by a continuous rotational symmetry. This is quite different from a conventional first order transition, where, at \(J_c\), the two competing phases are not even related by a discrete symmetry, and have (in the classical case) different energy and entropy.

We argue in three steps: first for the first-order nature of the transition, then for the presence of O(4) symmetry, then for the presence of effective O(4) long range order.

A. Evidence for first order nature of transition

We first give evidence that the transition is first order rather than continuous. Since the transition is certainly

4 While this perturbation is related to the previous one by a \(\pi/4\) rotation of the order parameter, higher order terms in \(\phi\) that break the \(U(1)\) symmetry in the ordered phase are not invariant under this rotation.
not strongly first order, we cannot access the very large system sizes $L$ required to see conventional first order signatures such as double-peaked histograms for the energy. Instead we examine the size-dependence of the order parameters at $J_c$. We give evidence that as $L \to \infty$ both order parameters extrapolate to a nonzero value, indicating coexistence between the two phases at $J_c$, i.e., a first order transition.

The two panels in Fig. 9 show the Néel and VBS order parameters, $N_x = \sqrt{\langle N_x^2 \rangle}$ and $\varphi = \sqrt{\langle \varphi^2 \rangle}$, as a function of system size at three values of $J$ close to $J_c$. (Here the quantity in the expectation value is averaged over the system volume.) The continuous lines are fits to the form $a + b/L + c/L^2$ for the $J$ value closest to $J_c$ (shaded areas are 95% confidence intervals for these fits). Extrapolated values at $L = \infty$ are:

$$N_x = 0.1569(20), \quad \varphi = 0.0986(20). \quad (22)$$

Fits to similar forms, including $a + bL^{-c}$, give compatible results, while putting the data on a log-log plot (Appendix A) shows that a power-law fit with $a = 0$ is not good. Note that the numerical values in Eq. 22 are not expected to be the same for both order parameters, as they depend on the arbitrary normalizations of the lattice operators.

**B. Evidence for approximate $O(4)$ symmetry**

If $O(4)$ symmetry emerges it fixes relations between various moments of the order parameters at $J_c$. We will give evidence for approximate symmetry under a subgroup of $O(4)$, which is the $U(1)$ acting on $(N_x, \varphi)$. (The $SO(3)$ acting on $N$ is an exact microscopic symmetry.)

First we examine the ratio between the order parameters, $\varphi/N_x \equiv \sqrt{\langle \varphi^2 \rangle} / \langle N_x^2 \rangle$, in Fig. 10. In the presence of emergent symmetry, this ratio should be $L$-independent at $J_c$ (see e.g. [19, 20]), yielding a crossing of curves for different $L$. Fig. 10 indeed shows a well-defined crossing if the smallest size, $L = 8$, is excluded, despite the fact that the order parameters are individually varying strongly with $L$.

The $J$-values of the crossings between consecutive $L$s are shown in the inset to Fig. 10. A weighted average of these crossings yields the estimate $J_c = 0.0993916(8)$ for the transition point.

Next we examine some moments of the joint probability distribution for $N_x$ and $\varphi$ [19, 20]. Let
\( (N_x, \varphi) = r(\cos \theta, \sin \theta) \), and let \( F_2^a = \langle r^a \cos(\ell \theta) \rangle \). This should vanish for \( \ell > 0 \) in the presence of \( U(1) \) symmetry relating these two order parameter components.

In Figs. 11 and 12 we show
\[
F_2^4 = \langle \tilde{N}_x^4 - \tilde{\varphi}^4 \rangle, \quad F_4^4 = \langle \tilde{N}_x^4 - 6\tilde{N}_x^2\tilde{\varphi}^2 + \tilde{\varphi}^4 \rangle. \tag{23}
\]

Here \( \tilde{N}_x = N_x / \sqrt{\langle N_x^2 \rangle} \) and \( \tilde{\varphi} = \varphi / \sqrt{\langle \varphi^2 \rangle} \) are the order parameters normalized to have unit variance.

In Fig. 11 the quantities \( F_2^4 \) and \( F_4^4 \) are shown as a function of system size for various \( J \) values close to \( J_c \). Strikingly, at \( J = 0.0993915 \) (the value closest to \( J_c \)) \( F_2^4 \) is zero to within errors for system sizes \( 16 \leq L \leq 128 \). \( F_4^4 \) approaches zero quite closely, consistent with approximate \( O(4) \). There appears to be a small but measurable difference from zero over this size range, indicating that \( O(4) \) is not perfect.

\( F_2^4 \) and \( F_4^4 \) are also plotted as a function of \( J \) in Fig. 12. The \( J \) values of the crossings of \( F_2^4 \) with zero, which are shown in the inset of Fig. 12, can be used to obtain a different estimate of the transition point, which is \( J_c = 0.0993911(14) \). This is the estimate in Eq. 21.

The curves for \( F_4^4 \) in the lower panel of Fig. 12 feature a peak at \( J_c \) with a maximum close to zero. This peak gets abruptly narrower with increasing system size. For \( L = 256 \), the width of this peak may lie within the unsampled interval \( 0.099390 < J < 0.099395 \) (we do not have data for \( J = 0.0993915 \) for this size).

### C. Evidence for \( O(4) \)-ordered regime

We now give evidence that at the longest scales we can access the system is in a regime which is described approximately by the \( O(4) \) sigma model in its ordered or Goldstone phase, as discussed in Sec. II.
A first indication of this is that for $L \sim 128$ the order parameter values are to fairly close to their extrapolated $L = \infty$ values (Sec. IV A), while at the same time the moment ratios are close to the $O(4)$ values. This is consistent with being in the $O(4)$-ordered regime. It is not consistent with a standard critical regime (where the order parameters would be scaling to zero with $L$) and it is not consistent with a standard first order regime (where there would be no $O(4)$ symmetry).

For a concrete check, we compare the probability distribution of a component of the order parameter with that expected for the sigma model in the ordered phase. Deep in the ordered phase, the 4-component order parameter can be treated as spatially constant, and has a uniform probability distribution on the sphere

$$|\mathbf{n}|^2 = R^2. \quad (24)$$

Integrating out 3 components gives the probability distribution for a single component, which is a semicircle:

$$P(n_1) = \frac{2}{\pi R^2} \sqrt{R^2 - n_1^2}. \quad (25)$$

This semicircle distribution is a hallmark of $O(4)$ order.

First, the probability distribution for $N_x$ is shown in Fig. 13 for several system sizes. We fit each curve to Eq. 25, with $R$ as the only parameter (continuous lines). The extrapolated $L = \infty$ value of the order parameter in Eq. 22 would correspond to the the height of the peak of the curve in Fig. 13 being $\sim 2.0$.

In Fig. 14 we show the probability distributions for the normalized order parameter components, $\tilde{N}_x$ and $\tilde{\phi}$ with variance 1. We see that the shape of the probability distribution changes more weakly than the overall width. The expected semicircle form is shown as a black line (without any fitting parameter, since the variance is now fixed). Error bars are smaller for $N_x$ than for $\varphi$.

While deviations from the semicircle are apparent for the smaller sizes, the distributions for $L = 64$ and $L = 128$ match extremely well to the semicircle. The amount of weight in the tails $|\tilde{N}_x| > 2$ is clearly decreasing as $L$ is increased, as expected from the semicircle form which has a bounded support.

Finally, for a more quantitative analysis, we compare cumulants of the order parameters with the values expected from the symmetric $O(4)$ sigma model in its ordered phase. Consider the cumulants (recall that $N_x$ is
normalized to have unit variance)

\[ C_4 = \left\langle \tilde{N}_x^4 \right\rangle - 3 \left\langle \tilde{N}_x^2 \right\rangle^2, \quad \text{(26)} \]

\[ C_6 = \left\langle \tilde{N}_x^6 \right\rangle - 15 \left\langle \tilde{N}_x^4 \right\rangle \left\langle \tilde{N}_x^2 \right\rangle + 30 \left\langle \tilde{N}_x^2 \right\rangle^3, \quad \text{(27)} \]

and similarly for \( \tilde{\varphi} \). In the \( O(4) \) ordered regime, we expect from Eq. 25:

\[ C_4 = -1, \quad C_6 = 5, \quad \text{(28)} \]

for both \( N_x \) and \( \varphi \). These values are very different from those that would be obtained for a Gaussian distribution (zero) or at a conventional first order transition.\(^5\)

In Fig. 15 we show these cumulants at \( J = J_c \) as a function of the inverse of the system size, for both order parameters. Both \( C_4 \) and \( C_6 \) are relatively close to the values expected from the ordered sigma model even for the smaller sizes, and for the larger sizes they are very close. This suggests that the system at \( J_c \) is well described by the ordered phase of the symmetric sigma model for \( L \sim 128 \) and even \( L \sim 64 \), despite the fact that the ordered moment at \( L = 64 \) is still quite far from its extrapolated value (Fig. 9).

\section{OUTLOOK}

We have exhibited a phase transition with emergent \( O(4) \) symmetry and a regime where the \( O(4) \) vector is effectively ordered. This symmetry is only expected to be approximate, and therefore the description using the long-range ordered \( O(4) \) sigma model is also only approximate even in the relevant range of length scales. However, the usefulness of this concept in organizing our understanding of this phase transition is clear. We have shown that it allows us to predict various ‘quasiuniversal’ features with good accuracy. As a zeroth order description for length scales of order, say, 100, the ‘\( O(4) \) spin flip’ description is clearly far more useful than standard expectations for first order transitions, which are strongly violated because of the effective continuous symmetry relating the two phases at coexistence.

The description of the data using the sigma model description could be further improved by considering Goldstone fluctuation corrections, as well as the leading weak anisotropies in the Lagrangian. Many other quantities, such as two-point functions or off-critical scaling forms, could also be understood with this approach.

The phenomenon we have argued for in the present model is likely to be more general [22]. Examples may exist with a range of emergent symmetry groups \( G \), and for a given \( G \), there will be many different possibilities for the (smaller) microscopic symmetry group.

The present \( O(4) \) regime may also appear in several other contexts. From the renormalization group picture one would naively expect that at large scales the ‘easy-plane’ Néel-VBS transition [11, 15–17, 31, 32] behaves similarly to the model discussed here [22, 23, 33]. (The easy plane transition involves competition between a two-component Néel order parameter and a two-component VBS order parameter.) However, recent work has argued that this transition can be continuous rather than first order [16, 17]. This should be understood better. The classical 3D dimer model, with appropriate anisotropy, is another platform that could be used to study the physics of the easy-plane NCCP\(^5\) model [20, 29].

The regime demonstrated here should also be looked for in two-flavour QED\(_3\), and is an alternative possibility to flow to a scale-invariant fixed point argued for previously on numerical grounds [54]. (The effect of \( O(4) \)-breaking perturbations within the \( O(4) \)-ordered phase is expected to be much weaker in that context [22].)

A long-range-ordered \( SO(5) \) regime may occur for deconfined criticality with 5 components, for example \( SU(2) \)-symmetric magnets at the Néel-VBS transition on

\(^5\) At a conventional first order transition between Néel and VBS there is a probability \( p(J, L) \) for the system to be in the VBS phase and \( 1 - p(J, L) \) to be in the Néel phase, with \( p \) determined by the free energy difference between the two phases in the finite system (here \( L \) is large). Using the values in the Néel phase (from averaging over the sphere) and the VBS phase (\( \varphi^2 \) ~ const.) gives, for a component of \( N \), \( C_{4(N)}^N = (3/5)(5p - 2)/(1 - p) \) and \( C_{6(N)}^N = (3/7)(16 - 77p + 70p^2)/(1 - p)^2 \), and for \( \varphi \), \( C_{4(\varphi)}^\varphi = (1 - 3p)/p \) and \( C_{6(\varphi)}^\varphi = (30p^2 - 15p + 1)/p^2 \). Strictly at \( J_c \), the free energy densities of the two phases are equal, but in a finite system with periodic boundary conditions the Néel phase has an \( O(\ln L) \) entropy associated with continuous symmetry breaking. As a result \( p \gg e \) as a power law at large \( L \). In this limit \( C_{4(N)}^N = -6/5 \), \( C_{6(N)}^N = 48/7 \), and \( C_{4(\varphi)}^\varphi \) and \( C_{6(\varphi)}^\varphi \) both diverge.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig15.png}
\caption{Cumulants \( C_4 \) and \( C_6 \) at \( J = 0.0993915 \) as function of the inverse of the system size, \( 1/L \). Dashed lines are the expected values for the \( O(4) \)-symmetric ordered sigma model, \( C_4 = -1 \) and \( C_6 = 5 \).}
\end{figure}

\[ C_4 = \left\langle \tilde{N}_x^4 \right\rangle - 3 \left\langle \tilde{N}_x^2 \right\rangle^2, \quad \text{(26)} \]

\[ C_6 = \left\langle \tilde{N}_x^6 \right\rangle - 15 \left\langle \tilde{N}_x^4 \right\rangle \left\langle \tilde{N}_x^2 \right\rangle + 30 \left\langle \tilde{N}_x^2 \right\rangle^3, \quad \text{(27)} \]
the square lattice [22]. Existing data sees features that seem compatible with a pseudocritical regime, for example drifting exponents that at large size tend to values that are incompatible with the exponents of a conformal fixed point [18, 26, 52, 53], at least if conventional finite-size scaling is assumed. However if the flow is eventually to the long-range-ordered state, the lengthscale needed to see this regime is very large and appears to be beyond the reach of current simulations [18]. Indeed on the presently accessible length scales the $SO(5)$ symmetry in various models resembles an exact symmetry of the infrared theory [19, 20].

In the future it will be useful to quantify more precisely the the accuracy of the emergent approximate $O(4)$ symmetry in the model studied here as a function of $L$. A more careful comparison with expectations from the ordered sigma model, taking finite size effects into account, as well as the effects of finite $J - J_c$, would also be enlightening. Simulations at larger $L$ might be able to probe the eventual flow away from the symmetric sigma model.

Finally, here we have focussed only on the critical point at $J_A = J_c$, $J_B = 0$. It will also be important to investigate the transition both in the presumably more strongly first-order regime at negative $J_B$ and in the presumably more weakly first-order regime at larger $J_B$. In Sec. II we noted an alternative scenario in which approximate $O(4)$ arises because the model is by accident fine-tuned close to an unstable $O(4)$–invariant tricritical point. We have argued this is unlikely as it would require fine-tuning (and an appropriate such fixed point may not exist). This could be checked directly by checking that the $O(4)$ ordered regime is robust against small changes of the microscopic parameters.

**Related Work:** After completion of this work we became aware of a numerical study of a deformed $JQ$ model by Zhao et al. [58]. That model also has a transition with 4 order parameter components, and the authors also find a first order transition with emergent $O(4)$ symmetry, as here.

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The deformation of the loop model studied here was suggested to one of us (PS) by Anders Sandvik and Ribhu Kaul, before the advent of emergent symmetries, as a way to interpolate between the DCP in the symmetric model and a strongly first order transition. We thank them for discussions. We thank G. J. Sreejith and S. Powell for discussions and collaboration on recent related work, and J. Chalker for discussions. AN acknowledges EPSRC Grant No. EP/N028678/1.

**Appendix A: Comparison of two VBS components**

In Fig. 16 we show the two components of the VBS order parameter in Eq. 17, $\phi_x$ and $\phi_y$, both as a function of $L$ at $J_c$, and as a function of $J$ for $L = 8$. The figure shows that at the transition $\phi_y$ is a massive field with a short correlation length, and that there is a strong asymmetry between $\phi_x$ and $\phi_y$ even at short scales. This confirms that the coupling values we have chosen (i.e. $J_B = 0$) are sufficiently far from the symmetric critical point with $J_A = J_B$. The symmetric critical point has very accurate $SO(5)$ symmetry. If we studied a weakly asymmetric model (i.e. $J_A - J_B$ too small) then there would be an intermediate range of scales with approximate $SO(5)$, and we would see $O(4)$ as a trivial consequence of this. It is clear from Fig. 16 that this is not the explanation for the $O(4)$ that we see.

**FIG. 16.** Main panel: we show the two components of $\phi$ (see Sec. III) as a function of system size at $J = 0.0993915$ (close to $J_c$). Note the log-log scale. The definition is $\phi_i = \sqrt{\langle \phi_i^2 \rangle}$, where the observable inside the expectation value is averaged over the full system volume. First, observe that for our choice of couplings (Eq. 19) there is a very strong asymmetry between $\varphi = \phi_x$ and $\phi_y$ even at small scales. The magnitude of $\phi_y$ decreases as $L^{-3/2}$ (dashed line), as expected for a massive field. This shows that the $O(4)$ symmetry we find is not just a consequence of proximity to the $SO(5)$ invariant critical (or pseudocritical) point in the symmetric model with $J_A = J_B$.

Second, note that the log-log plot for $\varphi = \phi_x$ (red line) is not straight, showing that the power law scaling that would be expected at a critical point does not apply here. Instead, $\varphi$ extrapolates to a finite value as $L \rightarrow \infty$ (Sec. IV.A). Inset: we show the two components of $\phi$ as a function of $J$ in a small system ($L = 8$). Again the strong asymmetry between $\varphi = \phi_x$, which orders at the transition, and $\phi_y$, which remains massive, is apparent.
In the presence of an appropriate dangerously irrelevant variable, the assumption of finite size scaling can be invalid \cite{14, 18}. 

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\footnote{In the presence of an appropriate dangerously irrelevant variable, the assumption of finite size scaling can be invalid \cite{14, 18}.}
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