Evidence for Deconfined Quantum Criticality in a Two-Dimensional Heisenberg Model with Four-Spin Interactions

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Using ground-state projector quantum Monte Carlo simulations in the valence-bond basis, it is demonstrated that nonfrustrating four-spin interactions can destroy the Néel order of the two-dimensional $S = 1/2$ Heisenberg antiferromagnet and drive it into a valence-bond solid (VBS) phase. Results for spin and dimer correlations are consistent with a single continuous transition, and all data exhibit finite-size scaling with a single set of exponents, $z = 1$, $\nu = 0.78 \pm 0.03$, and $\eta = 0.26 \pm 0.03$. The unusually large η and an emergent $U(1)$ symmetry, detected using VBS order parameter histograms, provide strong evidence for a deconfined quantum critical point.

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Since the discovery in 1986 of high-T_c superconductivity in layered cuprates, quantum phase transitions in two-dimensional (2D) antiferromagnets have formed a central topic in condensed matter physics [1,2]. While superconductivity is induced in the CuO_2 planes of the cuprates by doping with charge carriers, other mechanisms for destroying the Néel order and stabilizing different ground states have also been intensely investigated theoretically. Considerable effort has been devoted to possible spin liquid (''RVB'' [3]) and valence-bond solid (VBS) states driven by magnetic frustration [4–6]. This work has been partially motivated by the hope that an understanding of generic features of quantum phase transitions in 2D antiferromagnets could shed light also on the mechanisms at work in the cuprates [7]. Quantum fluctuation driven phase transitions are also of broader relevance in the context of strongly correlated systems [8].

A quantum phase transition occurs as a function of some parameter at temperature $T = 0$ and corresponds to a $T > 0$ transition in an effective classical system with an imaginary-time dimension—the path integral [9]. The standard Landau-Ginzburg-Wilson framework for critical phenomena should thus be applicable, with the dimensionality $d \rightarrow d + z$, where the dynamic exponent z depends on the way space and time correlations are related. In the paradigm prevailing until recently, the ''Landau rules'' for the nature of the transition—continuous or first order—were also assumed to remain valid for quantum phase transitions. A direct transition between two ordered phases should thus be generically first order if two different symmetries are broken. This notion has recently been challenged by Senthil *et al.*, who argued that quantum phase transitions separating two ordered phases can be generically continuous, even when different symmetries are broken [10]. This theory of ''deconfined'' quantum critical points was first developed for the transition between an antiferromagnetic (AF) and a VBS state. Both these states have confined $S = 1$ excitations—gapless magnons and gapped ''triplons'', respectively. The critical point is characterized by deconfined $S = 1/2$ spinons coupled to an emergent $U(1)$ gauge field [10]. In 2D the deconfined state is unstable and exists only at a point separating the two ordered phases. The AF and VBS order parameters arise as a consequence of spinon confinement. In this Letter, quantum Monte Carlo (QMC) results are presented which support this theory.

Preceding the theory of deconfined quantum critical points, continuous transitions between two ordered quantum states had been suggested based on numerical simulations [11,12]. However, in more detailed studies following the theoretical developments it has proved difficult to confirm their existence. Instead, many studies have pointed to weakly first-order AF-VBS transitions [13–17] or other scenarios inconsistent with deconfined quantum criticality [18]. To date, large-scale QMC studies of potential deconfined quantum critical points have focused on spin (or hard-core bosonic) models with spin-anisotropic interactions [13–16]. Frustrated $SU(2)$ (Heisenberg) symmetric interactions, which cannot be studied using QMC simulations due to the infamous ''sign problem'', have been considered in exact diagonalization studies [19]. Because of the limitations to very small lattices, it has not been possible to study phase transitions in detail, however. In fact, not even the nature of the VBS state has been completely settled in basic models such as the J_1-J_2 frustrated Heisenberg model [20].

Here it will be shown that the AF order of the square-lattice Heisenberg model can be destroyed also by nonfrustrated isotropic interactions accessible to QMC simulations. The following Hamiltonian will be discussed:

$$H = J\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j - Q\sum_{\langle ijkl\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \tfrac{1}{4})(\mathbf{S}_k \cdot \mathbf{S}_l - \tfrac{1}{4}), \quad (1)$$

where $\langle ij\rangle$ denotes nearest-neighbor sites and $\langle ijkl\rangle$ refers to the corners of a plaquette, such that ij and kl form two parallel adjacent horizontal or vertical links. This interaction contains a subset of the four-site ring exchange, and with $Q > 0$ there is no QMC sign problem. Note that the

purpose here is not to model any specific material, but simply to construct a model system in which an AF-VBS transition can be investigated. It will be shown below that the ground state of the J-Q model has AF order for $J/Q \gtrsim 0.04$ and VBS order for $J/Q \lesssim 0.04$.

To study the ground state of the Hamiltonian (1), an approximation-free projector technique in the valence-bond basis [21] is employed which is ideally suited for multispin interactions formed out of singlet projection operators $(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4})$. Here $L \times L$ lattices with L up to 32 are considered. Larger systems may be reachable using loop algorithms in the standard S^z basis, which have been used for $U(1)$ models with four-site interactions [22,23]. The valence-bond basis has its advantages, however, including an improved estimator for the singlet-triplet gap.

Results will be presented for spin-spin (s) and dimer-dimer (d) correlation functions,

$$C_s(\mathbf{r}) = \langle \mathbf{S}(\mathbf{0}) \cdot \mathbf{S}(\mathbf{r}) \rangle, \tag{2}$$

$$C_d(\mathbf{r}) = \langle [\mathbf{S}(\mathbf{0}) \cdot \mathbf{S}(\hat{\mathbf{x}})][\mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r} + \hat{\mathbf{x}})] \rangle, \tag{3}$$

where $\hat{\mathbf{x}}$ denotes a lattice unit vector in the x direction. The AF order parameter is the staggered magnetization, the square of which is calculated

$$M^2 = \frac{1}{N} \sum_{\mathbf{r}} C_s(\mathbf{r}) (-1)^{r_x + r_y}. \tag{4}$$

The VBS state can have either columnar or plaquette order, both of which break Z_4 symmetry. An important aspect of the theory is that these order parameters should both exhibit divergent fluctuations at the deconfined critical point. Only at some length-scale diverging as a power of the correlation length should one of them be singled out [10]. This is analogous to the irrelevance of Z_4 anisotropy in the 3D XY model [24] and corresponds directly to the predicted emergent $U(1)$ symmetry. The $\mathbf{q} = (\pi, 0)$ dimer order parameter,

$$D^2 = \frac{1}{N} \sum_{\mathbf{r}} C_d(\mathbf{r}) (-1)^{r_x}, \tag{5}$$

is divergent for both columnar and plaquette VBS order and will be studied here.

Extrapolations of the AF and VBS order parameters, shown in Fig. 1, demonstrate that there is long-range VBS order but no AF order at maximal four-spin interaction, $J/Q = 0$ (note that there are still two-site interactions present when $J = 0$; simulations for $J < 0$ are sign problematic). Also shown are results at $J/Q = 0.1$, where the situation is the reverse; there is AF order but the VBS order vanishes. Thus there is an AF-VBS transition somewhere in the range $0 < J/Q < 0.1$, or there could be a region of AF-VBS coexistence (which would be analogous to a supersolid state). The nature of the VBS order—columnar or plaquette—is not clear from these calculations. However, simulations of open-boundary rectangular lattices, in which a unique columnar or plaquette pattern can be stabilized [12], indicate that columnar order is preferred.

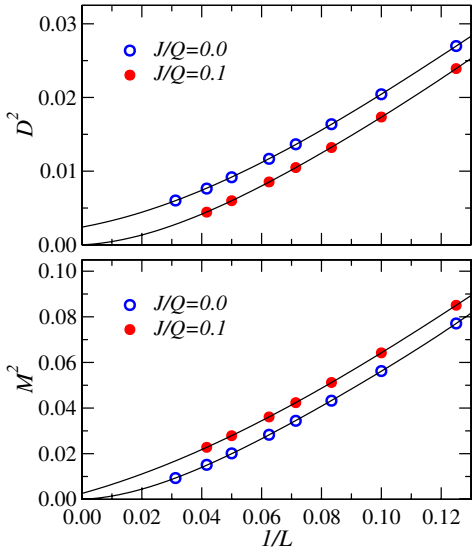

FIG. 1 (color online). Finite-size scaling of the squared spin (M) and dimer (D) order parameters at $J/Q = 0$ and 0.1. The curves are cubic fits. Statistical errors are much smaller than the symbols.

The extrapolated VBS correlation at $J/Q = 0$ is $D^2 \approx 0.0024$.

The deconfined theory has dynamic exponent $z = 1$ [10]. This exponent can be directly accessed through the finite-size scaling of the singlet-triplet gap; $\Delta \sim L^{-z}$. To demonstrate consistency with $z = 1$, the scaling of $L\Delta$ is shown in Fig. 2 for $J/Q = 0$ and 0.1, as well as for $J/Q = 0.04$ which will be shown below to be close to criticality. Here $L\Delta$ extrapolates to a nonzero value, supporting $z = 1$, and at $J/Q = 0$ and 0.1 the behaviors are what would be expected off criticality. The inset of Fig. 2 shows an infinite-size extrapolation of the gap at $J/Q = 0$, giving $\Delta/Q \approx 0.07$.

Correlation lengths ξ_s and ξ_d for spins and dimers are defined in the standard way as the square roots of the second moments of the correlation functions (2) and (3). Also useful is the Binder cumulant, defined for the spin as $q_s = \langle M^4 \rangle / \langle M^2 \rangle^2$. Finite-size scaling of these quantities is used to extract the critical coupling and the correlation length exponent ν. To achieve good data collapse, a subleading correction is also included. With $g = J/Q$, the scaling ansatz is

$$A(g, L) = L^{\kappa}(1 + aL^{-\omega}) f[(g - g_c)L^{1/\nu}], \tag{6}$$

where $A = \xi_s$, ξ_d, or q_s, and $\kappa = 1$ for ξ_s, ξ_d and 0 for q_s. As seen in Fig. 3, these quantities can be scaled using $g_c = 0.040 \pm 0.003$ and a common $\nu = 0.78 \pm 0.03$. In all cases, the subleading exponent $\omega \approx 2$, and the scaling is nearly as good if $\omega = 2$ is fixed throughout. Interestingly, the best prefactor a is then almost equal for ξ_s and ξ_d, $a \approx 8$, but this may be coincidental.

Next, the correlation functions $C_{s,d}(\mathbf{r})$ at the longest lattice distance, $\mathbf{r} = (L/2, L/2)$, are analyzed to extract the correlation function exponent η. The expected scaling

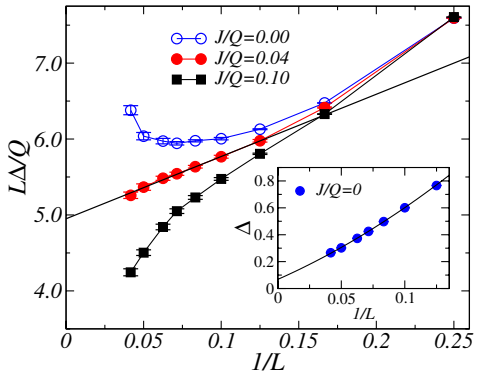

FIG. 2 (color online). Finite-size scaling of the singlet-triplet excitation gap multiplied by the system size L. The behavior at $J/Q = 0.04$ corresponds to $z = 1$.

is as in Eq. (6) with $\kappa = -(1 + \eta)$. Now g_c and ν are kept fixed at the values determined above. As shown in Fig. 4, a single exponent describes both the spin and dimer data, and in this case a subleading correction is not needed ($a = 0$). The exponent, $\eta = 0.26 \pm 0.03$, is unusually large. In the 3D $O(3)$ universality class, describing transitions between the AF and a featureless gapped state [1,25], $\eta \approx 0.04$. A larger η for deconfined quantum criticality was argued for on physical grounds by Senthil *et al.* [10]. The universality class was argued to be that of the hedgehog suppressed $O(3)$ transition, for which $\beta/\nu = (1 + \eta)/2 = 0.80 \pm 0.05$ was obtained in simulations of a classical model in [26]. This is larger than $\beta/\nu = 0.63 \pm 0.02$ found here, but on the other hand smaller lattices were used in [26] and there may also be issues with how hedgehogs were suppressed. The direct study of an actual AF-VBS transition presented above can thus be expected to be more reliable.

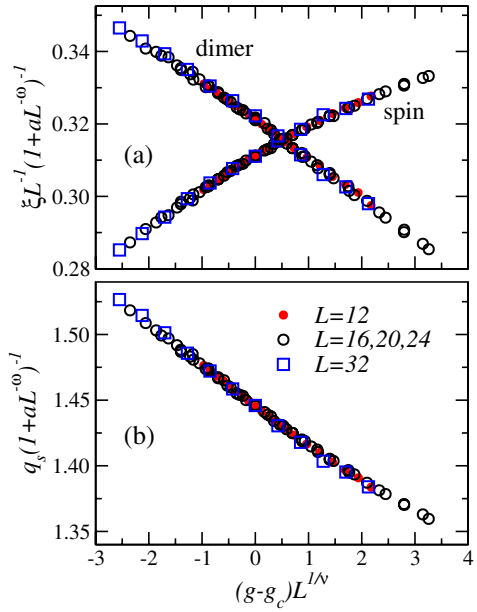

FIG. 3 (color online). Scaling with $\nu = 0.78$ and $g_c = 0.04$ of the correlation lengths (a) and the spin Binder ratio (b).

It is also interesting to study the probability distribution $P(D_x, D_y)$ of the dimer order parameter. In the VBS phase, one would expect this distribution to reflect the Z_4 symmetry; i.e., for a columnar VBS there should be peaks at $D_x = 0$, $D_y = \pm D$ and $D_x = \pm D$, $D_y = 0$ (whereas a plaquette state would give rise to peaks rotated by 45°). It should be noted, however, that $P(D_x, D_y)$ is a basis dependent function. In the valence-bond simulations [21] the order parameters used to construct $P(D_x, D_y)$ are matrix elements (with $\hat{\mathbf{e}} = \hat{\mathbf{x}}, \hat{\mathbf{y}}$),

$$D_e = \frac{\langle \Psi_b | \frac{1}{N} \sum_r \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r} + \hat{\mathbf{e}})(-1)^{r_e} | \Psi_a \rangle}{\langle \Psi_b | \Psi_a \rangle}, \qquad (7)$$

where $|\Psi_a\rangle$, $|\Psi_b\rangle$ are valence-bond states generated by operating with a high power H^n on a trial state (stochastically sampling valence-bond state evolutions). Although $P(D_x, D_y)$ is not a physically measurable quantity, any symmetry detected in it should reflect an underlying symmetry of the projected state. Figure 5 shows a color-coded $P(D_x, D_y)$ histogram generated at $J/Q = 0$. The expected Z_4 symmetry of the VBS is not seen; instead the histogram is ring shaped, which indicates a $U(1)$ symmetric order parameter. Such an emergent $U(1)$ symmetry is in fact predicted [10] by the deconfined theory in the VBS phase below a length scale Λ which diverges faster than the VBS correlation length; $\Lambda \sim \xi_d^a$, with $a > 1$. Thus, inside the VBS phase, if the system length $L \ll \Lambda$ one should expect to find an $U(1)$ symmetric order parameter, with the Z_4 becoming relevant only for larger sizes (and then seen as four peaks emerging in the histogram). Here, apparently, even at $J/Q = 0$ the system is close enough to the critical point for the system length ($L = 32$) to be less than Λ and, hence, Z_4 to be irrelevant. Recalling that the VBS gap is small, $\Delta/Q \approx 0.07$, and that $\Lambda \sim \xi_d^a \sim \Delta^{-a}$, this seems reasonable. On moving closer to the critical point, $P(D_x, D_y)$ smoothly evolves into a single broad peak centered at $(0, 0)$, as is expected for a continuous transition. Note that the finite-size extrapolation of the order parameter in Fig. 1 is not sensitive to the nature of the VBS state—plaquette or columnar—and should give the correct mag-

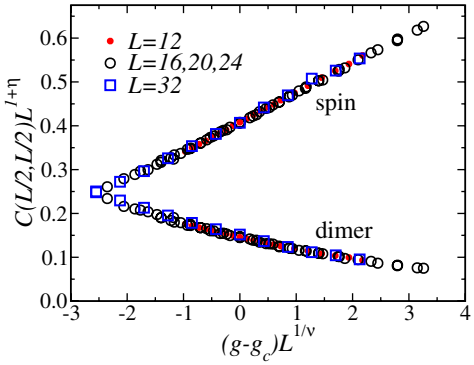

FIG. 4 (color online). Long-distance spin and dimer correlations scaled using $\nu = 0.78$, $\eta = 0.26$, and $g_c = 0.04$.

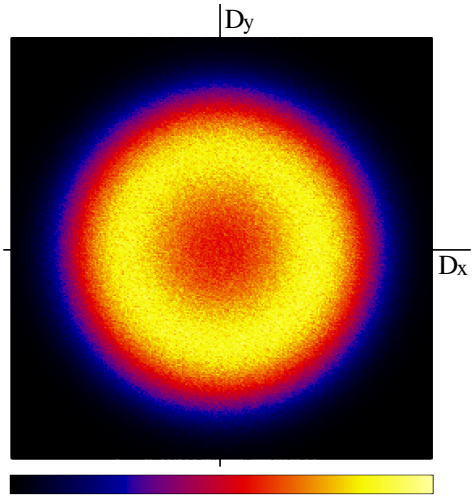

FIG. 5 (color online). Histogram of the dimer order parameter for an $L = 32$ system at $J/Q = 0$. The ring shape demonstrates an emergent $U(1)$ symmetry, i.e., irrelevance of the Z_4 anisotropy of the VBS order parameter.

nitude of the order parameter even though no Z_4 features are yet seen in the histogram for these system sizes.

The above analysis points consistently to a deconfined quantum critical point as the most likely scenario for the AF-VBS transition in the J-Q model. One set of exponents describes both spin and dimer correlations, the value of η is unusually large, and there is an emergent $U(1)$ symmetry in the VBS order parameter. In principle, one cannot rule out a weakly first-order transition on the basis of finite-size data. However, although the lattice sizes used in this work are not extremely large, it would be hard to explain why a first-order transition should lead to the kind of scaling observed. A narrow region of AF-VBS coexistence is also unlikely, as there would then be two transitions and there is no reason to expect the spin and dimer critical exponents to be the same (in particular, the unusually large η). It is difficult to say anything more quantitative regarding a possible first-order transition or coexistence based on the calculations presented here.

An emergent $U(1)$ symmetry may also explain why it has been so difficult to determine the nature of the VBS state in the J_1-J_2 Heisenberg model [20]. Even if the transition would turn out to be weakly first order in this case [17,27], an emergent $U(1)$ symmetry could still affect small lattices, thus making it difficult to distinguish between columnar and plaquette VBS patterns. Emergent $U(1)$ symmetry may be more common than deconfined quantum criticality and could hence affect many models with VBS states. The high density of low-lying singlets associated with $U(1)$ symmetry may also affect exact diagonalization studies [6] of level spectra.

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