**Rapid Communications**

# Theory of deconfined pseudocriticality

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(Received 24 March 2020; revised 30 June 2020; accepted 1 July 2020; published 21 July 2020)

It has been proposed that the deconfined criticality in $(2+1)d$—the quantum phase transition between a Néel antiferromagnet and a valence-bond solid (VBS)—may actually be pseudocritical, in the sense that it is a weakly first-order transition with a generically long correlation length. The underlying field theory of the transition would be a slightly complex (nonunitary) fixed point as a result of fixed points annihilation. This proposal was motivated by existing numerical results from large scale Monte Carlo simulations as well as a conformal bootstrap. However, an actual theory of such a complex fixed point, incorporating key features of the transition such as the emergent SO(5) symmetry, is so far absent. Here we propose a Wess-Zumino-Witten (WZW) nonlinear sigma model with level $k=1$, defined in $2+\epsilon$ dimensions, with target space $S^{3+\epsilon}$ and global symmetry $SO(4+\epsilon)$. This gives a formal interpolation between the deconfined criticality at $d=3$ and the $SU(2)_1$ WZW theory at $d=2$ describing the spin-1/2 Heisenberg chain. The theory can be formally controlled, at least to leading order, in terms of the inverse of the WZW level $1/k$. We show that at leading order there is a fixed point annihilation at $d^* \approx 2.77$, with complex fixed points above this dimension including the physical $d=3$ case. The pseudocritical properties such as correlation length, scaling dimensions, and the drifts of scaling dimensions as the system size increases, calculated crudely to leading order, are qualitatively consistent with existing numerics.

DOI: 10.1103/PhysRevB.102.020407

Going beyond the Landau paradigm has been a modern theme in the study of phase transitions. In the context of quantum magnetism, the prime example is the so-called deconfined quantum critical point (DQCP)—a direct continuous transition between a Néel antiferromagnet and a valence-bond-solid (VBS) state on a square lattice [1,2]. These two states break very different symmetries (spin rotation for Néel and lattice rotation for VBS) so a direct, continuous transition is forbidden in Landau theory without further fine tuning. For $SU(N)$ spin systems with sufficiently large $N$, the existence of such a non-Landau continuous transition has been firmly established both theoretically [1,2] and numerically [3], so there is no question on whether such a non-Landau transition can exist. However for SU(2) spins—the most interesting case for condensed matter physicists—the situation has been murky since the early days.

The continuum field theory describing the DQCP, known as the (noncompact) $CP^1$ theory, is a strongly coupled gauge theory with little theoretical control. Therefore, large scale numerical simulations are needed to determine whether the transition is truly continuous. Many such Monte Carlo simulations have been carried out in the past decade, on different lattice realizations of the DQCP [4–23], with linear system size $L$ measured in units of lattice spacing as large as 125–256 (quantum spin model [8,12]) or 640 (classical loop model [13]). Standard signatures of first-order transition (such as double-peaked probability distributions) have not been seen at the transitions in these simulations. Rather the correlation length appears to exceed the (already quite large) system size at the transition. The critical exponents extracted from finite-size scaling behaviors are roughly consistent across different simulations. However, the transition does not behave like a conventional continuous transition either: the critical exponents show significant dependence on system size up to the largest size simulated. Specifically, the two exponents $\nu$ and $\eta$ drift systematically to smaller values as the system size grows. Even worse, the correlation length exponent $\nu$ extracted from the largest system size ($\sim$0.44 from Refs. [12,13]) is smaller than the lower bound on $\nu$ ($\sim$0.511) for a continuous transition with a single tuning parameter, found using a numerical conformal bootstrap [24,25].

Another confusing issue is the emergent SO(5) symmetry at the DQCP. At the Néel-VBS critical point, an emergent SO(5) symmetry, rotating among the three components of Néel vector $\mathbf{n}$ and the real and imaginary parts of the VBS order parameter $\Phi$, was observed numerically [14]. This SO(5) symmetry, absent in both the lattice models and the continuum gauge theories (such as $CP^1$), was later rationalized using dualities between different gauge theories [26,27] (with hints from earlier works on nonlinear sigma models [28,29]). However, assuming such an SO(5) symmetry at a true critical point without further fine tuning, the scaling dimension of the SO(5) vector (in this case the Néel and VBS order parameters) is required by the conformal bootstrap [25] to be greater than 0.76. Numerically this scaling dimension was found to be $\sim$0.62 on the largest systems, significantly smaller than the bootstrap bound.

To resolve these discrepancies, it was proposed [13,26] that the DQCP for SU(2) spins may actually be "pseudocritical." Essentially, one postulates that there is a coupling constant $\lambda$, with a flow equation under renormalization group (RG) around $\lambda = 0$ given by (up to some redefinition)

$$\frac{d\lambda}{dl} = \varepsilon + \lambda^2 + \cdots, \tag{1}$$

where $\cdots$ are terms higher order in $\lambda$ and $\varepsilon$ is a small constant that is not flowing under RG. For $\varepsilon < 0$, there are two fixed points: an attractive one at $\lambda_- = -\sqrt{|\varepsilon|}$, and a repulsive one at $\lambda_+ = +\sqrt{|\varepsilon|}$. As $\varepsilon$ changes gradually from negative to positive, the two fixed points collide and annihilate with each other, and there is no real fixed point left. The pseudocritical scenario corresponds to a slightly positive $\varepsilon$ (ideally $0 < \varepsilon \ll 1$). Some simple observations immediately follow:

(1) Assuming $\lambda$ flows from $\ll -\sqrt{\varepsilon}$ to $\gg +\sqrt{\varepsilon}$. The correlation length, defined as exponential of the "RG time" $l$ spent along the flow, is given by

$$\xi = \xi_0 \exp\left(\frac{\pi}{\sqrt{\varepsilon}}\right), \tag{2}$$

where $\xi_0$ is a nonuniversal constant $\sim O(1)$ depending on the UV value of $\lambda$. This can be quite large even for mildly small values of $\varepsilon$. This is sometimes also called a "walking" coupling constant.

(2) Most of the RG time is spent around $-\sqrt{\varepsilon} \lessapprox \lambda \lessapprox \sqrt{\varepsilon}$. So for small $\varepsilon$ the point $\lambda = 0$ can be approximately viewed as a "fixed point" for system size $L \ll \xi$. One can then define notions of scaling dimensions and "relevant/irrelevant" perturbations around this pseudocritical point. In particular, the aforementioned SO(5) symmetry emerges (up to the correlation length $\xi$) if the microscopic symmetry-breaking terms are irrelevant around this fixed point $\lambda \approx 0$.

(3) Even though the $\lambda \approx 0$ region behaves almost like a fixed point for $L \ll \xi$, the parameter $\lambda$ is nevertheless slowly flowing. This implies that the scaling dimensions, generically as functions of $\lambda$, will be slowly drifting as the system size increases.

(4) The flow equation (1) does have two complex fixed points at $\lambda_\pm = \pm i\sqrt{\varepsilon}$. The pseudocritical behavior near $\lambda = 0$ on the real axis can be viewed as ultimately controlled by the complex fixed points (even though the fixed points themselves are unreachable due to unitarity of the underlying quantum mechanical system).

The above features of the pseudocriticality scenario could potentially resolve the existing issues in numerics. However an actual theory of the DQCP that naturally incorporates features like pseudocriticality and the emergent SO(5) symmetry, is currently absent—although a tentative theory for pseudocriticality in $CP^{N-1}$ models has been qualitatively discussed in Ref. [13]. The goal of this work is to develop such a theory, and to gain a clearer picture of the origin and contents of Eq. (1) in the DQCP. Such theories of pseudocriticality have been developed for certain $(3+1)d$ gauge theories [30–32] and $(1+1)d$ $q$-state Potts models with $q > 4$ [33–38].

We adopt the sigma-model approach to the DQCP. It is known that the DQCP has a "caricature" representation in terms of a nonlinear sigma model [28,29]

$$S = \int d^3x \frac{1}{4\pi g}(\nabla\widehat{N})^2 + k\Gamma^{\mathrm{WZW}}[\widehat{N}], \tag{3}$$

where $\widehat{N} = [n_1, n_2, n_3, \mathrm{Re}(\Phi), \mathrm{Im}(\Phi)] \in S^4$ represents the combined Néel-VBS order, $g$ is the coupling strength, and $\Gamma^{\mathrm{WZW}}$ is the standard Wess-Zumino-Witten (WZW) term [well defined since $\pi_{3+1}(S^4) = \mathbb{Z}$] with a quantized coefficient $k$, and in the case of the DQCP $k = 1$. The physical significance of $\Gamma^{\mathrm{WZW}}$ is that a vortex of the complex operator $\Phi$ traps a spin-1/2 moment, manifested as an effective $(0+1)d$ WZW term for $(n_1, n_2, n_3)$—this is exactly the feature expected for the DQCP from the lattice scale [39].

However, Eq. (3) is only a caricature because, as a continuum field theory, its dynamics is only well defined in the weak-coupling regime, where the SO(5) symmetry is spontaneously broken and $\langle\widehat{N}\rangle \neq 0$. Turning on a Néel-VBS anisotropy $n_1^2 + n_2^2 + n_3^2 - |\Phi|^2$ will induce a Néel-VBS transition, but a strongly first-order one. Realizing the DQCP, even in the pseudocriticality scenario, requires accessing some strong-coupling regime which is not well defined on its own.

It is instructive to look at what happened in a much better understood case: the WZW sigma model at $k = 1$ in $(1+1)d$, with target space $S^3$ [so the order parameter is an SO(4) vector]. The Lagrangian takes the same form as Eq. (3) except every term lives in one dimension lower and $\widehat{N} \in S^3$. This theory is asymptotically free, so the free Gaussian fixed point is unstable in IR (as required also by Hohenberg-Mermin-Wagner). The coupling strength will always flow to a critical value $g_c$ which is nothing but the famous $\mathrm{SU}(2)_1$ CFT [recall that $\mathrm{SU}(2) \sim S^3$] [40]. This is also the theory describing the critical spin-1/2 Heisenberg-Bethe chain [41], and can be viewed as the close relative of the DQCP in $(1+1)d$.

We now propose a theory of the WZW nonlinear sigma model, formally defined in space-time dimension $d = 2 + \epsilon$, with target space $S^{3+\epsilon}$ [so the symmetry is $\mathrm{SO}(4+\epsilon)$]. We do not attempt to explicitly write down the corresponding action (especially the WZW term) since we do not know how to precisely define the winding number of $S^{3+\epsilon}$ on another $S^{3+\epsilon}$. We simply postulate the existence of such theory as some kind of analytic continuation of WZW theories in general (positive integer) $d$ space-time dimensions with target space $S^{d+1}$—actions like Eq. (3) are always well defined for these theories since $\pi_{d+1}(S^{d+1}) = \mathbb{Z}$.

Let us first ask what are the possible scenarios based on qualitative considerations. We expect the RG flow of $g$ to look like Fig. 1. At $\epsilon = 0$ there is a stable fixed point at $g = g_c$ and an unstable Gaussian fixed point at $g = 0$. At small positive $\epsilon$, the attractive fixed point will continue in some fashion from $g_c$, but the Gaussian fixed point turns from unstable to stable because Hohenberg-Mermin-Wagner no longer applies in dimension higher than two. Therefore, another repulsive fixed point must emerge between the Gaussian ($g = 0$) and the attractive one (around $g_c$). As $\epsilon$ increases, both the repulsive and attractive fixed points will continue in some fashion, but we expect them to collide and annihilate each other at some critical $\epsilon^*$—otherwise this would lead to interacting, nonsupersymmetric CFTs in arbitrarily high dimensions, which is hard to imagine. As for the physical case of $\epsilon = 1$, there are three possible scenarios: (a) $1 < \epsilon^*$, and the attractive fixed point describes the truly continuous DQCP, (b) $\epsilon^*$ significantly below 1, and the transition is strongly first order, and (c) $\epsilon^*$ slightly below 1, and the system shows pseudocritical behavior before eventually crossing over to first-order transition at large system size. Based on existing numerical results, we expect scenario (c)

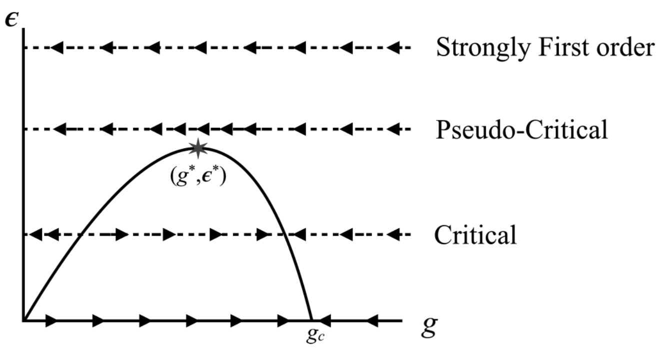


FIG. 1. Schematic RG flow of the coupling strength $g$ of the WZW sigma model in $2+\epsilon$ space-time dimensions with target manifold $S^{3+\epsilon}$, at different values of $\epsilon$. Depending on whether the physical dimension of the DQCP ($\epsilon = 1$) is below, well above, or slightly above $\epsilon^*$, the system will show critical, strongly first order, or pseudocritical behavior, respectively.

to be the physical one, and the small constant in Eq. (1) is $\varepsilon \propto (1-\epsilon^*)$.

Let us now try to be slightly more quantitative. The WZW sigma model can be perturbatively controlled if the WZW level $k$ is large. In this case $g_c(\epsilon = 0) \sim 1/k$, and we will see that we also have $g^* \sim \epsilon^* \sim 1/k$. Of course $k = 1$ for the physical case, so an expansion in $1/k$ (especially to low order) may not be trusted quantitatively. Nevertheless, just like usual small $\epsilon$ or large $N$ expansions, such a calculation can offer valuable insights, especially when combined with other approaches such as lattice simulations. We note that another scheme for a perturbatively controlled study of a nonlinear sigma model with a WZW term in $(2+1)d$ was proposed in Ref. [42].

The next question is how to compute the perturbative RG equation in $2+\epsilon$ dimensions with a WZW term for $S^{3+\epsilon}$—after all we do not even have a Lagrangian for such theories. However we do not need to have a Lagrangian—all we need to do is to analytically continue the perturbative RG flow equations in integer dimensions $d$ with target manifold $S^{d+1}$. The flow equations for integer $d \geqslant 2$ take the form

$$\begin{aligned} \frac{dg}{dl} &= -\epsilon g + 2g^2 - F(d)k^2 g^{2+d} + \cdots, \\ \frac{dk}{dl} &= 0, \end{aligned} \tag{4}$$

where the second equation simply comes from level quantization of the WZW term, the $2g^2$ term in the first equation is a standard result for a nonlinear sigma model, the $k^2 g^{2+d}$ term is the leading order contribution from WZW term (see the Supplemental Material [43] for more details), and $F(d)$ is some function of $d$. It is known [40] that $F(2) = 2$. We assume that the continuation of the second equation to fractional $\epsilon$ is trivially $dk/dl = 0$, namely we assume that the WZW level is quantized even for fractional $\epsilon$ [something like $\pi_{3+\epsilon}(S^{3+\epsilon}) = \mathbb{Z}$]. Now assuming an analytic continuation of $F(d)$ exists, then for $d = 2+\epsilon$ with $g \sim \epsilon \sim 1/k$, the leading order flow equation simply becomes

$$\frac{dg}{dl} = -\epsilon g + 2g^2 - 2k^2 g^4 + \cdots. \tag{5}$$

In particular, we only need the zeroth order value of the $F(2+\epsilon)$ term—the calculation would otherwise be much more complicated.

The fixed points from Eq. (5) are given by

$$\frac{\epsilon}{2} = g - k^2 g^3, \tag{6}$$

which indeed behave as Fig. 1. The critical dimension and coupling strength are given to leading order in $1/k$ by

$$\begin{aligned} \epsilon^* &= \frac{4}{3\sqrt{3}k} \approx \frac{0.77}{k}, \\ g^* &= \frac{1}{\sqrt{3}k}. \end{aligned} \tag{7}$$

Now consider the theory just above the critical dimension $\epsilon = (1+\alpha)\epsilon^*$ with $0 < \alpha \ll 1$. Equation (5) then reduces to Eq. (1) to leading order in $\alpha$, with $\lambda = 2(g - g^*)$. The correlation length is now (again to leading order in both $1/k$ and $\alpha$)

$$\xi = \xi_0 \exp\left(\frac{\pi}{\sqrt{2\alpha\epsilon^* g^*}}\right) = \xi_0 \exp\left(\frac{3\pi k}{\sqrt{8\alpha}}\right). \tag{8}$$

Putting $k = 1$ into the above results, we get $\epsilon^* \approx 0.77$. The physical case of $\epsilon = 1$ corresponds to $\alpha \approx 0.3$, which then gives the estimated correlation length $\xi \approx 440\xi_0$. These are indeed consistent with pseudocriticality! This is also qualitatively consistent with existing numerics, in the sense that it can be easily larger (but not too much larger) than the simulated system size.

We can also estimate critical exponents at the deconfined pseudocritical point to leading order. The scaling dimensions of rank-$l$ (symmetric traceless) tensors of the SO$(4+\epsilon)$ group are given by

$$\Delta_l = \frac{l(l+2)}{2} g^* = \frac{l(l+2)}{2\sqrt{3}k}, \tag{9}$$

where the first identity comes from standard nonlinear sigma model calculations without the WZW term—the WZW only affects the result through $g^*$ (Table I) (see the Supplemental Material [43]). At $k = 1$ this gives $\Delta[l = 1] \approx 0.87$ and $\Delta[l = 2] \approx 2.3$. For $l = 1$ (Néel/VBS order parameter) the numerical simulations give $\Delta[l = 1]_{\text{Num}} = (1+\eta)/2 \approx 0.62 \pm 0.1$, while for $l = 2$ (Néel-VBS anisotropy) the numerical value is roughly $\Delta[l = 2]_{\text{Num}} = 3 - 1/\nu \approx 1.0 \pm 0.3$. The error bar comes from sampling different works, on difference system sizes, with different schemes used to extract the exponents. Our estimated value (in $1/k$) for the vector order parameter is in qualitative agreement with the numerical values. In fact, the estimation is far better than a similar $O(1/k)$ estimation in two dimensions (2D), where the

TABLE I. Comparison of scaling dimensions of rank-$l$ tensors $\Delta[l]$ obtained by leading order perturbative calculations with numerical results $\Delta[l]_{\text{Num}}$.

| | $l = 1$ | $l = 2$ |
|---|---|---|
| $\Delta[l]$ | 0.87 | 2.3 |
| $\Delta[l]_{\text{Num}}$ | $0.62 \pm 0.1$ | $1.0 \pm 0.3$ |

exact result is known to be $\Delta[l=1]_{2D} = 3/2(k+2) = 1/2$ while the $O(1/k)$ estimation gives 3/2. In some sense this means that theories at $\epsilon > 0$ are less strongly coupled than the 2D $SU(2)_1$ theory so perturbative calculations become more reliable. Our estimation for the rank-2 tensor is less impressive—this is perhaps not too surprising since a similar estimation in 2D gives even larger error than the vector case. Furthermore, an estimation of rank-4 tensor shows that it is strongly irrelevant—this is crucial for the emergence of SO(5) at the DQCP since, in the context of DQCP, rank-4 tensors are allowed by microscopic symmetries as perturbations [1,2].

Equation (9) also implies that the scaling dimensions will drift downward as the system size grows, since $g$ flows slowly to smaller and smaller values. This feature is also in agreement with numerical results. We can estimate the amount of drift at $O(1/k, \alpha)$. Assuming at system size $L_0$ the coupling constant reaches $g^*$, then for $L$ not too far away from $L_0$ [specifically $|\ln(L/L_0)| \ll \ln(\xi/\xi_0)$], the relative drift in $\Delta_l$ is roughly (see the Supplemental Material for more details [43])

$$\frac{\Delta_l(L) - \Delta_l(L_0)}{\Delta_l(L_0)} \approx -0.23 \ln(L/L_0), \qquad (10)$$

which appears to be qualitatively consistent with the numerically observed drifts for the correlation length exponent $\nu$ [12,13].

We can also consider the $k = 2$ case. Repeat the analysis above one obtains $\xi(k=2) \sim 190\xi_0$, which means a weaker but potentially observable pseudocritical behavior—the actual number is less reliable since $\epsilon^*(k=2) \sim 0.38$ is further away from the physical dimension, and therefore the small $\alpha$ expansion is not justified. Note that since we expect operator scaling dimensions to reduce as $k$ becomes larger, the $k = 2$ theory may have additional relevant operators such as the rank-4 tensors. The $k = 2$ theory may potentially describe the Néel-columnar VBS transition of spin-1 antiferromagnets on a square lattice [44]. However, further fine tuning will be required, which makes the theory multicritical, if the rank-4 tensors are relevant—this is consistent with recent numerics on spin-1 systems on a square lattice [45] in which a strong first-order transition was observed.

In summary, we have proposed a WZW nonlinear sigma model in a $(2+\epsilon)$ space-time dimension, with target space $S^{3+\epsilon}$ and global symmetry $SO(4+\epsilon)$, as an interpolation between the $SU(2)_1$ WZW CFT in 2D and the DQCP in 3D. We argued on general ground that a fixed-point annihilation should happen at some finite $\epsilon^*$, above which there is no real fixed point. We then argued, based on a crude $O(1/k)$ estimation and its consistency with existing numerics, that $\epsilon^*$ is slightly smaller than the physical value $\epsilon = 1$ for the DQCP. Therefore the DQCP shows pseudocritical behavior before eventually crossing over to a first-order transition as the system size exceeds the large correlation length. The pseudocritical properties, calculated crudely in $O(1/k)$, are in qualitative agreement with existing numerics. We emphasize that, just like many other calculations in critical phenomena like $O(\epsilon)$ or $O(1/N)$, our $O(1/k)$ calculation is by no means a proof of pseudocriticality in the DQCP since in reality $k = 1$. Rather it gives a scenario, or a picture, that potentially describes the correct physics and is broadly consistent with existing numerics.

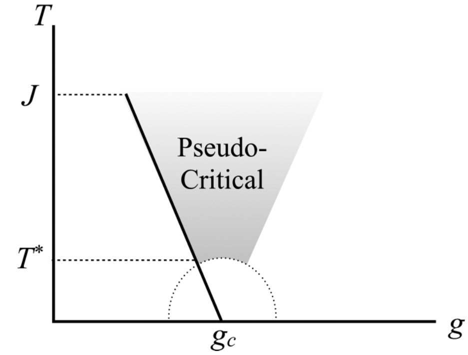


FIG. 2. Schematic phase diagram of pseudocriticality at finite temperature. The classic critical fan appears as long as the temperature is well below the microscopic energy scale $J$ and well above a very low crossover temperature $T^* \sim J\exp(-\pi/\sqrt{\varepsilon})$. Below $T^*$ the system crosses over to a conventional first-order transition.

There are many possible future directions following our work. The most obvious one is to try to give the $S^{3+\epsilon}$ WZW theory an intrinsic definition, instead of simply assuming that a reasonable analytic continuation from integer dimensions exists (as we did here). More practically, how do we compute the perturbative RG flow equation beyond leading order? Another open problem is to extend the pseudocritical theory to the easy-plane DQCP (which received stronger numerical support of the pseudocritical scenario recently [46,47]). Yet another question is how one could further generalize such theories, for example to other types of target space beyond spheres. Specifically, can we find another type of target space that pushes $\epsilon^*$ well above 1, so that a true critical point of this type appears in $(2+1)d$? Can we even push it far enough to have a nontrivial fixed point in $(3+1)d$? These are all open questions to be explored in the future.

We end by emphasizing that pseudocriticality is particularly interesting for quantum phase transitions: at finite temperature, the classic "critical fan" appears as long as the temperature is well below the microscopic energy scale $J$ and well above a very low crossover temperature $T^* \sim J\exp(-\pi/\sqrt{\varepsilon})$. Below $T^*$ the system crosses over to a conventional first-order transition. The schematic phase diagrams is shown in Fig. 2.

*Note added.* During the completion of this manuscript, we became aware of an independent work [48] by Adam Nahum which overlaps significantly with ours.

We thank Bert Halperin, Yin-Chen He, Adam Nahum, Djordje Radicevic, T. Senthil, Ashvin Vishwanath, and Cenke Xu for helpful discussions and comments. We thank Adam Nahum for sharing results prior to publication. Research at Perimeter Institute is supported in part by the Government of Canada through the Department of Innovation, Science and Economic Development Canada and by the Province of Ontario through the Ministry of Colleges and Universities.

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