Symmetry enhanced first-order phase transition in a two-dimensional quantum magnet

Bowen Zhao,1 Phillip Weinberg,1 and Anders W. Sandvik1,2

1Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA
2Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

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Theoretical studies of quantum phase transitions have suggested critical points with higher symmetries than those of the underlying Hamiltonian. Here we demonstrate a surprising emergent symmetry of the coexistence state at a strongly discontinuous phase transition between two ordered ground states. We present a quantum Monte Carlo study of a two-dimensional $S = 1/2$ quantum magnet hosting the antiferromagnetic (AFM) and plaquette-singlet solid (PSS) states recently detected in SrCu$_2$(BO$_3$)$_2$. We observe that the O(3) symmetric AFM order and the $Z_2$ symmetric PSS order form an O(4) vector at the transition. The control parameter $g$ (a coupling ratio) rotates the vector between the AFM and PSS sectors and there are no energy barriers between the two at the transition point $g_c$. This phenomenon may be observable in SrCu$_2$(BO$_3$)$_2$.

Introduction.—Theoretical studies of exotic quantum states of matter and the phase transitions between them can provide new perspectives on many-body physics and stimulate experimental investigations. A prominent example is the quantum phase transition between antiferromagnetic (AFM) and spontaneously dimerized valence-bond solid (VBS) ground states in two-dimensional (2D) spin $S = 1/2$ magnets [1,2]. Here the theory of deconfined quantum critical points (DQCPs) suggests that the Landau-Ginzburg-Wilson (LGW) paradigm for phase transitions is inapplicable, as a consequence of quasi-particle fractionalization [3,4]. Over the past decade, likely DQCPs have been identified in lattice models, using “designer Hamiltonians” constructed for their amenability to large-scale quantum Monte Carlo (QMC) simulations of the AFM–VBS transition [5–16]. Recently, a potential experimental realization of this type of DQCP was reported in the quasi-2D Shastry-Sutherland (SS) compound SrCu$_2$(BO$_3$)$_2$ under pressure [17]. Though the SS model [18] is difficult to study numerically, due to its geometrical frustration (which causes sign problems in QMC simulations), a specific type of VBS—a two-fold degenerate plaquette-singlet solid (PSS) located between AFM and bond-singlet phases—was demonstrated convincingly by tensor-network calculations [19]. Za-yed et al. [17] showed that a PSS also exists in SrCu$_2$(BO$_3$)$_2$ and suggested that the AFM–PSS transition may be a DQCP. The phase transition was not studied in the experiment, however, and it is not immediately clear if the two-fold degenerate PSS can support spinon deconfinement in the same way as a four-fold degenerate VBS. QMC studies of rectangular lattices with two-fold degenerate VBS states point to a first-order transition [15], as was also found in the SS model [19].

Here we study a sign-free model that mimics the SS compound, in the sense that it shares the same kinds of AFM and PSS ground states. The Hamiltonian, illustrated in Fig. 1(a), along with the SS model, is a new member in the “$J$–$Q$” family [5], with Heisenberg exchange $J$ supplemented by four-spin interactions $Q$ that weaken and eventually destroy the AFM order. Our QMC simulations demonstrate a first-order AFM–PSS transition with emergent O(4) symmetry.

Non-LGW critical points with emergent symmetries have been extensively investigated recently [20,30]. In the case discussed here, the order parameters exhibit clear discontinuities but conventional phase coexistence is not observed. Using order-parameter distributions, we show that the AFM order is rotated by the control parameter into PSS order. Phase coexistence at the transition takes the form of an O(4) symmetric vector arising out of the O(3) AFM and $Z_2$ PSS order parameters, with no energy barrier separating the two phases. In further support of this scenario, we demonstrate a characteristic logarithmic form of the PSS ordering temperature versus the tuning parameter $g$, as expected for a 2D O($N \geq 3$) quantum system deformed by a $Z_2$ interaction [31,32].

Ground states.—Our Hamiltonian can be defined using singlet projection operators $P_{ij} = (1/4 - S_i \cdot S_j)$:

$$H = -J \sum_{(ij)} P_{ij} - Q \sum_{ijkl \in C} (P_{ij}P_{kl} + P_{ik}P_{jl}),$$

(1)

where all indicated site pairs are nearest neighbors on a periodic square lattice with $L^2$ sites and $C$ denotes the $2 \times 2$ $Q$-plaquettes in Fig. 1(b). We define $g = J/Q$. For $g \rightarrow \infty$, this checker-board $J$–$Q$ (CBJQ) model reduces to the usual AFM ordered (at temperature $T = 0$) Heisenberg model, and for $g \rightarrow 0$ we will demonstrate a two-fold degenerate PSS. The model does not have any phase corresponding to the $J'$-bond singlet state of the SS model for large $J'/J$. However, for elucidating the nature of the AFM–PSS transition, we can invoke symmetries and universality to propose that the two
Figure 2. Dimer order distribution $P(D_x, D_y)$ in the ground state of the CBJQ model at $g = 0.20$ (in the PSS phase) and at $g = 0.24$ (in the AFM phase), from valence-bond QMC on $L = 96$ lattices.

models, as well as SrCu$_2$(BO$_3$)$_2$, contain the same physics.

We use two different QMC methods to study the CBJQ model: ground-state projection in the basis of valence bonds [33] and the stochastic series expansion (SSE) method [34]. Both techniques deliver exact results to within statistical errors. The projector method is very useful for studying spin-rotationally averaged quantities, while the SSE method is more efficient for finite-size scaling when the finite-$L$ ground states do not have to be fully reached but $T \to 0$ as $L \to \infty$.

To demonstrate the PSS ground state for large $g$, we first study a conventional dimer order parameter

$$D_{\mu} = \frac{1}{L^2} \sum_{\bf r} (-1)^{r_\mu} \bf S(r) \cdot S(r + \mu), \quad \mu = x, y, \quad (2)$$

where the sum is over the lattice sites at $\bf r = (r_x, r_y)$. In a VBS, $\langle D_x \rangle \neq 0, \langle D_y \rangle = 0$ for $x$-oriented bond order and the same with $x \leftrightarrow y$ for $y$-orientation. Since a singlet plaquette can be regarded as a resonance between horizontal and vertical bond pairs, a two-fold degenerate PSS should have $|\langle D_x \rangle| = |\langle D_y \rangle| \neq 0$ due to modulated singlet density on the plaquette rows and columns in Fig. 1. On a finite lattice the symmetry is not broken, and the system fluctuates between the two states. We use the projector method to generate the probability distribution $P(D_x, D_y)$. While strictly not a quantum mechanical observable, this distribution nevertheless properly reflects the fluctuations and symmetries of the system. Results on either side of the AFM–PSS transition (the location of which will be determined below) are shown in Fig. 2. We see the two-fold symmetry of a PSS, instead of the four-fold symmetry of the columnar VBS [9,35].

If the $Q$ terms are included on all plaquettes we arrive back to the original $J$-$Q$ model, whose AFM–VBS transition appears to be continuous [19]. In accord with the DQCP theory, an emergent U(1) symmetry of its microscopically $Z_4$ invariant VBS order parameter has been confirmed [5,7,35]. The proposed field theory description with spinons coupled to an U(1) gauge field [34] therefore seems viable. Unusual finite-size scaling behaviors not contained within the theory (but not contradicted by it) have also been observed [10,15,16] and interpreted by some as a weak first-order transition [7,8,11]. An interesting proposal is that the O(3) symmetry of the AFM and the emergent U(1) symmetry of the VBS may combine into an SO(5) symmetry exactly at the critical point [20,36]. In a spin-planar $J$-$Q$ model, it has instead been demonstrated that the U(1) AFM order parameter and the emergent U(1) VBS symmetry combine into a emergent O(4) symmetry [26]. In yet another example, it was proposed that a system with O(3) AFM order and $Z_2$ Kekule VBS states exhibits a DQCP with emergent SO(4) symmetry [27]. The O(3) and $Z_2$ symmetries apply also to the CBJQ model, and we therefore pay attention to a potential O(4) or SO(4) symmetry [37].

Finite-size scaling.—To analyze the AFM–PSS transition, we perform SSE calculations at $T = 2/L$. This way of taking the limit $T \to 0, L \to \infty$ is appropriate for a quantum phase transition with dynamic exponent $z = 1$, as well as for a first-order transition. We use order parameters defined solely with the $S^z$ spin components,

$$m_z = \frac{1}{L^2} \sum_{\bf r} \phi(r) S^z(r), \quad m_p = \frac{2}{L^2} \sum_{\bf q} \theta(q) \Pi^z(q), \quad (3)$$

where the subscripts $z$ (spin component) and $p$ (plaquette) mark the AFM and PSS order parameters, respectively. In $m_z, r$ runs over all $L^2$ lattice sites and $\phi(r) = \pm 1$ is the staggered AFM sign. In $m_p$, we have defined an operator

$$\Pi^z(q) = S^z(q) S^z(q + \hat{x}) S^z(q + \hat{y}) S^z(q + \hat{x} + \hat{y}), \quad (4)$$

detecting plaquette modulation, and the index $\bf q$ runs over the lower-left corners of the $Q$ plaquettes in Fig. 1. The signs $\theta(q) = \pm 1$ correspond to even or odd plaquette rows.

We will primarily analyze the Binder cumulants,

$$U_z = \frac{5}{2} \left( 1 - \frac{\langle m_z^4 \rangle}{3\langle m_z^2 \rangle^2} \right), \quad U_p = \frac{3}{2} \left( 1 - \frac{\langle m_p^4 \rangle}{3\langle m_p^2 \rangle^2} \right), \quad (5)$$

shown in Fig. 3(a), where the coefficients are chosen such that $U_z \to 1, U_p \to 0$ in the AFM phase while $U_z \to 0, U_p \to 1$ in the PSS. If there is a single transition, we can use the crossing point $g = g^*(L)$ at which $U_z(g, L) = U_p(g, L)$ to define a finite-size critical point $g^*(L)$. We also study the more commonly used crossing points of curves for two different system sizes, $bL$ and $L$ (where we use $b = 1/2$), locating the $g$ value where $U_z(g, bL) = U_z(g, L)$ or $U_p(g, bL) = U_p(g, L)$. The three definitions should flow to the same $g_c$ when $L \to \infty$.

From the slopes of the cumulants we can extract the correlation-length exponents $\nu_z$ and $\nu_p$ [16,38]:

$$\frac{1}{\nu_p} = \frac{1}{\ln(b)} \ln \left[ \frac{dU_p(g_c(L), L)}{dg} \right]_{g = g_c(L)}, \quad (6)$$

where $g_c(L)$ is the relevant ($bL, L$) cross point. The derivatives can be evaluated directly in the QMC simulations, and we interpolate to obtain the cross points and slopes from data on a dense $g$-grid in the neighborhood of $g_c$.

The analysis is presented and explained in Fig. 3. We find a single transition with $g_c = 0.2175 \pm 0.0001$ based on all three cross point estimators in Fig. 3(b). Most notably, in Fig. 3(c) the order parameters at their respective Binder crossing points...
do not vanish as \( L \to \infty \). This coexistence of AFM and PSS order is a decisive indicator of a first-order transition. Another first-order indicator is seen in the exponents \( 1/\nu_{z} \) and \( 1/\nu_{p} \):

\[
\text{Emergent O}(4) \text{ symmetry.—Due to energy barrier separating coexisting phases at a conventional first-order transition, the squared order parameter follows a double-peaked distribution, which causes a divergent negative peak in the Binder cumulant [40, 41]. Such peaks are present at the first-order transition in a } J \cdot Q \text{ model with a staggered } Z_{4} \text{ VBS [42], but are absent in Fig. 3(a). This lack of negative cumulant peaks leads us to consider alternative scenarios for coexisting order parameters, without energy barriers. A well known case is a system with long-range order driven through a point at which the Hamiltonian has a higher symmetry. As an example, we have studied an XXZ-deformed 3D classical Heisenberg O(3) model in its ordered phase. As shown in detail in Supplemental Material (SM) [39], it behaves very similar to the CBJQ model if we make an analogy between the } xy \text{ magnetization and the AFM order parameter on the one hand and the Ising magnetization and the PSS order parameter on the other hand.}
\]

The CBJQ model does not have any obvious enhanced symmetry, but the above results suggest that the O(3) AFM and the \( Z_{2} \) PSS combine to form an emergent O(4) symmetry at \( g_{c} \) [37]. In the transition region the system can then be described by an effective deformed quantum O(4) model, where the control parameter \( g = J/Q \) tunes the order parameter from the ordered O(3) phase through the O(4) point into the \( Z_{2} \) phase.

As an explicit test of emergent O(4) symmetry, we use the valence-bond projector QMC method and now define the PSS order parameter with the rotationally invariant operator

\[
\Pi(q) = S(q) \cdot S(q + \hat{x}) + S(q + \hat{y}) \cdot S(q + \hat{y} + \hat{x}) + S(q) \cdot S(q + \hat{y}) + S(q + \hat{x}) \cdot S(q + \hat{x} + \hat{y}),
\]

in place of \( \Pi(q) \) in Eq. (3). For the AFM, we still use the \( z \)-component of the order parameter Eq. (3). In a state with both AFM and PSS order, the commutator \( [m_{z}, m_{p}] \propto L^{-2} \), and we can safely use the c-numbers corresponding to \( m_{z} \) and \( m_{p} \) from a given transition graph [33] to accumulate the joint probability distribution \( P(m_{z}, m_{p}) \). For the putative O(4) symmetry to be manifest, we further normalize \( m_{z} \) and \( m_{p} \) by factors involving \( \langle m_{z}^{2} \rangle \) and \( \langle m_{p}^{2} \rangle \) [39].

For a point on an O(4) sphere of radius \( R \), the projection onto two components results in a uniform distribution within a circle of radius \( R \). However, in a finite quantum system we also expect fluctuations of \( R \) and therefore compare our CBJQ results with a distribution obtained from an O(4) sphere with mean radius \( R = 1 \) and standard deviation \( \sigma \). Examples are shown Fig. 4. At the transition, the CBJQ distribution is rotation symmetric with radial profile similar to O(4) sampling with \( \sigma \approx 0.15 \). Inside the phases the distributions are shifted as expected—deep in the PSS we should eventually, for \( L \to \infty \), obtain a point on the \( y \)-axis, and in the AFM state a line on the \( x \)-axis. Quantitative tests of the symmetry are presented in SM [39]. As expected for an emergent symmetry, we find clear O(4) violations for small system sizes.

At a classical first-order transition, \( 1/\nu \to 0 \) in \( d \) dimensions, and in \( 2+1 \) dimensions we might expect \( 1/\nu_{ZP} \to 3 \). The larger values seen in Fig. 3(d) indicate a particular type of first-order transition, as explained below.
The parameter of the higher symmetry (though no convincing evidence has been presented) may be expected at certain weak first-order transitions, where the system is close to a fine-tuned point with order parameter $m_z$, while the $y$-axis is the PSS order parameter $m_p$.

$(L = 8, 16)$, but no detectable deviations at $g_c$ for the largest systems studied (up to $L = 96$).

Having concluded that there is emergent $O(4)$ symmetry, we can also understand why $1/\nu_{z,p} > 3$ in Fig. 3(b): The dynamic exponent of the Anderson-Goldstone rotor states associated with $O(N \geq 3)$ order is $z = 2$, and therefore one may expect the exponents to eventually tend to $d + z = 4$ when $L \rightarrow \infty$ at $T = 0$. The deviations may be due to $T > 0$ effects when $T$ is scaled as $L^{-1}$ (instead of $L^{-2}$). As we show in SM [39], quantitative measures of the emergent $O(4)$ symmetry in our $T = 0$ calculations exhibit $L^{-1}$ scaling of the size of the $g$-window in which the symmetry is emergent.

Another interesting consequence of $O(4)$ symmetry should be a specific logarithmic (log) form of the critical PSS temperature $T_c$ versus the distance $\delta = g_c - g$ from the $T = 0$ transition point, $T_c \propto \log^{-1}(C/\delta)$, as in an $O(N \geq 3)$ model with an Ising deformation [41, 42]. This form is very different from that expected close to an Ising quantum-critical point, where $T_c \propto \delta^{-\nu_\text{Is}}$, where $\nu_\text{Is}$ is the 3D Ising correlation-length exponent. Neither form should apply at a conventional first-order transition extending from $(g_c, T = 0)$ to some $T > 0$. If the (O(4) breaking) perturbation is very weak, one should still expect the log form to hold down to some low temperature.

We have computed $T_c(g)$ for the PSS by the cumulant-crossing method using SSE data for $L \leq 160$. We can reliably extrapolate $T_c$ to the thermodynamic limit for $g \leq 0.216$ (0.0015), as shown in Fig. 5. The behavior for $\delta \approx 0.02$ is very well described by the log form, lending strong indirect support to the emergent $O(4)$ symmetry through an important physical observable in the thermodynamic limit.

Discussion.—We cannot exclude that the $O(4)$ symmetry is present only up to some length scale above the largest system, $L = 96$, studied here. Such symmetry violations at a long scale may be expected at certain weak first-order transitions, either when the system is close to a fine-tuned point with order parameter of the higher symmetry (though no convincing evidence has been presented), or in proximity of a quantum-critical point at which the higher symmetry is emergent [20, 24, 28].

In the CBJQ model studied here, the observed discontinuities are rather strong: from Fig. 3(c), the magnitude of the $O(4)$ vector in AFM units is $m_z = (4m_z^2)^{1/2} \approx 0.12$, almost 25% of the maximum staggered magnetization $1/2$. The first-order nature of the transition is apparent even on small lattices, e.g., as seen in the flow of $1/\nu_\text{Z}$ toward an anomalously large value in Fig. 3(d). Thus, in the scenario of Ref. [25], we have $\xi/L \ll \xi' \sim (\xi/L)^{1/4}$, where the exponent $\alpha$ must be rather large in order to give the clear separation of length scales needed to account for the observed behavior. Such behavior has not been previously anticipated; rather, emergent symmetry on large length scales has been cited as support for continuous non-LGW transitions [20, 27].

In an alternative scenario of an asymptotic $O(4)$ symmetry, the dominant symmetry-breaking field is tuned to zero at the AFM-PSS transition and higher-order $O(4)$ violating perturbations would vanish upon renormalization, perhaps by an extension of the DQCP framework, or by some more general mechanism. While emergent $O(N)$ multicritical points arising from $O(N - 1)$ and $Z_2$ order parameters have been extensively discussed within the LGW framework [43, 44], the influence of the higher symmetry on associated first-order lines has not been addressed until recently in the weakly first-order DQCP context [25]. In order to exclude that the CBJQ model is accidentally fine-tuned to vanishing or extremely small perturbations of the $O(4)$ symmetry, we have also studied a model extended by additional interactions; see SM [39].

We designed the CBJQ model with SrCu$_2$(BO$_3$)$_2$ in mind.
The expected Ising-type $T > 0$ PSS transition would be a good target for detecting the still incompletely characterized PSS phase and the putative O(4) symmetry. In 2D we have demonstrated a characteristic log form of $T_c$ (Fig. 5), and this form will hold down to some low temperature in the presence of sufficiently weak inter-layer couplings; presumably the 3D $T = 0$ transition is a conventional first-order one.

The O(4) AFM–PSS transition is reminiscent of the SO(5) theory of high-$T_c$ superconductivity [49], where O(3) AFM and O(2) superconducting order parameters form the higher symmetry; a scenario not confirmed, neither experimentally nor in models. After the completion of the present work, an SO(5) analogue of the AFM–PSS was demonstrated in a spin-1 $J\cdot Q$ model [50], and an O(4) transition very similar to ours was discussed in the context of a classical 3D loop model [51].

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* sandvik@bu.edu

[1] S. Sachdev, Quantum magnetism and criticality, Nature Phys. 4, 173 (2008).
[2] R. K. Kaul, R. G. Melko, and A. W. Sandvik, Bridging Lattice-Scale Physics and Continuum Field Theory with Quantum Monte Carlo Simulations, Annu. Rev. Condens. Matter Phys. 4, 179 (2013).
[3] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Deconfined Quantum Critical Points, Science 303, 1490 (2004).
[4] T. Senthil, L. Balents, S. Sachdev, A. Vishwanath, and M. P. A. Fisher, Quantum criticality beyond the Landau-Ginzburg-Wilson paradigm, Phys. Rev. B 70, 144407 (2004).
[5] A. W. Sandvik, Evidence for Deconfined Quantum Criticality in a Two-Dimensional Heisenberg Model with Four-Spin Interactions, Phys. Rev. Lett. 98, 227202 (2007).
[6] R. G. Melko and R. K. Kaul, Scaling in the Fan of an Unconventional Quantum Critical Point, Phys. Rev. Lett. 100, 017203 (2008).
[7] F.-J. Jiang, M. Nyfeler, S. Chandrasekharan, and U.-J. Wiese, From an antiferromagnet to a valence bond solid: evidence for a first-order phase transition, J. Stat. Mech. (2008) P02009.
[8] A. B. Kuklov, M. Matsumoto, N. V. Prokofev, B. V. Svistunov, and M. Troyer, Deconfined Criticality: Generic First-Order Transition in the SU(2) Symmetry Case, Phys. Rev. Lett. 101, 050405 (2008).
[9] J. Lou, A. W. Sandvik, and N. Kawashima, Antiferromagnetic to valence-bond-solid transitions in two-dimensional SU(N) Heisenberg models with multispin interactions, Phys. Rev. B 80, 180414(R) (2009).
[10] A. W. Sandvik, Continuous Quantum Phase Transition between an Antiferromagnet and a Valence-Bond Solid in Two Dimensions: Evidence for Logarithmic Corrections to Scaling, Phys. Rev. Lett. 104, 177201 (2010).
[11] K. Chen, Y. Huang, Y. Deng, A. B. Kuklov, N. V. Prokofev, and B. V. Svistunov, Deconfined Criticality Flow in the Heisenberg Model with Ring-Exchange Interactions, Phys. Rev. Lett. 110, 185701 (2013).
[12] K. Harada, T. Suzuki, T. Okubo, H. Matsuo, J. Lou, H. Watanabe, S. Todo, and N. Kawashima, Possibility of deconfined criticality in SU(N) Heisenberg models at small N, Phys. Rev. B 88, 220408(R) (2013).
[13] M. S. Block, R. G. Melko, and R. K. Kaul, Fate of CP$^{N-1}$ Fixed Points with q Monopoles, Phys. Rev. Lett. 111, 137202 (2013).
[14] S. Pujari, K. Damle, and F. Alet, Néel-State to Valence-Bond-Solid Transition on the Honeycomb Lattice: Evidence for Deconfined Criticality, Phys. Rev. Lett. 111, 087203 (2013).
[15] A. Nahum, J.T. Chalker, P. Serna, M. Ortuño, and A.M. So moza, Deconfined Quantum Criticality, Scaling Violations, and Classical Loop Models, Phys. Rev. X 5, 041048 (2015).
[16] H. Shao, W. Guo, and A. W. Sandvik, Quantum criticality with two length scales, Science 352, 213 (2016).
[17] M. Zayed, Ch. Rüegg, J. Larrea, A. M. Lüiáchli, C. Panagopoulos, S. S. Saxena, M. Ellerby, D. McMor, Th. Strässle, S. S. Klotz, G. Hamel, R. A. Sadykov, V. Pomjakushin, M. Boehm, M. Jiménez-Ruiz, A. Schneidewin, E. Pomjakushin, M. Stingaciu, K. Conder, and H. M. Romnow, 4-spin plaquette singlet state in the Shastry-Sutherland compound SrCu$_2$(BO$_3$)$_2$, Nat. Phys. 13, 962 (2017).
[18] B. S. Shastry and B. Sutherland, Exact ground state of a quantum mechanical antiferromagnet, Physica B+C 108, 1069 (1981).
[19] P. Corboz and F. Mila, Tensor network study of the Shastry-Sutherland model in zero magnetic field, Phys. Rev. B 87, 115144 (2013).
[20] A. Nahum, P. Serna, J. T. Chalker, M. Ortuño, and A. M. So moza, Emergent SO(5) Symmetry at the Néel to Valence-Bond-Solid Transition, Phys. Rev. Lett. 115, 267203 (2015).
[21] A. Karch and D. Tong, Particle-Vortex Duality from 3D Bosonization, Phys. Rev. X 6, 031043 (2016).
[22] M. A. Metlitski and A. Vishwanath, Particle-Vortex Duality of Two-Dimensional Dirac Fermion from Electric-Magnetic Duality of Three-Dimensional Topological Insulators, Phys. Rev. B 93, 245151 (2016).
[23] D. F. Mross, J. Alicea, and O. I. Motrunich, Explicit Derivation of Duality between a Free Dirac Cone and Quantum Electrodynamics in (2+1) Dimensions, Phys. Rev. Lett. 117, 016802 (2016).
[24] S. Kachru, M. Mulligan, G. Torroba, and H. Wang, Non-supersymmetric Dualities from Mirror Symmetry, Phys. Rev. Lett. 118, 011602 (2017).
[25] C. Wang, A. Nahum, M. A. Metlitski, C. Xu, and T. Senthil, Deconfined Quantum Critical Points: Symmetries and Dualities Phys. Rev. X 7, 031051 (2017).
[26] Y. Q. Qin, Y.-Y. He, Y.-Z. You, Z.-Y. Lu, A. Sen, A. W. Sandvik, C. Xu, and Z. Y. Meng, Duality between the Deconfined Quantum-Critical Point and the Bosonic Topological Transition, Phys. Rev. X 7, 031052 (2017).
[27] T. Sato, M. Hohenadler, and F. F. Assaad, Dirac Fermions with Competing Orders: Non-Landau Transition with Emergent Symmetry, Phys. Rev. Lett. 119, 197203 (2017).
[28] M. A. Metlitski and R. Thorngren, Intrinsic and emergent anomalies at deconfined critical points, Phys. Rev. B 98, 085140 (2018).
[29] S. Gazit, F. F. Assaad, S. Sachdev, A. Vishwanath, and C. Wang, Confinement transition of $Z_2$ gauge theories coupled to mass-
less fermions: emergent QCD3 and SO(5) symmetry, Proc. Nat. Acad. Sci. 115, E6987 (2018).

[30] G. J. Sreejith, S. Powell, and A. Nahum, Emergent SO(5) symmetry at the columnar ordering transition in the classical cubic dimer model, arXiv:1803.11218

[31] V. Yu. Irkhin and A. A. Katanin, Thermodynamics of isotropic and anisotropic layered magnets: Renormalization-group approach and 1/N expansion, Phys. Rev. B 57, 379 (1998).

[32] A. Cuccoli, T. Roscilde, V. Tognetti, R. Vaia, and P. Verrucchi, Quantum Monte Carlo study of $S = 1/2$ weakly anisotropic antiferromagnets on the square lattice, Phys. Rev. B 67, 104414 (2003).

[33] A. W. Sandvik and H. G. Evertz, Loop updates for variational and projector quantum Monte Carlo simulations in the valence-bond basis, Phys. Rev. B 82, 024407 (2010).

[34] A. W. Sandvik, Computational Studies of Quantum Spin Systems, AIP Conf. Proc. 1297, 135 (2010).

[35] A. W. Sandvik, Finite-size scaling and boundary effects in two-dimensional valence-bond solids, Phys. Rev. B 85, 134407 (2012).

[36] T. Senthil and M. P. A. Fisher, Competing orders, nonlinear sigma models, and topological terms in quantum magnets, Phys. Rev. B 74, 064405 (2006).

[37] Our calculations cannot distinguish between O(4) and SO(4) symmetry, since we only test for the rotational symmetry common to both.

[38] J. M. Luck, Corrections to finite-size-scaling laws and convergence of transfer-matrix methods, Phys. Rev. B 31, 3069 (1985).

[39] See Supplemental Material for analogous results for a 3D classical XXZ model, detailed quantitative analysis of order-parameter distributions, and a generalized CBJQ model with two different $Q$ terms.

[40] K. Vollmayr, J. D. Reger, M. Scheucher, and K. Binder, Finite size effects at thermally-driven first order phase transitions: A phenomenological theory of the order parameter distribution, Z. Phys. B 91, 113 (1993).

[41] S. Iino, S. Morita, A. W. Sandvik, and N. Kawashima, Detecting signals of weakly first-order phase transitions in two-dimensional Potts models, arXiv:1801.02786

[42] A. Sen and A. W. Sandvik, Example of a first-order Néel to valence-bond-solid transition in two dimension, Phys. Rev. B 82, 174428 (2010).

[43] M. E. Muller, A note on a method for generating points uniformly on n-dimensional spheres, Commun. ACM 2(4), 19 (1959).

[44] A. Kuklov, N. Prokofev, and B. Svistunov, Weak First-Order Superfluid-Solid Quantum Phase Transitions, Phys. Rev. Lett. 93, 230402 (2004).

[45] A. Pelissettp and E. Vicari, Multicritical behavior of two-dimensional anisotropic antiferromagnets in a magnetic field, Phys. Rev. B 76, 024436 (2007).

[46] M. Hasenbusch and E. Vicari, Anisotropic perturbations in three-dimensional O(N)-symmetric vector models, Phys. Rev. B 84, 125136 (2011).

[47] A. Eichorn, D. Mesterházy, and M. M. Scherer, Multicritical behavior in models with two competing order parameters, Phys. Rev. E 88, 042141 (2013).

[48] F. Hébert, G. G. Batrouni, R. T. Scalettar, G. Schmid, M. Troyer, and A. Dorneich, Quantum phase transitions in the two-dimensional hardcore boson model, Phys. Rev. B 65, 014513 (2001).

[49] E. Demler, W. Hanke, and S.-C. Zhang, SO(5) theory of antiferromagnetism and superconductivity, Rev. Mod. Phys. 76, 909 (2004).

[50] J. Wildeboer, J. D’Emidio, and R. K. Kaul, Emergent symmetry at a transition between intertwined orders in a $S=1$ magnet, [arXiv:1808.04731]

[51] P. Serna and A. Nahum, Emergence and spontaneous breaking of approximate O(4) symmetry at a weakly first-order deconfined phase transition, [arXiv:1805.03759]

[52] U. Wolff, Collective Monte Carlo Updating for Spin Systems, Phys. Rev. Lett. 62, 361 (1989).

[53] K. S. D. Beach and A. W. Sandvik, Some formal results for the valence bond basis, Nucl. Phys. B 750, 142 (2006).

[54] S. Liang, B. Doucot, and P. W. Anderson, Some New Variational Resonating-Valence-Bond-Type Wave Functions for the Spin-1/2 Antiferromagnetic Heisenberg Model on a Square Lattice, Phys. Rev. Lett. 61, 365 (1988).

[55] P. Weinberg and A. W. Sandvik, Dynamic scaling of the restoration of rotational symmetry in Heisenberg quantum antiferromagnets, Phys. Rev. B 96, 054442 (2017).
SUPPLEMENTAL MATERIAL

Symmetry enhanced first-order phase transition in a two-dimensional quantum magnet

Bowen Zhao, Phillip Weinberg, and Anders W. Sandvik

We present additional results supporting the existence of an emergent O(4) symmetry in the CBJQ model at its AFM–PSS transition. In Sec. 1, as a benchmark for finite-size scaling, we discuss results for the phase transition between an xy-ordered state and a z-ordered state in a deformed classical O(3) model (the XXZ model) below its critical temperature. In Sec. 2 we carry out a quantitative analysis of the order parameter histograms exemplified in Fig. 4 of the main paper. In Sec. 3 we deform the CBJQ model by introducing alternating plaquette terms of strength $Q_A$ and $Q_B$, such that the case $Q_A = Q, Q_B = 0$ corresponds to the original CBJQ model discussed in the main text. We find emergent O(4) symmetry also with $Q_B = Q_A/2$, showing that the O(4) symmetry of the original CBJQ model is not accidental due to some implicit fine-tuning.

1. Classical XXZ model

In the 3D classical O(N) model at $T < T_c$, a deformation of one of the N interaction terms by a factor $\Delta$ leads to an ordered phase breaking O(N − 1) symmetry for $\Delta < 1$ and $Z_2$ (Ising) symmetry for $\Delta > 1$. We have argued that the CBJQ model corresponds to this situation with $N = 4$, with the O(3) and $Z_2$ phases corresponding to the AFM and PSS, respectively. However, in the CBJQ model the O(4) symmetry is not explicitly present at the Hamiltonian level but is emergent on long length scales.

We will here study the deformed 3D classical O(3) model and demonstrate finite-size scaling behaviors analogous to those that we found for the CBJQ model. We could also have studied an O(4) model, but the same physics is manifest already with $N = 3$, which is the minimum number of components for which one of the deformed phases breaks a continuous symmetry and the other one breaks the discrete $Z_2$ symmetry. The Hamiltonian of the XXZ model is:

$$H = -\sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \Delta \sigma_i^z \sigma_j^z,$$

(S1)

where $\langle ij \rangle$ corresponds to nearest-neighbor interactions between the unit vectors $\sigma_i$ on a simple cubic lattice. We could also consider the 2D $S = 1/2$ AFM Heisenberg model at $T = 0$ with a similar deformation, which was done in Ref. [32] but with a different focus.

The 2D $S = 1/2$ XXZ model with nearest-neighbor interactions on the square lattice has long-range order at $T = 0$ for all values of $\Delta$, and the order parameter symmetry changes with $\Delta$ in the same way as in the 3D classical model below $T_c$. When passing through the special point $\Delta = 1$, the elementary excitations change, as the Goldstone modes present in the O(2) phase and the O(3) point are gapped out continuously for $\Delta > 1$. In this sense, we can consider the change in symmetry as a phase transition with both first-order and continuous characteristics; a discontinuous flip of the direction of the order parameter but a continuously varying gap. Note that $T > 0$ in the quantum XXZ model corresponds to a finite size $L_3 \propto 1/T$ of one of the dimensions of the classical 3D model (here written as the third dimension). Here we will only consider the 3D model with equal size $L$ in all dimensions and, thus, obtain results corresponding to $T = 0$ in the quantum case when $L \rightarrow \infty$.

We have carried out Monte Carlo simulations of the classical 3D XXZ model at two different temperatures in the ordered phase, $T^{-1} = 0.7$ and 0.75, the former being close to $T_c^{-1}(\Delta_c = 1) \approx 0.6930$. We use the efficient Wolff cluster algorithm [52] and analyze the $xy$ and $z$ magnetizations individually. The Binder cumulants and slopes are defined in ways analogous to Eqs. (5) and (6).

As shown in Fig. S1(a) behaviors similar to those in the CBJQ model (Fig. 2) are observed at $T = 0.7$ if we make an analogy between the $xy$ magnetization and the AFM order parameter on the one hand and the Ising $z$ magnetization and the PSS order parameter on the other hand. There are no negative cumulant peaks in Fig. S1(b) in the neighborhood of the transition point $\Delta = 1$. In Fig. S1(b) we show that the transition point is accurately reproduced with the same curve-correcting method as we used for the CBJQ model. Looking at the coexistence values of the order parameters in Fig. S1(c), which obey $(m_x^2 + m_y^2) = 2m_z^2$, the length $|m|$ of the vector $m$ is about 25% of the maximum value 1. This is similar to the relative length of the O(4) vector extracted from Fig. 3(c) for the CBJQ model, where we can define $|m| = \sqrt{4|m_z^2|}$, with maximum value $|m| = 1/2$.

In Fig. S1(d) we see that $1/\nu_{xy}$ extrapolates close to the standard first-order value 3, while $1/\nu_z$ is somewhat lower. One may question the standard first-order value in this case because of the lack of free-energy barriers, but a simple mean-field argument gives that the relevant scaling variable is $(\Delta - 1)L^3$ also for the long-range ordered XXZ model. In Fig. S1(d) we have only used a simple line fit to extrapolate both the exponents, and an asymptotically form with higher-order corrections and larger system sizes would likely explain why the values are less than 3. Similar to the CBJQ model, Fig. 3(d), there is a rather sharp cross-over from one slope at small system sizes to a higher slope for the larger sizes. The cross-over region should correspond to $L \approx \xi$, $\xi$ being the correlation length of the infinite system in the neighborhood...
of the transition. Because of the cross-over behavior, it is difficult to carry out reliable extrapolations with the rather small number of system sizes available.

In most respects, we see that the O(3) order–order transition looks in finite-size scaling like a first-order transition, with the glaring exception of the lack of negative Binder peak. Indeed, with phase coexistence in the form of a higher symmetry, the arguments behind the negative peak [40, 41] do not apply, since, thanks to the higher rotational symmetry, the two phases are not separated by a free-energy barrier at the transition point $\Delta = 1$. These results for the classical model provide support for a similar mechanism at play at the AFM–PSS transition of the CBJQ model, even though no exact higher symmetry is present in its Hamiltonian.

In Fig. S2 we show results at a slightly lower temperature, $T^{-1} = 0.75$. The results are qualitatively very similar to those at $T^{-1} = 0.7$, but the features are sharper due to the stronger order. The extrapolation of both exponents $1/\nu_{xy}$ and $1/\nu_z$ to 3 is also clearer in this case, with an overall weaker size dependence (though still the linear extrapolation somewhat underestimates the values of both the exponents) and no clear cross-over. The lack of cross-over here suggests that the correlation length in the infinite system remains small at this temperature.

Figure S2. The same quantities as in Fig. S1 for the 3D XXZ model at a lower temperature, $T^{-1} = 0.75$.

2. Quantitative check of emergent O(4) symmetry

Here we discuss further details of our tests of emergent O(4) symmetry in the CBJQ model based on order-parameter distributions (histograms) $P(m_z, m_p)$, such as those shown in Fig. 4. In addition, we also consider the distribution of $P(m_s, m_p)$, where $m_s$ is the magnitude of the full O(3) AFM order parameter,

$$m_s^2 = m_z^2 + m_y^2 + m_x^2.$$ (S2)
Like \( m_p \) defined in Eqs. 3 and 7, the c-number corresponding to \( m_z^2 \) is obtained in the valence-bond projector QMC method after each Monte Carlo updating sweep directly from the transition graph as a single unique number (in contrast to just the component \( m_z \), which is obtained by sampling one of the many spin configurations that contribute to the transition graph) \[ \text{[S5]} \text{[S3]} \text{[S4]}. \] Note that it is not possible to obtain independent equal-time values for all three components of the AFM order parameter from the transition graphs or the associated \( z \) basis spin configurations.

In the simulations, we generate and store a list of points \((m_z, m_z^2, m_p)\), \( i = 1, \ldots, M \). In order to obtain smooth probability distributions and small error bars on the associated integrated quantities that we use to test for the emergent symmetry, we need a very large number of points (\( M \) of the order of millions). To capture the point of maximal symmetry and study the scaling properties away from this point, we also need many values of \( g \). We have carried out the valence-bond QMC simulations with a very long projection time \( \tau \) in the imaginary-time evolution operator \( e^{-\tau H} \) and find that \( \tau = 8L \) is sufficient for \( T \to 0 \) convergence of the distributions for the system sizes considered here; up to \( L = 96 \).

Symmetry tests with two components.—The definitions of the two order parameters by Eqs. 3 and 7 are not unique. Therefore, even if there is an emergent symmetry between the order parameters, \( m_z \) and \( m_p \) are not directly comparable as to their overall magnitudes. To investigate a possible emergent O(2) symmetry of the distribution \( P(m_z, m_p) \), as a proxy for the full O(4) symmetry of all four components, we need to remove the ambiguity by properly normalizing the sampled numbers. To this end, post-simulation, we compute the corresponding variances \( \langle m_z^2 \rangle \) and \( \langle m_p^2 \rangle \). We can then define the radius \( R \) of the distribution as

\[
\langle R^2 \rangle = \langle m_z^2 \rangle + a^2 \langle m_p^2 \rangle, \quad R \equiv \langle R^2 \rangle^{1/2}, \tag{S3}
\]

while also requiring that

\[
\langle m_z^2 \rangle = a^2 \langle m_p^2 \rangle. \tag{S4}
\]

Thus, the parameter \( a \) that puts the two sampled order parameters on an equal scale is defined by

\[
a^2 = \frac{\langle m_z^2 \rangle}{\langle m_p^2 \rangle}. \tag{S5}
\]

We can now define normalized point pairs as

\[
(\tilde{m}_z, \tilde{m}_p) = R^{-1}(m_z, a m_p), \tag{S6}
\]

and test for emergent O(2) symmetry in the distribution \( P(\tilde{m}_z, \tilde{m}_p) \) at the AFM–PSS transition.

To quantify the degree of O(2) symmetry of a distribution \( P(\tilde{m}_z, \tilde{m}_p) \) we use the integrals

\[
I_g = \int d\tilde{m}_z d\tilde{m}_p P(\tilde{m}_z, \tilde{m}_p) \cos(q\phi(\tilde{m}_z, \tilde{m}_p))
= \frac{1}{M} \sum_{i=1}^{M} \cos(q\phi(|\tilde{m}_z|, |\tilde{m}_p|))_i, \tag{S7}
\]

where on the second line \( i \) is the index corresponding to the \( M \) QMC sampled points \((\tilde{m}_z, \tilde{m}_p)\), from which angles \( \phi(|\tilde{m}_z|, |\tilde{m}_p|)_i \in [0, \pi/2] \) are extracted (with the absolute values taken to transform to the positive quadrant). We will here consider the integrals with \( q = 2, 4, 6, 8 \), all of which should vanish if the distribution is O(2) symmetric. For larger \( q \), the results become increasingly noisy, but since there is no reason to expect distributions with \( I_2 = I_4 = I_6 = I_8 = 0 \) and \( I_{q>8} \neq 0 \), what we do here is sufficient for demonstrating O(4) symmetry.

There is a remaining ambiguity in the normalization, as to the point at which the scale factor \( a \) should be evaluated. In Fig. 4(b) of the main paper, \( a \) was evaluated at \( g = 0.21755 \) (the data in the middle panel) and used at the other \( g \) values as well. If the distribution is O(2) symmetric at \( g_c \), as it appears to be, we argue that the best way to proceed is to fix \( a \) at this point, instead of using a \( g \)-dependent value \( a^2(g) \) computed from a distribution that is not O(2) symmetric when \( g \neq g_c \). This choice is motivated by the fact that the O(4) symmetry should only apply to a single point, the transition point, and there is no reason why the normalization condition Eq. (S4) should be applied elsewhere. If the varying \( a^2(g) \) is used for all \( g \) values, then the distribution away from \( g_c \) will artificially be drawn out in one direction, thus making the signals (the values of \( I_4 \)) less sensitive to the control parameter. The fact that the mean vector projection in the different directions should not be the same when the vector flips from the AFM sector to the PSS direction would then be missed. Note that fixing \( a^2(L) \) at \( g_c \) also in no way can artificially introduce a false symmetry in the quantities we study.

Given the above arguments, we use the following two-step procedure to analyze the distribution: At the first stage, we compute the scale factor \( a^2(g) \) in Eq. (S5) for each of the \( g \) values considered. Results for various system sizes up to \( L = 96 \) are shown in Fig. [S5]. We can observe that the curves for different system sizes cross each other around the transition point \( g \approx 0.2175 \). Based on closer inspection and extrap-
I exhibit minimums at the point \( L = 96 \) for all \( g \) and \( L \) we fix \( a(L) \) in Eq. (S4) at their values obtained at \( g = 0.21755 \), which is full consistent with the transition point \( g_c = 0.2175 \pm 0.0001 \) extracted in the main paper.

The results are shown in Fig. S4. Here we can see that the \( I_q \) curves for odd \( q \) go through zero at \( g_c \), while for even \( q \) they exhibit minimums at \( g_c \). For the larger system sizes, \( I_4 \) and \( I_8 \) have minimum values equal to 0 to within statistical errors. Thus, we conclude that there is an emergent O(4) symmetry at the transition point. Deviations from O(4) behaviour are seen in \( g_q \) and \( I_8 \) for the smallest system sizes, which is expected if the symmetry is emergent upon increasing \( L \). For the largest system sizes, up to \( L = 96 \), no deviations from O(4) symmetry can be detected at \( g_c \) in any of the \( I_q \) integrals.

We next carry out a data-collapse procedure with the data in Fig. S4. At a classical first-order phase transition, the exponent \( \nu \) relevant for finite-size scaling slightly away from the phase transition takes the trivial value \( \nu = 1/d \) \([40,41]\). In analogy with the case of quantum-critical points, one would expect that \( d \) at a quantum first-order phase transition should be replaced by \( d + z, z \) being the dynamic exponent that relates time and length scales. In the case at hand, one would expect \( z = 2 \), which corresponds to the scaling of the finite-size excitation gap, \( \epsilon \propto L^{-2} \), in a 2D O(N) system. The time scale \( \epsilon^{-1} \) corresponding to this energy is exactly that of the angular fluctuations of the order parameter, as in Anderson’s analogy between the finite-size excitations of an AFM and quantum rotor states (as studied explicitly in QMC calculations in Ref. [55]). Thus, we expect \( 1/\nu = z + 2 = 4 \) to be the relevant scaling exponent describing the rotation of the O(4) vector as the transition point is traversed, and we attempt to describe the data by the finite-size scaling form

\[
I_q(g, L) = f_q((g - g_c)L^4).
\]  

In Fig. S5 we re-graph the data from Fig. S4 versus \((g-g_c)L^4\). We indeed observe very good collapse of the data, except for the smallest systems. These results lend additional support to an emergent O(4) symmetry.

It should be noted here that we did not see clearly that \( 1/\nu_{xy} \) and \( 1/\nu_z \) extrapolate to 4 in Fig. S4(d). There could be two reasons for this. First, as we mentioned also in Sec. 1 above, we have neglected corrections to the assumed leading linear scaling forms in Fig. S4(d). Second, since the excitation gap at the transition should scale as \( 1/L^2 \), there may be some effects of using \( 1/T \propto L \), instead of \( 1/T \propto L^2 \), in the SSE simulations. This would not affect any of the other extrapolated quantities in Fig. S4 as it is still true that \( T \to 0 \) when \( L \to \infty \) and the O(4) coexistence state should have an exponentially large correlation length \( \xi(T) \) as \( T \to 0 \). i.e., \( \xi(T) \gg L \) when \( T \to 1/L \). The projector QMC simulations used here to generate the order-parameter simulations are also fully consistent with coexisting long-range orders and the value of the transition point extracted based on SSE simulations. As we have seen above, the quantitative scaling analysis of the symmetry properties gives further support to the emergent O(4) symmetry in the complete absence of any finite-\( T \) effects.

Along with a finite order parameter at the transition, the O(4) symmetry projected down to two components also implies a flat radial distribution between 0 and the radius \( R \) of the sphere. As we pointed out in the main text and demonstrated in Fig. S4, the not completely flat behavior close to the rim observed in the CBJQ histogram can be explained by finite-size fluctuations of the radius, which should vanish only in the limit \( L \to \infty \). Furthermore, since the O(3) symmetry between the three components of the AFM order parameter is explicitly enforced by the Hamiltonian and is also not violated in any way in the simulations, the demonstration of O(2) symmetry in the distribution \( P(m_z, m_y) \) immediately also implies O(4) symmetry at the AFM-PSS coexistence point.

Thus, we have shown here that for the largest system size available, \( L = 96 \), the CBJQ model has a point at which its combined AFM and PSS order parameters exhibit O(4) symmetry to a high degree, with any potential violation too small to be detectable within the rather small error bars of our results. For the smallest system sizes we do see some deviations.
from perfect symmetry, which is expected when the symmetry is not present in the Hamiltonian but emerges as the system size increases.

Tests with four components.—We complement the above analysis of two out of the four components of the putative O(4) vector with a test where all four components are used, projected down to two dimensions by using the magnitude of the full O(3) AFM order parameter in Eq. (S2) and the PSS order parameter, i.e., the distribution \( P(m_s, m_p) \). We carry out a process similar to the one discussed above to put the overall lengths of the AFM and PSS components on equal footing.

For an ideal O(4) sphere with fixed \( R \) projected down to two dimensions in this manner, the distribution \( P(m_s, m_p) \) has the shape of arc of infinitesimal thickness and radius \( R \), with the density varying proportionally to \( m_z^2 \) along the arc, due to the different contents (number of components of the 4-dimensional vector) of the two dimensions. Fig. S6(a) shows the distribution for three different values of the standard deviation \( \sigma \) of the fluctuating radius about the mean value \( R = 1 \). In the case of the CBJQ model, as shown in Fig. S6(b), there is indeed very little weight close to the y-axis as expected. As we go from the PSS state to the AFM state the weight shifts clockwise from large \( y \) \( (m_p) \) values down toward the x-axis (large \( m_s \)). At the transition point we see a distribution very similar to the O(4) sphere with \( \sigma \approx 0.20 \).

It should be noted that \( m_z^2 \) in the valence-bond basis is obtained from the transition graph as a sum of squared loop lengths, and this corresponds to a sum over \( 2^n \) spin configurations in the basis of \( S^z \) spins, \( n_l \) being the number of loops (each loop having two compatible staggered spin configurations). This implicit averaging over points on the putative O(4) sphere may cause some additional smearing in \( P(m_z, m_p) \), beyond just the projection down to two dimensions and the fluctuations of the radius associated with finite system size. The somewhat larger \( \sigma \) required to match the O(4) sphere in Fig. S6 than what was needed in the case of \( P(m_s, m_p) \) in Fig. S4 likely reflects this effect. In addition, for finite system size, the loop estimator for \( m_s \) has a strict lower bound \( \propto L^{-2} \), with a de facto large prefactor, and this also seems to cause some visible deviations from the O(4) sphere results at the left tip of the distribution. For these reasons, we believe that the \( P(m_z, m_p) \) distribution is better for quantitatively characterizing the degree of symmetry.

3. The CBJQ model with \( Q \Lambda \neq Q_W \)

One might wonder whether the CBJQ model could have an accidental emergent symmetry, i.e., that a generically present symmetry-breaking perturbation at the transition point could
be absent, or extremely small, in this particular model. In order to exclude such a fine-tuning scenario, we here deform the CBJQ model in a significant way by introducing four-spin coupling of strength $Q_B$ on the plaquettes without Q-couplings in Eq. (1) and Fig. 1. We refer to the previously present plaquette couplings as $Q_A$. Calling the two sets of plaquettes $\square_A$ and $\square_B$, the Hamiltonian of this extended CBJQ model is

$$H = -J \sum_{ij} P_{ij} - Q_A \sum_{ijkl \in \square_A} (P_{ij} P_{kl} + P_{ik} P_{jl}) - Q_B \sum_{ijkl \in \square_B} (P_{ij} P_{kl} + P_{ik} P_{jl}).$$

(S9)

When $Q_A = Q_B$, this model becomes the ordinary $J$-$Q$ model on the square lattice, which hosts a four-fold degenerate columnar VBS and where no convincing signs of a first-order transition between it and the AFM has been detected. The non-magnetic state in the extended CBJQ model is likely a two-fold degenerate PSS for any $Q_A \neq Q_B$, though this is not completely clear because of the checkerboard deformation of the square-lattice system is still also compatible with a four-fold degenerate columnar VBS. If indeed we have the PSS for all $Q_A \neq Q_B$, then for $Q_A$ very close to $Q_B$ there will be interesting cross-over behaviors as the system size is increased, from an almost $Z_4$ symmetric columnar VBS to a $Z_2$ symmetric PSS. However, the first-order behavior we have found here for $Q_B = 0$ may in principle end at a tricritical point at some $0 < (Q_B/Q_A)_t < 1$, with a continuous AFM-PSS transition obtaining for $(Q_B/Q_A)_t < Q_B/Q_A < 1$. In a future study, we plan to investigate these and other issues for the extended CBJQ model in its full range of the ratio $Q_B/Q_A$.

Here we only consider $Q_B/Q_A = 1/2$, for which we find that the transition is still first-order and the nonmagnetic state is indeed the PSS. We focus on the histogram approach for detecting emergent O(4) symmetry. The added interaction is sufficiently strong so that an accidental emergent symmetry cannot be the explanation for our finding for $Q_B/Q_A = 0$ if we also find O(4) symmetry when $Q_B/Q_A = 1/2$—unless this whole class of extended CMQJ models is automatically fine-tuned, which by itself would be remarkable and an indication that symmetry perturbations can be broadly avoided (likely beyond the CBJQ models) under previously overlooked circumstances.

We proceed using the same methods as previously, here up to system size $L = 96$. We find $g_c = 0.139 \pm 0.001$ and the length of the O(4) vector with the same normalization as in the previous section is about 10% of the maximum value, or 40% of the value found when $Q_B = 0$. Scaled results for the integrals $I_q$ are shown in Fig. S7. Here we observe the same kind of behavior as in Fig. S5 with good data collapse and no discernible deviations from 0 of the $I_q$ values at $g_c$. Thus, we conclude that the emergent O(4) symmetry is not due to some accidental fine-tuning but an intrinsic feature of the CBJQ class of models.

Comparing Figs. S5 and S7 we see that the scaled integrals are close to zero over a wider range of $(g - g_c)L^4$ when the first-order transition is weaker, i.e., for $Q_B/Q_A = 1/2$. This is natural in light of the larger fluctuations as the discontinuities of the order parameters weaken. The behavior also points to an important role of a quantum-critical point that may be reachable as $Q_B/Q_A$ is further increased (but not up to $Q_B/Q_A = 1$, where the non-magnetic state is different, a columnar VBS breaking $Z_4$ symmetry). The emergent symmetry may ultimately be connected to some extension of the DQCP scenario, as also mentioned in the main paper.

These results of course do not prove that the emergent symmetry exists up to infinite length scale. In the scenario of an approximate symmetry at the first-order transition being due to a nearby critical point with exact emergent symmetry, one would expect the length scale up to which the approximate symmetry applies to be larger when the order parameter is smaller. Therefore, it would clearly be useful to also study a model where the coexisting order parameters are larger than for the case $Q_B = 0$. However, so far we have not found any way to make the transition more strongly first-order within the CBJQ models.