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Emergent SO(5) Symmetry at the Néel to Valence-Bond-Solid Transition

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We show numerically that the “deconfined” quantum critical point between the Néel antiferromagnet and the columnar valence-bond solid, for a square lattice of spin 1/2, has an emergent SO(5) symmetry. This symmetry allows the Néel vector and the valence-bond solid order parameter to be rotated into each other. It is a remarkable (2 + 1)-dimensional analogue of the SO(4) = [SU(2) × SU(2)]/Z₂ symmetry that appears in the scaling limit for the spin-1/2 Heisenberg chain. The emergent SO(5) symmetry is strong evidence that the phase transition in the (2 + 1)-dimensional system is truly continuous, despite the violations of finite-size scaling observed previously in this problem. It also implies surprising relations between correlation functions at the transition. The symmetry enhancement is expected to apply generally to the critical two-component Abelian Higgs model (noncompact CP¹ model). The result indicates that in three dimensions there is an SO(5)-symmetric conformal field theory that has no relevant singlet operators, so is radically different from conventional Wilson-Fisher-type conformal field theories.

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Many condensed matter systems show higher symmetry in the infrared than they do in the ultraviolet. The liquid-gas critical point is a classical example: although there is no microscopic Z₂ symmetry exchanging liquidlike and gaslike configurations, the fixed point has an emergent Z₂ symmetry and is simply the Ising fixed point. Microscopically, this fixed point is perturbed by operators that break the Z₂ symmetry, but it nevertheless governs the critical behavior because these perturbations are irrelevant under the renormalization group.

To reach this critical point two variables, say temperature and pressure, must be tuned. The spin-1/2 Heisenberg chain provides an example of emergent symmetry without such fine-tuning in a quantum setting. The ground state of this model is well known to be critical. Its microscopic symmetries are SU(2) spin rotations, together with spatial symmetries. However the scaling limit of the spin-1/2 chain is the SU(2)₁ Wess-Zumino-Witten conformal field theory [1], and this has an SO(4) = [SU(2) × SU(2)]/Z₂ symmetry that is much larger than the global symmetry present microscopically.

Physically, this arises as follows [2]. The Néel vector \vec{N} has three components. There is also a spin-Peierls parameter φ that distinguishes between the two different patterns of dimer (singlet) order and which changes sign under appropriate reflections or translations. We may form the four-component superspin $\vec{\Phi} = (\vec{N}, \varphi)$, and the emergent SO(4) corresponds to rotations of this vector. Although the dimer and Néel order parameters are utterly inequivalent microscopically, a symmetry between them arises in the infrared. Technically, this again relies on the

SO(4)-breaking perturbations of the conformal field theory (CFT) being irrelevant or marginally irrelevant.

Naively, one might expect this phenomenon to be special to one spatial dimension, where the enlarged symmetry is related to special properties of 2D conformal invariance (the doubling of conserved currents [1]). We show here however that an analogous symmetry enhancement occurs for the spin-1/2 magnet on the square lattice, at the celebrated “deconfined” quantum critical point [3–5]. This is a transition between the antiferromagnetically ordered Néel state and a columnar valence-bond solid (VBS), and is reached by tuning a single parameter. For example, the nearest-neighbor Heisenberg model can be driven into the VBS using either a four-spin interaction [6] or a next-nearest-neighbor exchange [7,8]. The emergent symmetry we put forward is an SO(5) symmetry that mixes the components of the Néel vector \vec{N} , which has three components, and the VBS order parameter $\vec{\varphi}$, which has two. We test it by examining the joint probability distribution for these quantities.

Numerically, the critical behavior can be studied efficiently with a 3D classical loop model [9], and we use this approach here. The order of the transition has been controversial as a result of violations of conventional finite-size scaling [10–16], which we discussed in detail previously [9]. We will return to this below, arguing that the present results support the continuity of the transition.

The Néel-VBS transition is usually described with the noncompact CP¹ (NCCP¹) Lagrangian [4,17]

$$\mathcal{L} = |(\nabla - iA)z|^2 + \kappa(\nabla \times A)^2 + \mu|z|^2 + \lambda|z|^4. \quad (1)$$

The two-component bosonic spinon field $\mathbf{z} = (z_1, z_2)$ is related to the Néel vector \vec{N} by $\vec{N} = \mathbf{z}^\dagger \vec{\sigma} \mathbf{z}$. The U(1) gauge field A_μ is related by duality to the VBS order parameter $\vec{\varphi} = (\varphi_x, \varphi_y)$, which distinguishes the different columnar singlet patterns [4,18]. Although we will use the language of the Néel-VBS transition, our conclusions apply more generally to the above field theory, indicating that it flows to an SO(5)-symmetric fixed point at the critical value of μ . In the language of this 3D gauge theory, the VBS order parameter is the operator $\mathcal{M} = \varphi_x + i\varphi_y$ that inserts a Dirac monopole in A_μ [4,19,20].

SO(5) symmetry cannot be made explicit in the formulation of Eq. (1). Fortunately, Senthil and Fisher [21], building on the work of Tanaka and Hu [22], have argued that an alternative field theory describes the Néel-VBS transition and is equivalent to Eq. (1). This is a nonlinear σ model (NL σ M) for the five-component superspin

$$\vec{\Phi} = (N_x, N_y, N_z, \varphi_x, \varphi_y), \quad (2)$$

augmented with (i) anisotropies that break the global symmetry from SO(5) down to the spin rotation and spatial symmetries present microscopically, and (ii) a topological Wess-Zumino-Witten term at level 1 [23,24], which is analogous to that in the CFT for the spin chain. The leading anisotropy plays the role of the mass term in Eq. (1): it drives the transition between the Néel and VBS ordered phases.

The NL σ M formulation makes the emergent symmetry a more natural possibility, since it could arise at the critical point if all the higher anisotropies happen to be renormalization-group irrelevant [22,25]. We will discuss below the phase diagram for the NL σ M (with the WZW term) that is implied by this conjecture. Because there is at present no perturbatively accessible description of the transition that would permit an analytical calculation of scaling dimensions, we approach the problem using large-scale simulations.

In previous work we characterized various observables at the deconfined transition in detail, using a three-dimensional loop representation to reach system sizes up to $L = 512$. See Ref. [9] for details of the model, which is in the Néel phase for coupling $J < J_c$ and the VBS phase for $J > J_c$, with $J_c = 0.088501(3)$. We found a remarkable similarity between the critical Néel and VBS correlation functions. The anomalous dimensions determined from the correlators at separations $r \ll L$ are $\eta_{\text{Néel}} = 0.259(6)$ and $\eta_{\text{VBS}} = 0.25(3)$ [26]; the two correlators also behave similarly in the regime $r \sim L$, despite the scaling violations discussed in Ref. [9]. This suggests searching for an emergent SO(5) symmetry that would explain these apparent coincidences.

Probability distribution.—Consider the joint distribution for the Néel and VBS order parameters in a system of linear size L . If SO(5) symmetry emerges, then this will be a

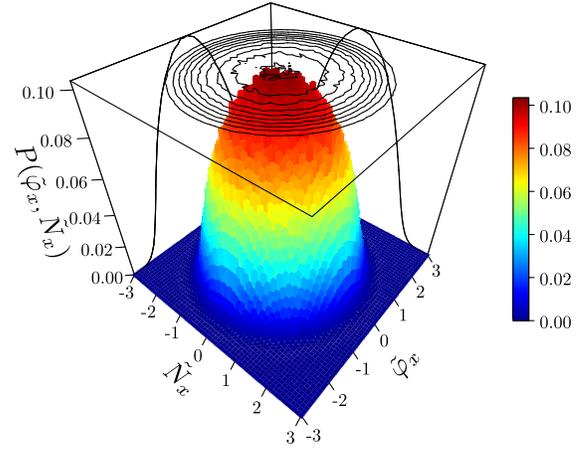


FIG. 1 (color online). The joint probability distribution $P(\tilde{N}_x, \tilde{\varphi}_x)$, after rescaling N_x and φ_x to have unit variance, in a critical system of size $L = 100$. The upper plane shows the contour plot.

function only of $\vec{\Phi}^2 = \vec{N}^2 + \vec{\varphi}^2$ at the critical point (after a trivial rescaling of $\vec{\varphi}$). Spin rotation symmetry of course already guarantees that the distribution depends on \vec{N} only via \vec{N}^2 . Also, while microscopic spatial symmetry only allows $\vec{\varphi}$ to be rotated by multiples of $\pi/2$, it is well established numerically that symmetry under continuous U(1) rotations of $\vec{\varphi}$ emerges near the transition [6,27,29]. This was checked for the present model in Ref. [9] (see also Supplemental Material [30], and see Ref. [33] for related phenomena). The crucial point is therefore whether the distribution is invariant under U(1) rotations that mix a component of $\vec{\varphi}$ with a component of \vec{N} .

Let the standard deviations of N_x and φ_x be denoted σ_N and σ_φ , respectively, and use a tilde to denote quantities rescaled to have unit variance: $\tilde{N}_x = N_x/\sigma_N$ and

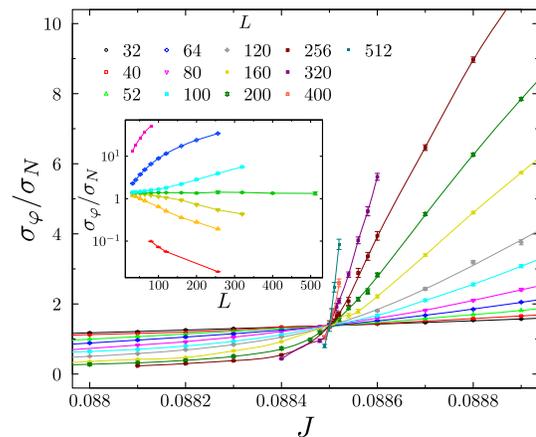


FIG. 2 (color online). Main panel: variance ratio σ_φ/σ_N plotted against J for various L . Curves cross at J_c as expected from SO(5) symmetry. Inset: same quantity as a function of L for several J around $J_c \approx 0.0885$ (key in Fig. 3).

$\tilde{\varphi}_x = \varphi_x/\sigma_\varphi$. Figure 1 shows the joint probability distribution for these quantities at the critical point $J = J_c$ in a system of size $L = 100$. The visual evidence for emergent symmetry between Néel and VBS orders is striking.

Before turning to a quantitative analysis of the distribution, a basic test is that the variances σ_N and σ_φ of the order parameters depend on system size in the same way at criticality [34], i.e., that σ_φ/σ_N is L -independent at J_c . In Fig. 2 this is confirmed to high precision over a wide range of length scales. Plots of σ_φ/σ_N versus J for different L values cross at J_c [35] (the value of σ_φ/σ_N at J_c depends on the nonuniversal normalization of the lattice operators).

For a quantitative analysis of the probability distribution we examine the moments

$$F_\ell^a = \langle r^a \cos(\ell\theta) \rangle, \quad (3)$$

where $(\tilde{N}_x, \tilde{\varphi}_x) = r(\cos\theta, \sin\theta)$. Emergent symmetry requires these to vanish for $\ell > 0$. We have computed F_2^4 and F_4^4 for large sizes:

$$F_2^4 = \langle \tilde{N}_x^4 - \tilde{\varphi}_x^4 \rangle, \quad F_4^4 = \langle \tilde{N}_x^4 - 6\tilde{N}_x^2\tilde{\varphi}_x^2 + \tilde{\varphi}_x^4 \rangle. \quad (4)$$

Figure 3 shows F_2^4 as a function of L at and close to the critical point; the Supplemental Material contains F_4^4 [30]. For $J = J_c$, both moments are consistent with zero over the entire L range. The expected values [30] in the adjacent phases [including the regime of weak VBS order, which has an effective U(1) symmetry for rotations of $\tilde{\varphi}$] are also indicated in the figure.

The inset to Fig. 3 shows F_2^4 as a function of J : note the very clearly defined crossing at $J = J_c$, $F_2^4 = 0$. Further moments are shown for $L = 100$ in Table I [30]. It should be noted that the critical distribution is markedly non-Gaussian, with nonvanishing higher cumulants, e.g., $[\langle N_x^4 \rangle - 3\langle N_x^2 \rangle^2]/\langle N_x^2 \rangle^2 = -0.7549(13)$ for $L = 100$.

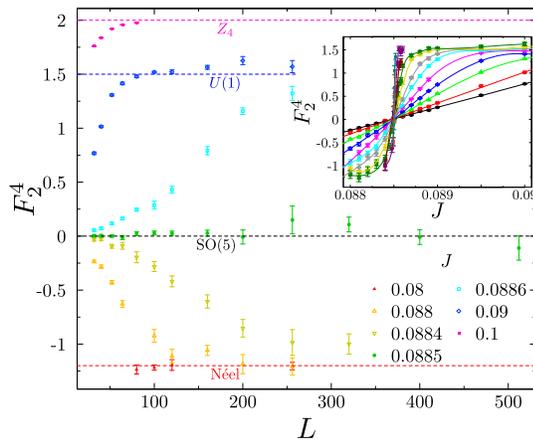


FIG. 3 (color online). Main panel: F_2^4 [Eq. (4)] versus L for a few J values close to $J_c \approx 0.0885$. Dashed lines: values in the Néel phase, at the SO(5)-symmetric critical point, and in the U(1) and \mathbb{Z}_4 -symmetric regimes of the VBS phase. Inset: J dependence of F_2^4 for various L (key in Fig. 2).

Equalities between scaling dimensions.—In addition to the equivalence between Néel and VBS vectors (manifested in the joint distribution and anomalous dimensions), SO(5) has consequences for operators transforming in higher representations. Take the leading operators in the symmetric two- and four-index representations:

$$\mathcal{O}_{ab}^{(2)} = \Phi_a \Phi_b - \frac{1}{5} \delta_{ab} \Phi^2, \quad \mathcal{O}_{abcd}^{(4)} = \Phi_a \Phi_b \Phi_c \Phi_d - C_{abcd}.$$

The subtractions [36] ensure irreducibility. $\mathcal{O}^{(2)}$ is relevant, with scaling dimension $x_2 < 3$. In fact, a component of $\mathcal{O}^{(2)}$ is the operator \mathcal{O}_J that drives us through the Néel-VBS transition as we vary J , by favoring one or the other order [\mathcal{O}_J therefore plays the role of the mass term in Eq. (1)]:

$$\mathcal{O}_J = \frac{5}{2} \sum_{a=1}^3 \mathcal{O}_{aa}^{(2)} = \vec{N}^2 - \frac{3}{2} \vec{\varphi}^2. \quad (5)$$

Remarkably, various *a priori* unrelated operators share the same scaling dimension x_2 since they are also components of $\mathcal{O}^{(2)}$. These include the spin-quadrupole moments $N_a N_b - \delta_{ab} \vec{N}^2/3$, and the relevant [29] operators $\varphi_a \varphi_b - \delta_{ab} \vec{\varphi}^2/2$ that in NCCP¹ language insert “strength-2” monopoles [37]. The same scaling dimension controls $\varphi_a N_b$, though microscopically this is maximally dissimilar from \mathcal{O}_J , as $\varphi_a N_b$ transforms under spin and spatial symmetries while \mathcal{O}_J is invariant under them.

To test these predictions, Fig. 4 shows the two-point functions of \mathcal{O}_J , $\varphi_x N_z$, and $\varphi_x \varphi_y$, or rather lattice versions [30] of these operators. (See Ref. [9] for a general discussion of critical correlators.) Note the striking similarity of the three curves, as expected from SO(5) symmetry. The slopes at $r \sim 10$ are around $x_2^{\text{eff}} \sim 1.5$. This effective exponent could be strongly affected by finite size effects, but it agrees well with a recent estimate of the two-monopole scaling dimension in Ref. [38]. [The two-monopole [39] and other dimensions are known at

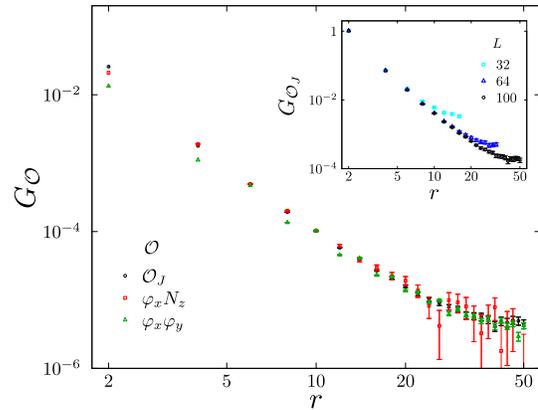


FIG. 4 (color online). Correlators $G_{\mathcal{O}}(r)$ for operators $\varphi_x N_z$, $\varphi_x \varphi_y$, and \mathcal{O}_J in a system of size $L = 100$. (The $G_{\mathcal{O}}$ have been normalized to agree at $r = 10$.) Inset: $G_{\mathcal{O}_J}$ for various L .

large n in the $SU(n)$ generalization of Eq. (1) [40–43], and show that a symmetry between Néel and VBS order parameters cannot persist in this limit.]

$\mathcal{O}^{(4)}$ allows us to write both a subleading operator that breaks the symmetry between Néel and VBS ($\sum_{a=1}^3 \sum_{b=4}^5 \mathcal{O}_{aabb}^{(4)}$), and one that breaks the remaining symmetry for $\vec{\varphi}$ down to fourfold rotations ($\sum_{a=4}^5 \mathcal{O}_{aaaa}^{(4)}$). Therefore, the same irrelevant exponent may control finite-size corrections to both types of symmetry enhancement [30]. Note that all the anisotropies that are allowed by microscopic symmetry in the bare action (with the exception of \mathcal{O}_J) must be irrelevant, as otherwise $SO(5)$ symmetry could not emerge at criticality.

Nonlinear σ model.—The $NL\sigma M$ proposed for the deconfined critical point in Ref. [21] (see also Ref. [22]) is

$$\mathcal{S}_\sigma = \int d^3x \left(\frac{1}{g} (\nabla \vec{\Phi})^2 + \sum_i \lambda_i \mathcal{O}_i \right) + \mathcal{S}_{WZW}, \quad (6)$$

where \mathcal{S}_{WZW} is a topological Wess-Zumino-Witten term at level 1 [associated with the homotopy group $\pi_4(S^4) = \mathbb{Z}$ of the target space]. Physically, this term ensures that a vortex in the VBS has an unpaired spin 1/2 at its core [18,21]. The \mathcal{O}_i are the various anisotropies, some discussed above, that break $SO(5)$ symmetry down to the microscopic physical symmetry.

Suppose that the Néel-VBS transition is continuous, with emergent $SO(5)$ symmetry, and is described by the $NL\sigma M$ with the WZW term. Since the critical point is reached by tuning a single parameter, there is only *one* RG-relevant coupling in Eq. (6), namely, the anisotropy \mathcal{O}_J of Eq. (5). The present results therefore show that the $SO(5)$ -symmetric $NL\sigma M$, without anisotropies, has a nontrivial infrared *stable* fixed point controlling a power-law correlated phase (Fig. 5). This fixed point also governs the deconfined transition. (The $NL\sigma M$ with the WZW term also has a stable ordered phase.)

The absence of a trivial disordered phase in Fig. 5 is counterintuitive, but one may argue that such an absence is inevitable in any field theory that describes the lattice magnet [21,44], essentially because of the higher-dimensional Lieb-Schultz-Mattis theorem [45–47].

The emergent $SO(5)$ symmetry therefore suggests the existence of a 3D $SO(5)$ -symmetric CFT that is radically unlike standard Wilson-Fisher CFTs, in that there are no

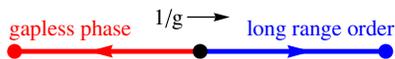


FIG. 5 (color online). Conjectured phase diagram for the fully $SO(5)$ -symmetric $NL\sigma M$ with the WZW term. The fixed point on the left also governs the deconfined critical point, where $SO(5)$ symmetry is emergent. Moving away from J_c introduces the relevant symmetry-breaking perturbation \mathcal{O}_J (not shown), leading to Néel or VBS order.

relevant singlet operators. It would be very interesting to investigate this using the conformal bootstrap [48], making use of numerical estimates for operator dimensions [9]. This should be simpler [49] than studying the critical NCCP¹ model without assuming $SO(5)$ symmetry.

Scaling violations.—The deconfined critical point shows strong violations of conventional finite-size scaling. We argued in Ref. [9] that these are not simply large scaling corrections of the conventional type (i.e., from irrelevant or marginally irrelevant operators)—but should instead be attributed *either* to an anomalously weak first order transition *or* to a genuine critical point with unconventional finite-size scaling due to a dangerously irrelevant variable. The present results strongly support the second scenario (a genuine continuous transition). This is because a critical point is the only natural explanation for emergent $SO(5)$ symmetry, which we have tested here to high precision. This symmetry therefore provides long-sought direct evidence for the continuity of the transition.

In more detail, if one attempts to account for the data in terms of an anomalously weak first order transition (i.e., without postulating a genuine 3D critical point), one is led to a scenario where the apparent criticality is due to a nearby fixed point at a spacetime dimension slightly below 3 [9]. Although this scenario can potentially explain pseudocritical behavior up to an extremely large length scale, it cannot naturally account for the emergent $SO(5)$ symmetry, which makes sense only for a 3D fixed point. While we can consider the NCCP¹ model in an arbitrary dimension, the operator $\vec{\varphi}$ —interpreted, for example, as a monopole insertion operator—is special to 3D, and is required for construction of the $SO(5)$ superspin.

Assuming therefore that the transition is continuous, a possible explanation for the scaling violations is that a dangerously irrelevant variable is required to cut off the fluctuations of a zero mode of the field [9]. (This is analogous to ϕ^4 theory above four dimensions, where the quartic term is irrelevant, but nevertheless necessary to prevent divergent fluctuations of ϕ 's zero mode [50].) This may suggest that an alternative field theory description exists that is more natural than the $NL\sigma M$ [51].

Future directions.—It would be interesting to investigate consequences of the emergent symmetry for finite temperature behavior, as well as to look for signs of it using methods complementary to Monte Carlo calculations such as exact diagonalization or density matrix renormalization group. Our results also motivate further analysis of $SO(5)$ -symmetric 3D CFTs (e.g., with the conformal bootstrap) and a general investigation of the role played by the WZW terms in field theories above 2D. For example, is there an analogous $SO(6)$ -symmetric CFT in 4D? Finally, we note that the critical behavior at the deconfined transition remains perplexing, and deserves further investigation.

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