

# Emergence of U(1) Symmetry in the 3D XY Model with $Z_q$ Anisotropy

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We study the three-dimensional XY model with a  $Z_q$  anisotropic term. At temperatures  $T < T_c$  this dangerously irrelevant perturbation is relevant only above a length scale  $\Lambda$ , which diverges as a power of the correlation length,  $\Lambda \sim \xi^{a_q}$ . Below  $\Lambda$  the order parameter is U(1) symmetric. We derive the full scaling function controlling the emergence of U(1) symmetry and use Monte Carlo results to extract the exponent  $a_q$  for  $q = 4, \dots, 8$ . We find that  $a_q \approx a_4(q/4)^2$ , with  $a_4$  only marginally larger than 1. We discuss these results in the context of U(1) symmetry at deconfined quantum-critical points separating antiferromagnetic and valence-bond-solid states in quantum spin systems.

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A remarkable feature of the recently proposed theory of “deconfined” quantum-critical points, which separate Néel and valence-bond-solid (VBS) ground states of antiferromagnets on the square lattice, is the emergence of U(1) symmetry [1]. The VBS either is dimerized on columns or forms a square pattern with plaquettes of four strongly entangled spins [2,3]. In both cases there are four degenerate patterns and, thus,  $Z_4$  symmetry is broken. However, as the critical point is approached, the theory predicts a length scale  $\Lambda$ , diverging faster than the correlation length,  $\Lambda \sim \xi^a$ ,  $a > 1$ , below which the distinction between columnar and plaquette VBS states disappears. The nature of the VBS state is manifested only when coarse graining on length scales  $l > \Lambda$ , whereas for  $l < \Lambda$  there is an emergent U(1) symmetry characterizing the fluctuations between columnar and plaquette order.

Quantum Monte Carlo simulations [4] of an  $S = 1/2$  Heisenberg model with four-spin couplings have recently provided concrete evidence for a continuous Néel-VBS transition, and also detected U(1) symmetry in the VBS order-parameter distribution. There was no trace of the expected  $Z_4$  anisotropy in the VBS phase although the finite-size scaling of the squared order parameter shows that the system is long-range ordered. This can be interpreted as the largest studied lattice size  $L = 32 < \Lambda$ . A distribution without  $Z_4$  features was also found in simulations of an SU(N) generalization of the Heisenberg model [5], which may be a consequence of proximity of this system to a deconfined quantum-critical point.

In order to better understand the U(1) features of these VBS states, and to guide future studies of them, we here exploit a classical analogy. In the three-dimensional XY model including a  $Z_q$ -anisotropic term,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - h \sum_i \cos(q\theta_i), \quad (1)$$

the anisotropy is dangerously irrelevant for  $q \geq 4$  [6–10]; i.e., the universality class is that of the isotropic XY model but the perturbation is relevant for  $T < T_c$  above a length

scale  $\Lambda$ . In the closely related  $q$ -state clock model, the anisotropy is dangerously irrelevant for  $q \geq 5$ . While numerical studies [11–13] have confirmed the irrelevance of the anisotropy at  $T_c$ , the associated  $\Lambda$  has, to our knowledge, not been extracted numerically, except for an analysis of the 3-state antiferromagnetic Potts model, which corresponds to  $Z_6$  [9,14].

Here we report results of Monte Carlo simulations for  $4 \leq q \leq 8$  on periodic-boundary lattices with  $N = L^3$  sites and  $L$  up to 32. In addition to METROPOLIS single-spin updates, we also use Wolff cluster updates [15] to reduce critical slowing down. We sample the order-parameter distribution  $P(m_x, m_y)$ , where

$$m_x = \frac{1}{N} \sum_{i=1}^N \cos(\theta_i), \quad m_y = \frac{1}{N} \sum_{i=1}^N \sin(\theta_i). \quad (2)$$

The standard order parameter can be defined as

$$\begin{aligned} \langle m \rangle &= \int_{-1}^1 dm_x \int_{-1}^1 dm_y P(m_x, m_y) (m_x^2 + m_y^2)^{1/2} \\ &= \int_0^1 dr \int_0^{2\pi} d\theta r^2 P(r, \theta). \end{aligned} \quad (3)$$

We will compare this with an order parameter  $\langle m_q \rangle$ , which is sensitive to the angular distribution:

$$\langle m_q \rangle = \int_0^1 dr \int_0^{2\pi} d\theta r^2 P(r, \theta) \cos(q\theta). \quad (4)$$

While the finite-size scaling of  $\langle m \rangle$  is governed by the correlation length  $\xi$ ,  $\langle m_q \rangle$  should instead be controlled by the U(1) length scale  $\Lambda$  [9], becoming large for a system of size  $L$  only when  $L > \Lambda$ . Figure 1 shows magnetization histograms at  $h/J = 1$  for  $Z_4$  and  $Z_8$  systems with  $L = 4$  and 32. The angular distribution  $P(\theta) = \int dr r P(r, \theta)$  is also shown. The average radius of the distribution is the magnetization  $\langle m \rangle$ , which decreases with increasing  $L$ . The anisotropy, on the other hand, increases with  $L$ . This is particularly striking for  $Z_8$ , where the  $L = 4$  histogram shows essentially no angular dependence, even though  $T$  is

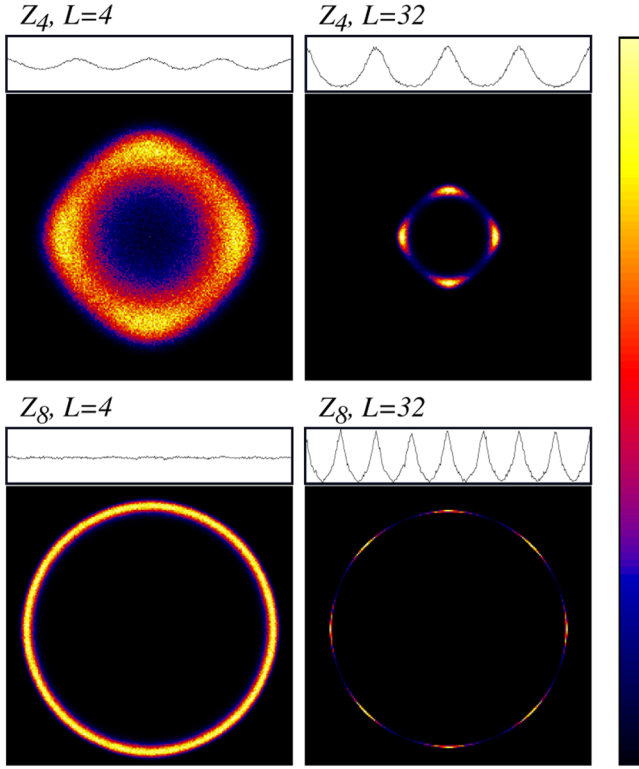


FIG. 1 (color online).  $P(m_x, m_y)$  at  $h/J = 1$  for  $q = 4, 8$ ,  $L = 4, 32$ . The temperature  $T/J = 2.17$  for  $Z_4$  and  $1.15$  for  $Z_8$ , both less than  $T_c/J \approx 2.20$ . The size of the histograms corresponds to  $m_{x,y} \in [-1, 1]$ . Angular distributions  $P(\theta)$  with  $\theta \in [0, 2\pi]$  are shown above each histogram.

very significantly below  $T_c$ , whereas there are 8 prominent peaks for  $L = 32$ . Thus, in this case the U(1) length scale  $4 < \Lambda < 32$ . For the  $Z_4$  system  $T$  is much closer to  $T_c$  but still some anisotropy is seen for  $L = 4$ ; it becomes much more pronounced for  $L = 32$ .

It is instructive to examine a spin configuration with  $m_x \approx m_y$ , i.e.,  $\theta \approx \pi/4$ . Figure 2 shows one layer of a  $Z_4$  system with  $L = 10$  below  $T_c$ . The spins align predominantly along  $\theta = 0$  and  $\theta = \pi/2$ , with only a few spins in the other two directions. Clearly there is some clustering of spins pointing in the same direction—the system consists of two interpenetrating clusters. Essentially, the configuration corresponds to a size-limited domain wall between  $\theta = 0$  and  $\theta = \pi/4$  magnetized states.

Hove and Sudbø studied the  $q$ -state critical clock model [13]. Upon course graining, they found that the structure in the angular distribution diminished with the size of the block spins for  $q \geq 5$ , as is expected for an irrelevant anisotropy. Here we want to quantify the length scale  $\Lambda$  at which the anisotropy becomes relevant for  $T < T_c$ . Consider first what would happen in a course-graining procedure for a single-spin configuration of an infinite system in the ordered state very close to  $T_c$ . With individual spins having  $q$  preferred directions, as seen clearly in Fig. 2, there would be  $q$  peaks in the probability distribution of angles  $\theta_i$ . Averaging over blocks of  $l^3$  spins, we

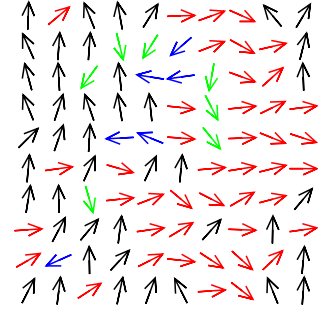


FIG. 2 (color online). Spins in one layer of the  $Z_4$  model with  $L = 10$  at  $h/J = 1$ ,  $T/J = 1.9 < T_c$ . Here  $m_x \approx m_y$ , corresponding to  $\theta \approx \pi/4$  in  $P(r, \theta)$ . Arrows are color-coded according to the closest  $Z_4$  angle;  $n\pi/2$ ,  $n = 0, 1, 2, 3$ .

would expect the angular dependence to become less pronounced because of the averaging over spins pointing in different directions (again, as is seen in Fig. 2). Sufficiently close to  $T_c$  we would expect the distribution to approach flatness. However, since we are in an ordered state, at some  $l \approx \Lambda$  one of the  $q$  preferred angles will become predominant and one peak in the histogram will start to grow. We cannot simulate the infinite system and instead carry out an analogous procedure versus the lattice size  $L$ , sampling a large number of configurations. We calculate the order parameters  $\langle m \rangle$  and  $\langle m_q \rangle$ , defined in Eqs. (3) and (4), and analyze them using

$$\langle m \rangle = L^{-\sigma} f(tL^{1/\nu}), \quad (5)$$

$$\langle m_q \rangle = L^{-\sigma} g(tL^{1/\nu_q}). \quad (6)$$

Here (5) is the standard finite-size ansatz with  $\sigma = \beta/\nu$ , and the XY exponents are  $\beta \approx 0.348$  and  $\nu \approx 0.672$  [16]. Equation (6) is an intuitive generalization of (5), which was proposed and used also in Ref. [9], but we can actually also derive the scaling function  $g(X)$  exactly.

Consider the scaling behavior of the order-parameter distribution  $P(\vec{m})$ . It depends on the system size  $L$  and the size of scaling operators perturbing the critical theory, the temperature deviation  $t = T_c - T$ , and the presumed irrelevant  $q$ -fold anisotropy strength  $h$ . By conventional scaling arguments, we expect

$$P(\vec{m}; L, t, h) = L^{\sigma/2} \hat{P}(L^\sigma \vec{m}, tL^{1/\nu}, H = hL^{3-\Delta_q}), \quad (7)$$

where  $\Delta_q > 3$  is the scaling dimension of the irrelevant anisotropy. The prefactor above is determined from normalization of the probability distribution. In the scaling regime,  $|t| \ll 1$ ,  $L \gg 1$ , so  $H$  is small. When the first two arguments are  $O(1)$ ,  $\hat{P}$  can be well approximated by taking  $H = 0$  [with “corrections to scaling” of  $O(H)$ , i.e., suppressed by  $L^{3-\Delta_q}$  for a large system]. At  $H = 0$ , the distribution is fully XY symmetric, and the integral in Eq. (4) vanishes. Thus, in this regime  $\langle m_q \rangle$  is small,  $O(H)$ , and should be considered as arising from corrections

to scaling. This simply reflects the irrelevance of the anisotropy at the critical point.

Because the anisotropy is *dangerously* irrelevant, a larger contribution, however, emerges when  $tL^{1/\nu} \gg 1$ , i.e.,  $L \gg \xi \sim t^{-\nu}$ . In this limit, the system can be regarded as possessing long-range XY order, and the only significant fluctuations are the *global* fluctuations of the XY phase  $\theta$ . This is biased by the anisotropy. The scale  $\kappa$  of the total anisotropy (free) energy can be estimated by its typical magnitude within an XY correlation volume,  $h\xi^{3-\Delta_q}$ , multiplied by the number of correlation volumes,  $(L/\xi)^3$ , i.e.,  $\kappa = hL^3\xi^{-\Delta_q}$ . Note that although the energy per correlation volume is small (due to the irrelevance of anisotropy at the critical point), the number of correlation volumes becomes very large and more than compensates for this smallness for  $L/\xi$  sufficiently large.

From this argument, we see that for  $L/\xi \gg 1$ , the distribution of angles  $\theta$  is just determined from a Boltzmann factor for a single XY spin with the  $q$ -fold anisotropy energy  $\sim -\kappa \cos q\theta$ . Furthermore, for  $L/\xi \gg 1$ , the magnitude  $|\vec{m}| \approx \langle m \rangle$  is approximately nonfluctuating. Thus the distribution factors into the form  $P(|m|, \theta) = \langle m \rangle^{-2} \delta(|m| - \langle m \rangle) P(\theta)$ , with  $P(\theta) = \frac{1}{Z} e^{\kappa \cos(q\theta)}$ , where  $Z = \int_0^{2\pi} d\theta e^{\kappa \cos(q\theta)}$  is the single-spin partition function. It is then straightforward to obtain from Eq. (4)

$$\langle m_q \rangle = \langle m \rangle \frac{I_1(\kappa)}{I_0(\kappa)}, \quad (8)$$

where  $I_n$  is the modified Bessel function of order  $n$ . Oshikawa obtained a similar expression in a different way [9], but we disagree about his scaling variable. Comparing (8) with the scaling form in Eq. (6), we see that  $\nu_q = \Delta_q \nu / 3$  ( $a_q = \Delta_q / 3$ ),  $\kappa = h(tL^{1/\nu_q})^{3\nu_q}$ , and

$$g(X) \propto \frac{I_1(\tilde{h}X^{3\nu_q})}{I_0(\tilde{h}X^{3\nu_q})}. \quad (9)$$

Here  $\tilde{h}$  should be viewed as a nonuniversal scale factor. From the above discussion, one sees that this form is valid for  $L/\xi \gg 1$  but  $L/\xi_q$  is arbitrary. For  $L/\xi$  of  $O(1)$  or smaller,  $L/\xi_q \ll 1$  (implying  $\kappa, X \ll 1$ ), and the scaling form for  $\langle m_q \rangle$  becomes small and of order the expected correction to scaling in the critical regime.

In Fig. 3 we show results for the two order parameters for systems with  $q = 4, 5, 6$ . We have studied several values of  $h/J$  and here show results for a different value for each  $q$ . We have extracted  $T_c$  using finite-size scaling of  $\langle m \rangle$  with Eq. (5) and the XY exponents. This works very well for all  $q$ , confirming the irrelevance of  $h$ . The magnetization for  $T < T_c$  is seen to decrease marginally with increasing  $q$  in Fig. 3. The  $Z_q$  order parameter  $\langle m_q \rangle$  changes more drastically, being strongly suppressed close to  $T_c$  for large  $q$ . This is expected, as  $\langle m_q \rangle$  should vanish for all  $T$  in the XY limit  $q \rightarrow \infty$ . For  $Z_4$ , the  $\langle m_q \rangle$  curves for different  $L$  cross each other, with the crossing points moving closer to  $T_c$  as  $L$  increases. This is consistent with the

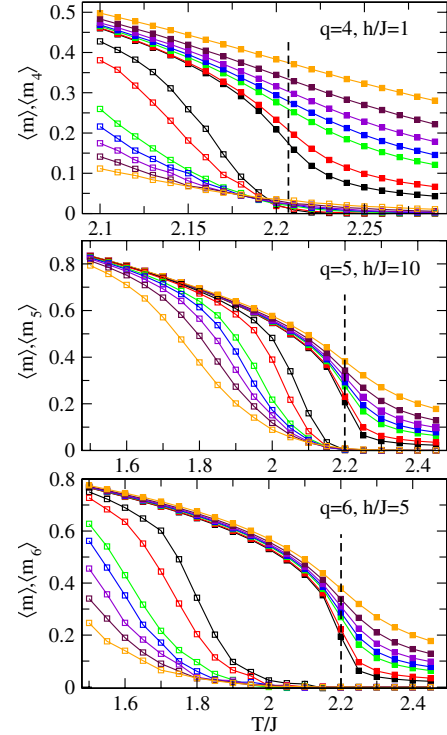


FIG. 3 (color online). The XY order parameter  $\langle m \rangle$  (solid curves) and the  $Z_q$  order parameter  $\langle m_q \rangle$  (dashed curves) vs temperature for  $q = 4, 5, 6$ . The system sizes are  $L = 8, 10, 12, 14, 16, 24$ , and  $32$ . The curves become sharper (increasing slope) around  $T_c$  (indicated by vertical lines). The ratios  $h/J$  used are indicated on the graphs.

above discussion of course graining: In the ordered state close to  $T_c$ ,  $\langle m_q \rangle$  should first, for small  $L$ , decrease with increasing  $L$  as the  $q$ -peaked structure in  $P(\theta)$  diminishes due to averaging over more spins. For larger  $L$ ,  $\langle m_q \rangle$  starts to grow with  $L$  as the length scale  $\Lambda$  is exceeded. This behavior is more difficult to observe directly for  $q = 5, 6$  because  $\langle m_q \rangle$  is small and dominated by statistical noise close to  $T_c$  where the curves cross.

Figure 4 shows finite-size scaling of the  $Z_q$  order parameter  $\langle m_q \rangle$ , using the hypothesis (6) and the XY value for  $\sigma$ . Adjusting  $\nu_q = a_q \nu$  for each  $q$  we find satisfactory data collapse using  $a_4 = 1.07(3)$ ,  $a_5 = 1.6(1)$ ,  $a_6 = 2.4(1)$ , and, not shown in the figure,  $a_8 = 4.2(3)$ . These results are consistent with the form  $a_q = a_4(q/4)^2$ , in qualitative agreement with the  $\epsilon$  expansion by Oshikawa, which gave  $a_q \rightarrow q^2/30$  for large  $q$  [9]. However, in the  $\epsilon$  expansion there are significant deviations from the  $q^2$  form in the range of  $q$  values considered here. Our  $a_6$  is smaller than the value  $\approx 3.5$  obtained on the basis of the 3-state Potts antiferromagnet [9].

In Fig. 4 we also show the scaling function (9). It does not match exactly the collapsed data, but the agreement improves as  $q$  increases. As we have discussed above, the scaling function represents the dominant behavior for  $T < T_c$ , but exactly at  $T_c$  this contribution vanishes and the

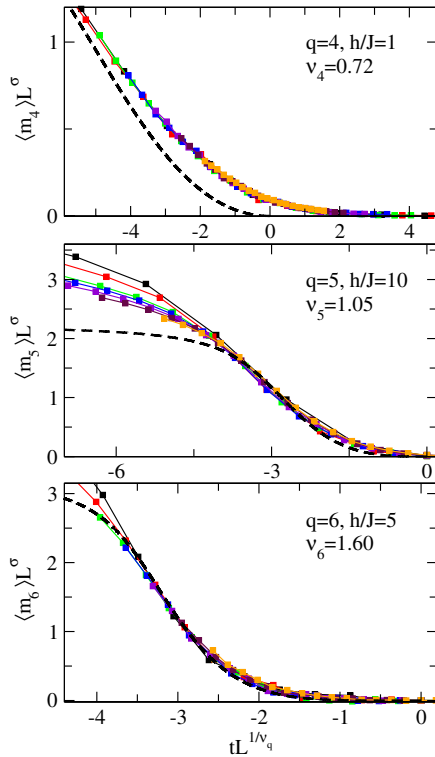


FIG. 4 (color online). Scaling of the  $Z_q$  magnetization. We use  $\sigma = 0.52$  for all  $q$ , and  $\nu_q$  as indicated in the plots. The colors of the curves correspond to  $L$  as in Fig. 3. The dashed curves are the predicted scaling functions with  $\tilde{h}$  and prefactors adjusted to fit the data approximately.

critical-point scaling behavior  $\langle m_q(T_c) \rangle \sim L^{3-\Delta_q}$  becomes dominant. For  $q = 4$ ,  $\Delta_4 - 3$  is small; our estimate is  $\Delta_4 - 3 = 0.21(9)$ , in good agreement with previous estimates of the scaling dimension [8,10]. Thus it is clear that very large systems would be required for this contribution to become invisible on the scale used in our graph. It is also clear that for  $t < 0$ , close to  $t = 0$ , there will be a similarly significant correction to the asymptotically dominant scaling function. As  $q$  increases, we have seen that  $\Delta_q = 3a_q$  increases rapidly, and we thus expect a significantly smaller correction to scaling. For  $q = 6$  the agreement is already seen to be quite good, considering that our lattices are not very large.

To conclude, we relate our results to the quantum VBS states discussed in the introduction. Returning to Fig. 2, associating  $\theta_i \approx 0$  arrows with two adjacent horizontal dimers on even-numbered columns and  $\theta_i \approx \pi/2$  with vertical adjacent dimers on even rows,  $\langle \theta \rangle = 0, \pi/2$  correspond to columnar VBS states. A plaquette is a superposition of horizontal and vertical dimer pairs, whence a plaquette VBS corresponds to  $\langle \theta \rangle = \pi/4$  [3]. Rotating the arrows by  $90^\circ$  corresponds to translating or rotating a VBS. Either a columnar or plaquette VBS should obtain in the infinite-size limit, but close to a deconfined quantum-

critical point, for  $L < \Lambda$ , the system fluctuates among all mixtures of plaquette and columnar states. This corresponds to a ring-shaped VBS order-parameter histogram. In numerical studies of quantum antiferromagnets [4,5] no 4-peak structure was observed in the angular distribution, and hence it is not clear what type of VBS finally will emerge (although a method using open boundaries favors a columnar state in [4]). It seems unlikely that the  $U(1)$  symmetry should persist as  $L \rightarrow \infty$ . In the classical  $Z_4$  model we never observe perfectly  $U(1)$ -symmetric histograms far inside the ordered phase, in contrast to Refs. [4,5]. On the other hand,  $a_q$  is larger for  $q > 4$ , and in Fig. 1 we have shown a prominently  $U(1)$ -symmetric histogram for the  $Z_8$  model deep inside the ordered phase. Thus, the exponent  $a$  may be larger for the  $Z_4$  quantum VBS than  $a_4 \approx 1$  obtained here for the classical  $Z_4$  model. There is, of course, no reason to expect them to be the same, as the universality class of deconfined quantum criticality is not that of the classical  $Z_4$  model [1,4]. Future numerical studies of VBS states and deconfined quantum criticality can hopefully reach sufficiently large lattices to extract the  $U(1)$  exponent using the scaling method employed here.

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