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Antiferromagnetic to valence-bond-solid transitions in two-dimensional SU(N) Heisenberg models with multispin interactions

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We study two-dimensional Heisenberg antiferromagnets with additional multispin interactions which can drive the system into a valence-bond-solid state. For standard SU(2) spins, we consider both four- and six-spin interactions. We find continuous quantum phase transitions with the same critical exponents. Extending the symmetry to SU(N), we also find continuous transitions for $N=3$ and 4. In addition, we also study quantitatively the crossover of the order-parameter symmetry from Z_4 deep inside the valence-bond-solid phase to $U(1)$ as the phase transition is approached.

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Two-dimensional quantum spin system with nonmagnetic ground states have been at the forefront of condensed-matter physics for more than two decades.[1–4] Frustrated system have been investigated intensely,[5] but large-scale unbiased computational studies of their ground states are not possible, due to the "sign problems" hampering quantum Monte Carlo (QMC) methods.[6] It was recently realized that one prominent class of nonmagnetic states—valence-bond solids (VBSs)—can be accessed also without frustration, by adding certain multispin interactions to the standard $S=1/2$ Heisenberg antiferromagnet.[7] These models enable detailed QMC studies of the antiferromagnetic (AF) to VBS quantum phase transition. It has been argued that this transition is associated with spinon deconfinement (hence the term deconfined quantum criticality) and should, due to subtle quantum interference effects, be continuous.[3] This scenario violates the "Landau rule," according to which a direct phase transition between ground states breaking unrelated symmetries should be generically first order.

The theory of deconfined quantum criticality has generated a great deal of interest, as well as controversy.[7–15] Numerical studies of a Heisenberg hamiltonian with four-spin interactions are generally in good agreement with the theory, showing a continuous transition with dynamic exponent $z=1$, large spin-correlation exponent η_s, and an emergent $U(1)$ symmetry.[7–9] Arguments for a first-order transition have also been put forward,[11,14] based on numerical studies of lattice versions of the CP^1 field theory proposed[3] to capture the AF-VBS transition. Other similar studies reach different conclusions however.[13] Further studies are thus called for.

In this paper, we advance computational studies of the AF-VBS transition in two different ways. First, we consider the $S=1/2$ Heisenberg model including four-spin and six-spin interactions. The unperturbed Heisenberg model is defined by the Hamiltonian

$$H_1 = J\sum_{\langle ij\rangle} \mathbf{S}_i\cdot\mathbf{S}_j = -J\sum_{\langle ij\rangle} C_{ij} + \frac{L^2 J}{2}, \tag{1}$$

where $\langle ij\rangle$ denotes nearest neighbors on a periodic square lattice with L^2 sites and

$$C_{ij} = \frac{1}{4} - \mathbf{S}_i\cdot\mathbf{S}_j \tag{2}$$

is the two-spin singlet projector. In the "J-Q" model introduced in Ref. 7 the following term is added to H_1;

$$H_2 = -Q_2 \sum_{\langle ijkl\rangle} C_{kl}C_{ij}. \tag{3}$$

The spin pairs ij and kl are located on adjacent corners of a four-site plaquette, as illustrated in Fig. 1. We denote the strength of the four-spin term Q_2, with the subscript indicating two singlet projectors, and also consider a similar term with three stacked singlet projectors,

$$H_3 = -Q_3 \sum_{\langle ijklmn\rangle} C_{mn}C_{kl}C_{ij}, \tag{4}$$

as also illustrated in Fig. 1. Using an improved version[16] of a ground-state QMC method operating in the valence-bond basis,[17] we have studied the J-Q_2 and J-Q_3 models on lattices with L up to 64. We find critical AF-VBS points with the same set of exponents for both models, providing additional evidence of a universal deconfined critical point in this class of systems.

In a second development, we have studied SU(N) symmetric versions of the J-Q_2 model, in the representation of

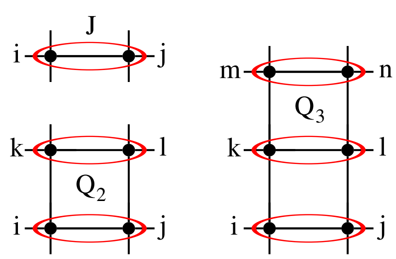

FIG. 1. (Color online) Interactions involving p singlet projectors (illustrated by ovals enclosing two sites) on the square lattice. The two-spin ($p=1$) interaction J is the Heisenberg exchange. Higher-order Q_p terms with $p=2$ and 3 are considered here. All translations and 90° rotations of the site groupings shown here are included in the hamiltonian.

the spin operators previously used in mean-field[2] and QMC calculations[18] of the SU(N) Heisenberg model. We find continuous AF-VBS transitions also for $N=3$ and 4 (whereas for $N>4$ the system is VBS ordered[18,19] for all $Q_2>0$).

An open problem in previous studies of the J-Q_2 model was that the order-parameter distribution inside the VBS phase did not show the expected fourfold symmetry. Instead, the distribution was always $U(1)$ symmetric.[7,9] An emergent $U(1)$ symmetry close to criticality is indeed predicted by the field theory[3] as a consequence of a dangerously irrelevant operator, but deep inside the VBS phase the order parameter should exhibit Z_4 symmetry (which has been observed in other quantum models[19,20]). With the J-Q_3 model and the $N>2$ versions of the J-Q_2 model, we can now reach sufficiently deep inside the VBS phase to observe the expected $U(1)-Z_4$ crossover. We present quantitative finite-size scaling results for the exponent governing the crossover.

For all the models, we compute the square of the staggered magnetization, $M^2=\langle \mathbf{M}\cdot\mathbf{M}\rangle$, where

$$\mathbf{M}=\frac{1}{L^2}\sum_{x,y}(-1)^{x+y}\mathbf{S}_{x,y} \tag{5}$$

is the operator of the AF (spin) order parameter. We define the columnar VBS order parameter in terms of nearest-neighbor (dimer) correlators

$$D_x=\frac{1}{L^2}\sum_{x,y}(-1)^{x}\mathbf{S}_{x,y}\cdot\mathbf{S}_{x+1,y}, \tag{6}$$

and D_y defined analogously. We compute the square $D^2=\langle D_x^2+D_y^2\rangle$ and also study the probability distribution $P(D_x,D_y)$, with D_x and D_y evaluated in the configurations generated in the QMC sampling (as in Ref. 7). To extract the critical points and exponents, we use standard finite-size scaling forms for the order parameters,

$$M^2=L^{-(1+\eta_s)}F_s([q-q_c]L^{1/\nu}), \tag{7}$$

$$D^2=L^{-(1+\eta_d)}F_d([q-q_c]L^{1/\nu}), \tag{8}$$

where η_s and η_d are the exponents governing the spin and dimer correlation functions, respectively, at criticality (the anomalous dimensions) and $1+\eta_{s,d}=2\beta_{s,d}/\nu$. Here we assume a dynamic exponent $z=1$, in accord with previous studies of the J-Q_2 model,[7,8] and use a single correlation length exponent ν, as in the theory.[3]

We first present results for the SU(2) models. Defining coupling ratios $q=Q_p/(J+Q_p)$, we find critical points $q_c=0.961(2)$ for $p=2$ and $q_c=0.600(5)$ for $p=3$. The former agrees with previous estimates.[7–9] Standard data collapse plots according to Eqs. (7) and (8) are shown in Fig. 2. The critical exponents are listed on the first two lines of Table I. Here it is very significant that all the exponents are the same for the two models. This supports the notion of a universal deconfined quantum-critical point. Note that the order parameters decay as $L^{-(1+\eta_{s,d})}$ at the common critical point $q=q_c$. At a first-order transition, the order parameters should instead be size independent at q_c, due to phase coexistence.

Comparing with previous results for the J-Q_2 model, the results for smaller systems in Ref. 7 were consistent with

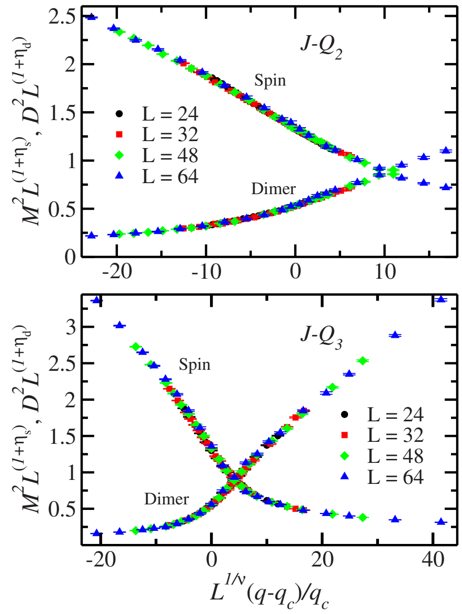

FIG. 2. (Color online) Finite-size scaling of the squared AF and VBS order parameters of the J-Q_2 and J-Q_3 models.

$\eta_s=\eta_d$ (with a value between those found here), but the present results for larger systems clearly show that the spin and dimer exponents are different. The theory does not make any specific predictions for a relationship between η_s and η_d, and they can be expected to be different. The exponents η_s and ν are in good agreement with values obtained using finite-temperature scaling[8] (where η_d was not determined).

Next, we discuss the J-Q_2 model generalized to SU(N) spins. Considering first the Heisenberg model, the Hamiltonian can be written as

$$H_{\mathrm{SU}(N)}=\frac{J}{N}\sum_{\langle ij\rangle}\mathbf{S}_i^{\alpha\beta}\mathbf{S}_j^{\beta\alpha}=-J\sum_{\langle ij\rangle}C_{ij}+\frac{2JL^2}{N^2}, \tag{9}$$

where $\mathbf{S}_i^{\alpha\beta}$ is the generator of the SU(N) algebra, with $\alpha,\beta=1,2,\ldots,N$ the different "colors," and C_{ij} is the generalization of Eq. (2) to SU(N). As in Ref. 18 we focus on the simplest case, where the spins on sublattice A are expressed in the fundamental representation (i.e., with a single-box Young tableau). Spins on sublattice B are SU(N) conjugates (dual representation) of those on A (a Young tableau with one column and $N-1$ rows). The states in this representation can be written in terms of permutations P of the boxes, with

TABLE I. Critical exponent for all the models studied. The crossover exponent a_4 cannot be determined for the SU(2) J-Q_2 model because no crossover is observed for $L\leq 64$.

Model, symmetry	η_s	η_d	ν	a_4
J-Q_2, SU(2)	0.35(2)	0.20(2)	0.67(1)	
J-Q_3, SU(2)	0.33(2)	0.20(2)	0.69(2)	1.20(5)
J-Q_2, SU(3)	0.38(3)	0.42(3)	0.65(3)	1.6(2)
J-Q_2, SU(4)	0.42(5)	0.64(5)	0.70(2)	1.5(2)

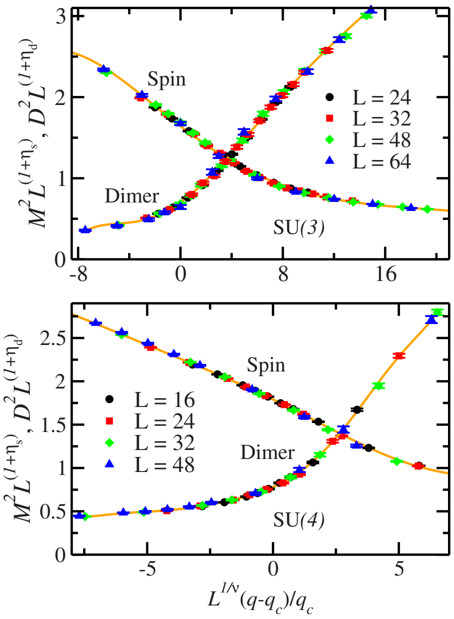

FIG. 3. (Color online) Scaling of the spin and dimer order parameters of the SU(3) and SU(4) J-Q_2 models.

$$|\bar{\alpha}\rangle_j \equiv \frac{1}{\sqrt{(N-1)!}}\sum_P (-1)^P |P(2)P(3)\cdots P(N)\rangle_j, \quad (10)$$

with $\alpha=1,2,\ldots,N$ and $P(1)=\alpha$. An SU(N) singlet of spins i and j on different sublattices is given by

$$|\mathrm{singlet}\rangle_{ij} \equiv \frac{1}{\sqrt{N}}\sum_{\alpha=1}^{N} |\alpha\rangle_i \otimes |\bar{\alpha}\rangle_j. \quad (11)$$

QMC algorithms using these SU(N) spins in the valence-bond basis are simple generalizations of the SU(2) case.[16,17,21] Instead of spins ↑ and ↓ for SU(2), there are N colors, and, thus, N states of the space-time loops in the loop algorithm.[16] The off-diagonal matrix elements of the singlet projection operators are $1/N$ instead of 1/2, and the overlap of two valence-bond states is generalized to $N^{n_\circ - L^2/2}$, where $n_\circ$ is the number of loops in the transposition graph. Four- and six-spin terms (3) and (4) are written explicitly using products of singlet projectors and have obvious generalizations to SU(N).

Our results for the SU(3) and SU(4) versions of the J-Q_2 model are consistent with continuous AF-VBS critical points, with no signs of first-order behavior. The critical couplings are $q_c=0.335(2)$ and $q_c=0.082(2)$ for $N=3$ and 4, respectively. Scaling plots giving the critical exponents are shown in Fig. 3 and numerical values are listed in Table I. As a function of N, ν does not change appreciably, η_s increases slowly, and η_d increases significantly. In the $N=\infty$ theory $\eta_s=1$.[3] A VBS exponent $\eta_d \propto (N-1)$ is expected for $N\to\infty$ on account of the divergent scaling dimension of monopoles in the CP^{N-1} field theory.[23] Our results are consistent with this behavior, $\eta_d \approx (N-1)/5$, already for $N=2,3,4$.

We could, in principle, consider still higher N, but with $J>0$ the system is always in the VBS state for $N=5$ and higher.[18,19] A transition could presumably be reached for $J<0$, but this causes QMC sign problems. Alternatively, without sign problems, one could use longer-range unfrustrated interactions to enforce antiferromagnetic correlations.

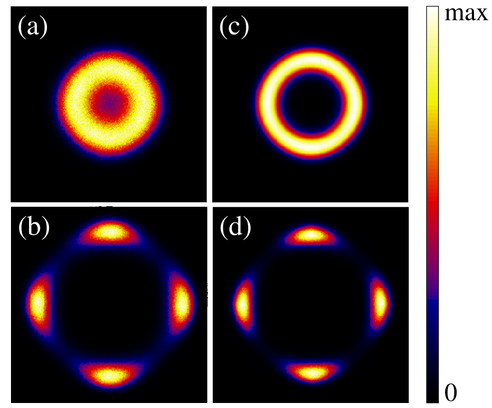

FIG. 4. (Color online) Dimer order distribution $P(D_x,D_y)$ for $L=32$ systems. The left panels are for the J-Q_3 model at (a) $q=0.635$ and (b) $q=0.85$, and the right panels are for the SU(3) J-Q_2 model at (c) $q=0.45$ and (d) $q=0.65$.

The dimer order distribution $P(D_x,D_y)$ can be used to investigate the VBS order-parameter symmetry.[7,18] As shown in Fig. 4, for large q the robust VBSs in the SU(2) J-Q_3 model and the SU(3) and SU(4) versions of the J-Q_2 model result in histograms with clearly visible columnar Z_4 features (i.e., peaks on the D_x and D_y axis, as opposed to 45° rotated histograms expected for a plaquette state). However, in the SU(2) J-Q_2 model the histograms are ring shaped for all system sizes currently accessible, even in the extreme case of $q=1(J=0)$. In all cases, we see $U(1)$ symmetric histograms as the critical point is approached, in agreement with one of the salient features of deconfined quantum criticality.[3]

Defining an order parameter sensitive to the symmetry,

$$D_4^2 = \int dD_x dD_y P(D_x,D_y)(D_x^2+D_y^2)\cos(4\theta) = \int dr \int_0^{2\pi} d\theta P(r,\theta) r^3 \cos(4\theta), \quad (12)$$

where θ is the angle corresponding to a point (D_x,D_y), we proceed as in Ref. 22 (which deals with a classical system with a dangerously irrelevant perturbation) to extract the exponent governing the length scale Λ of the $Z_4-U(1)$ crossover (and the spinon confinement). Z_4 features should appear for $L>\Lambda$, which is predicated[3] to scale as $\Lambda \sim \xi^{a_4}$ where ξ is the correlation length and $a_4>1$. We analyze D_4 assuming the scaling form;[22]

$$D_4^2 = L^{-(1+\eta_d)} F_4(qL^{1/a_4\nu}). \quad (13)$$

This form describes the crossover, as shown in Fig. 5 in two cases. The values of a_4 are listed in Table I. The large error-bars reflect slow evolution of the VBS angle in the QMC simulations. It is nevertheless clear that $a_4>1$ (and increasing with N), reflecting emergent $U(1)$ symmetry due to a

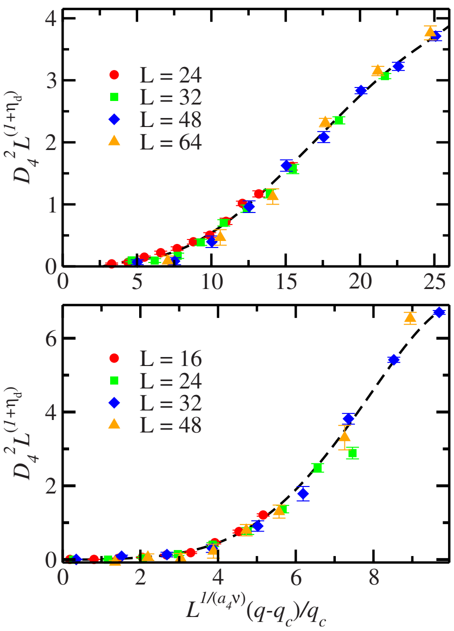

FIG. 5. (Color online) Finite-size scaling of the square of the anisotropic order parameter D_4 in the J-Q_3 model (upper panel) and SU(3) J-Q_2 model (lower panel).

dangerously irrelevant perturbation (which here is the lattice enforcing the fourfold degenerate VBS).

The results presented here support deconfined quantum criticality. Although one can still, in principle, not completely rule out very weakly first-order transitions based on these calculations, the universal behavior for the two SU(2) models makes this less likely. The common exponents for the J-Q_2 and J-Q_3 models at the very least suggest close proximity to a universal critical point. The detailed information now available from QMC simulations should be useful to further advance the theory.

In a very interesting experimental development, Itou *et al.* recently measured the spin-lattice relaxation rate $1/T_1$ in a layered organic compound which seems to be near critical.[24] It has been argued that, in spite of the triangular lattice, the AF-VBS transition in this kind of system should be in the same class of deconfined quantum-critical points discussed here.[25] The exponent η_s governs the temperature scaling of $1/T_1$, and the value $\eta_s \approx 0.35$ is in excellent agreement with the experiment over a wide range of temperatures. Further experiments should elucidate the nature of the ground state and whether it is indeed close to a deconfined quantum-critical point.

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