Continuous quantum phase transition between an antiferromagnet and a valence-bond-solid in two dimensions; evidence for logarithmic corrections to scaling

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The antiferromagnetic to valence-bond-solid phase transition in the two-dimensional J-Q model (an $S = 1/2$ Heisenberg model with four-spin interactions) is studied using large-scale quantum Monte Carlo simulations. The results support a continuous transition of the ground state, in agreement with the theory of “deconfined” quantum criticality. There are, however, large corrections to scaling, of logarithmic or very slowly decaying power-law form, which had not been anticipated. This suggests that either the SU($N$) symmetric noncompact CP$^N$ field theory for deconfined quantum criticality has to be revised, or that the theory for $N = 2$ (as in the system studied here) differs significantly from $N \to \infty$ (where the field theory is analytically tractable).

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Valence-bond solid (VBS) states of two-dimensional (2D) quantum spin systems have been studied for more than two decades [1] and have recently come into renewed focus with the theory of “deconfined” quantum criticality (DQC) [2, 3, 4], which describes the transition between an antiferromagnetic (AF) and a VBS ground state in terms of deconfinement of spinons. In addition to the interest in such AF–VBS transitions in condensed matter physics, there are also intriguing connections to deconfinement in gauge theories in particle physics [1]. To test the validity of the DQC scenario, and to obtain quantitative results for, e.g., predicted unusual critical exponents, unbiased numerical studies of quantum spin hamiltonians with AF–VBS transitions are necessary.

The “J-Q” model was introduced recently [5] as an SU(2) symmetric spin system realizing the 2D AF–VBS transition, following earlier work on related U(1) symmetric models [6, 7]. It combines the standard Heisenberg antiferromagnet with four-spin interactions, which lead to local correlated bond singlets (valence bonds) and reduce the amplitudes of the longer valence bonds required [8] in an AF state. The J-Q model is free from “sign problems” [9], which prohibit quantum Monte Carlo (QMC) studies of frustrated spin systems such as the J$_1$–J$_2$ Heisenberg model [10], on which much of the past computational (exact diagonalization) research on VBS states was focused. While series expansions [11] around various candidate states can give some insights, QMC methods [12], when applicable, are the only unbiased tools for studying 2D quantum phase transitions (in contrast to one dimension, where the density-matrix-renormalization-group method [13] is applicable) [14]. Being sign problem free, the J-Q model (and generalizations of it [15]) have opened up new avenues for exploring magnetically quantum-disordered states and quantum phase transitions.

In this Letter, a large-scale, high-precision QMC study of the AF–VBS transition in the J-Q model is presented in order to further test the he DQC theory, and to settle discrepancies between previous studies [5, 16, 17]. The main point of contention is the order of the transition. In the DQC theory, it was argued that AF–VBS transitions are generically continuous [2] and that the critical point for SU($N$) spins corresponds to a non-compact (NC) CP$^N$-1 field theory [3]. This is at odds with the long-standing Landau-Ginzburg paradigm, where a direct transition between two states breaking unrelated symmetries should be first-order (except at fine-tuned multi-critical points). Ground state [5, 15] and finite-temperature [16] QMC studies of the J-Q model show scaling behavior in good agreement with the DQC theory, including a dynamic exponent $z = 1$, a rather large anomalous dimension $\eta_{\text{spin}} \approx 0.35$, and an emergent U(1) symmetry in the VBS phase (which in the theory is associated with spinon deconfinement). On the other hand, a QMC finite-size analysis by Jiang et al. would, if correct, require a first-order transition [17]. A weakly first-order AF–VBS scenario has been elaborated by Kuklov et al. [18, 19], based on results for a lattice model claimed to realize the NCCP$^1$ action, but other studies of the action have reached different conclusions [3].

Here it will be shown that the claimed first-order signals in the study by Jiang et al. [17] can be attributed to over-interpretations of QMC data affected by significant systematical and statistical errors. The results to be presented below were obtained with the stochastic series expansion (SSE) method [20, 21], which is a finite-temperature QMC method free from systematical errors. There are no indications of a first-order transition, even in systems of space-time volume 20 times larger than in [17]. However, the data are now of high enough quality to detect logarithmically weak deviations from the scaling forms expected at a $z = 1$ critical point. Logarithmic corrections are well known consequences of marginal operators at criticality, which, although they have not been predicted theoretically in this case (in large-$N$ treatments of the NCCP$^{N-1}$ theories [2, 22, 23]), cannot a priori be ruled out for $N = 2$. A first-order transition would lead...
to much more dramatic deviations from $z = 1$.

Turning now to a quantitative discussion of the calculations, the J-Q Hamiltonian \[ H = -J \sum_{<ij>} C_{ij} - Q \sum_{<ijkl>} C_{ij} C_{kl}, \] (1)

where $C_{ij}$ is a bond-singlet projector for $S = 1/2$ spins; $C_{ij} = 1/4 - S_i \cdot S_j$. In the J term $ij$ are nearest neighbors on the square lattice, while $ij$ and $kl$ in the Q term are on opposite edges of a $2 \times 2$ plaquette. Lattices of $N = L^2$ spins with periodic boundaries are used. Assuming $z = 1$ (based on previous work \cite{5, 16}), the inverse temperature $\beta = Q/T$ is taken proportional to $L$ for finite-size scaling; $\beta = L$ and $\beta = L/4$ will be considered for $L$ up to 256. Calculations for $T/Q \geq 0.035$ are also carried out for systems sufficiently large, up to $L = 512$, to give results in the thermodynamic limit.

The focus here will be on magnetic properties. The staggered magnetization $m_s$ is computed along the $z$ (quantization) axis. To extract the critical coupling ratio $(J/Q)_c$, and to address the issue of a possible first-order transition, consider first the Binder cumulant \cite{24},

$$U_2 = \frac{5}{2} \left( 1 - \frac{1}{3} \langle m_s^2 \rangle \right),$$

(2)

which is defined so that $U_2 \to 0$ and $U_2 \to 1$ in an AF disordered and ordered state, respectively, when $L \to \infty$ (stemming from a Gaussian distribution of $|\vec{m}_s|$ around $|\vec{m}_s| = 0$ and a $\delta$-function at $|\vec{m}_s| > 0$, respectively). The factors in \cite{24} correspond to $m_{sz}$ being one component of a three-dimensional vector $\vec{m}_s$. At a continuous transition, curves of $U_2$ versus $J/Q$ for different system sizes should intersect at the critical coupling, with normally $0 < U_2 < 1$ \cite{24}. At a first-order transition, on the other hand, $U_2 \to -\infty$ when $L \to \infty$ \cite{24}, following from a distribution with peaks at both $|\vec{m}_s| > 0$ and $|\vec{m}_s| = 0$ when the ordered and disordered phases coexist (with weight transferring rapidly between the peaks as the transition is crossed for large finite $L$). It should be noted that $U_2$ can be negative also at a continuous transition \cite{24, 25} only a divergence signals a first-order transition.

As seen in Fig. 1 in the J-Q model there are no signs of $U_2$ becoming negative. The curves intersect at a point which moves very slowly toward larger $J/Q$ with increasing system size. The critical coupling for $L \to \infty$ can be extracted by extrapolating the crossing points for systems of size $L$ and $L/2$, as shown in Fig. 2.

Fig. 2 also shows results for the size-dependent critical coupling suggested by Kuklov et al. \cite{18} and used by Jiang et al. \cite{17}. It is based on the winding numbers,

$$W_a = \frac{1}{L} \sum_{p=1}^{n} J_a(p),$$

(3)

where $J_a(p)$, $a = x, y$, is the spin current in lattice direction $a$ at location $p$ in an SSE configuration containing $n$ operators \cite{20}. In the case of the J-Q model, these currents take the values $J_a(p) \in \{0, \pm 1, \pm 2\}$. The “temporal” winding number is essentially the magnetization,

$$W_r = 2M_z, \quad M_z = \sum_{i=1}^{N} S_{i}^z, \quad (4)$$

The squared winding numbers are related to two important thermodynamic quantities; the spin stiffness,

$$\rho_s = \frac{1}{2\beta} \left( \langle W_x^2 \rangle + \langle W_y^2 \rangle \right),$$

(5)

and the uniform magnetic susceptibility,

$$\chi = \frac{\beta}{N} \langle M_z^2 \rangle = \frac{\beta}{4N} \langle W_r^2 \rangle. \quad (6)$$

For $L \to \infty$ and $T \to 0$, in a magnetically disordered (here VBS) phase $\rho_s \to 0$ and $\chi \to 0$, while in the AF phase $\rho_s > 0$ and $\chi > 0$. A possible definition of the transition point (for finite $L$ and $\beta$) is the coupling at which the probability $P_0$ of all the winding numbers being zero is 1/2 (or any fixed fraction) \cite{18}. Fig. 2 shows results obtained by interpolating $P_0$ for several $J/Q$ values. They extrapolate to the same $(J/Q)_c \approx 0.0445$ as
The conclusion of this study is that the AF-VBS transition in the J-Q model is continuous, but with significant corrections to the $z = 1$ scaling that have not been discussed previously. The corrections appear to be logarithmic, although conventional scaling corrections $\sim L^{-\omega}$ with $\omega < 1$ cannot be ruled out based on the numerical data alone. The scaling fits away from the critical point give a correlation length exponent $\nu \approx 0.6$, but this is without considering possible corrections also to the conventional $L^{1/\nu}$ scaling. It is difficult to include logarithmic corrections in quantities where the leading exponent is not known, in contrast to $\rho_s$ and $\chi$ where $z = 1$ governs the leading behavior.

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correction \((L_0 = 0.9)\) for \(\beta = L\) systems. The curves show a fit to a common polynomial \(f[(J - J_c)L^{1/\nu}]\) with \(J_c/Q = 0.0447\) and \(\nu = 0.59\) (not including the \(L = 32\) data).



FIG. 5: (Color online) Scaling of the spin stiffness with a log-correction \((L_0 = 0.9)\) for \(\beta = L\) systems. The curves show a fit to a common polynomial \(f[(J - J_c)L^{1/\nu}]\) with \(J_c/Q = 0.0447\) and \(\nu = 0.59\) (not including the \(L = 32\) data).

mulated numerical evidence of scaling (and experiments on natural systems), along with non-rigorous analytical calculations, have established a consensus that critical points are ubiquitous. The system volumes \(\beta L^2\) used here for the J-Q model are similar to those in contemporary classical Monte Carlo simulations \(\cite{27}\). In the absence of any concrete signals of first-order behavior, the transition must therefore be regarded as continuous.

The scaling corrections will hopefully stimulate further field-theoretical work to explain them. Scaling anomalies that could be logarithmic have been seen in Monte Carlo studies of the NCCP\(^1\) action \(\cite{28}\), but it has also been claimed that this action always leads to a first-order transition \(\cite{19}\) (in which case a different field-theory for the J-Q model would have to be found). Marginal operators leading to logarithms appear in systems at their upper critical dimension, but this is not applicable here. Logarithmic corrections have been previously found in gauge field theories with fermions \(\cite{28}\). On the other hand, conventional power-law corrections due to irrelevant operators are always expected, but here the subleading exponent \(\omega\) would have to be very small, which has not been anticipated (although the dangerously irrelevant operator causing the VBS has a small scaling dimension \(\nu\) and is a potential source of a small \(\omega\)). Studies of the SU\((N)\) generalization of the J-Q model would be useful to determine whether \(N = 2\) is a special case. QMC calculations have already been carried out for \(N = 3\) and 4 \(\cite{15}\), but the quantities discussed here have not yet been investigated.

A consequence of the findings presented here is that the anomalous VBS transition in U\((1)\) symmetric systems \(\cite{7}\) should be re-evaluated. Scaling deviations very similar to (but stronger than) those in the J-Q model were found, which in \(\cite{18,19}\) was interpreted as a first-order transition. Considering scaling corrections, this class of models as well may in the end have continuous transitions \(\cite{6}\).

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