Nature of the antiferromagnetic to valence-bond-solid quantum phase transition in a 2D XY-model with four-site interactions

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We report large-scale quantum Monte Carlo calculations at the \(T = 0\) antiferromagnetic to valence-bond-solid (VBS) transition of a two-dimensional \(S = 1/2\) XY model with four-spin interactions. Finite-size scaling suggests a discontinuous spin stiffness, but a continuous VBS order parameter. We propose that this is a continuous VBS transition without critical spin fluctuations. We also argue that the system is close to a point, in an extended parameter space, where both the magnetic and VBS fluctuations are critical—possibly a deconfined quantum-critical point.

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Senthil et al. recently proposed a class of generic deconfined quantum-critical points describing phase transitions between \(O(2)\) or \(O(3)\) antiferromagnetic (AF) and four-fold degenerate valence-bond-solid (VBS) ground states in two dimensions (2D). These critical points fall outside the standard Landau-Ginzburg-Wilson framework, where order–order transitions are generically first-order (except at fine-tuned multi-critical points). A continuum field theory of spinons interacting with a \(U(1)\) gauge field was proposed in which the critical point is not explicitly described in terms of order parameters. Instead, AF or VBS order is a consequence of confinement of spinons. This remarkable, but so far untested, theory calls for numerical studies of lattice models that could potentially exhibit deconfined quantum-criticality. It was suggested that such a transition may already have been observed in a quantum Monte Carlo (QMC) study of an XY-model including four-site interactions. Such a model should also from a theoretical perspective be among the most natural candidates for the proposed physics.

The J-K model studied in \(^2\) is defined by

\[
H = J \sum_{ij} B_{ij} - K \sum_{ijkl} P_{ijkl},
\]

where \(B_{ij}\) and \(P_{ijkl}\) are, respectively, operators acting on nearest-neighbor sites and four sites on the corners of a plaquette on a 2D square lattice:

\[
B_{ij} = S_i^- S_j^- + S_i^+ S_j^+ = 2(S_i^x S_j^x + S_i^y S_j^y),
\]

\[
P_{ijkl} = S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+.
\]

This \(S = 1/2\) model is equivalent to a half-filled lattice of hard-core bosons. It was found to undergo a continuous AF-VBS transition at \(K/J \approx 7.9\), with no intervening coexistence region. However, recent simulations of related bosonic current models have instead shown weakly first-order transitions. This motivates us to revisit the J-K model and analyze the transition in greater detail.

Using a stochastic series expansion (SSE) QMC algorithm, we have carried out extensive simulations of the J-K model in the vicinity of the AF-VBS transition. We have performed ground-state (\(T \to 0\) converged) finite-size scaling for \(L \times L\) lattices with \(L\) up to \(\approx 100\). Although the spin stiffness shows signs of a discontinuity, we argue that the transition is not necessarily first-order. We propose a scenario in which VBS order can emerge continuously in a state where AF order is not suppressed by diverging VBS fluctuations. The spin correlations change continuously from long-ranged to exponentially decaying at the transition, while the stiffness is discontinuous because the VBS formation is associated with the opening of a spin gap. While our results show that the theory of deconfined quantum-criticality does not apply, we argue that such a transition may be located nearby in an extended parameter space.

The spin stiffness \(\rho_s\) is calculated with the the SSE method in the standard way in terms of winding number fluctuations. At a quantum phase transition with dynamic exponent \(z\), it should scale with size as

\[
\rho_s \sim L^{2-D-z/z} = L^{-z}.
\]

We also compute the squared VBS order parameter \(\langle m_P^2 \rangle\) and the associated susceptibility \(\chi_P\):

\[
\langle m_P^2 \rangle = \frac{1}{N^2} \sum_{a,b} \langle P_a P_b \rangle (-1)^{x_a + x_b},
\]

\[
\chi_P = \frac{1}{N^2} \sum_{a,b} \int_0^\beta d\tau \langle P_a(\tau) P_b(0) \rangle (-1)^{x_a + x_b}.
\]

Here \(P_{ijkl} = P_{ijkl}\) and the sums are over all plaquettes. The expected quantum-critical scaling is

\[
\langle m_P^2 \rangle \sim L^{-(z+n)},
\]

\[
\chi_P \sim L^{-\eta},
\]

where \(\eta\) is the correlation function exponent.

Analyzing the stiffness according to Eq. (4), we obtain \(z \approx 0.4\). In Fig. a, we show how \(L^{1.4} \rho_s\) versus \(K/J\) graphed for different lattice sizes produces a crossing point at \(K/J \approx 7.915\) (with \(z = 1\) the crossing points...
move significantly with $L$). As we will show below, this unusual value of the dynamic exponent is not consistent with the $T > 0$ behavior of the spin susceptibility. The discrepancy could be interpreted as a quantum-critical point violating hyperscaling, but a more plausible scenario is that the observed scaling is an artifact of the limited range of system sizes available. We therefore explore an alternative scenario.

Consider the anisotropic 2D Heisenberg model:

$$H_{\text{Heisenberg}} = J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z).$$

(9)

Its $xy$ spin stiffness is non-zero at $T = 0$ for $\Delta \leq 1$ and vanishes in the thermodynamic limit for $\Delta > 1$. This is not due to a phase transition, but a consequence of the order parameter flipping from the $xy$-plane to the $z$-axis. Exactly at the isotropic point the stiffness should approach a constant value; $2/3$ of the stiffness of the symmetry-broken state (reflecting rotational averaging). However, numerical results do not show a point at which $\rho_s$ becomes obviously size independent. Instead, as shown in Fig. 1(b), we find curve crossings for $L^{0.3} \rho_s$ very close to $\Delta = 1$, reminiscent of the results for the J-K model in Fig. 1(a). This shows that a discontinuity in the thermodynamic limit can easily be mistaken for a continuous transition with an anomalously small $z$—going to very large lattices we would eventually find $z = 0$. We therefore believe that the stiffness of the J-K model is also discontinuous. This does not have to imply a point with enhanced symmetry. A similar behavior can be expected also if $\rho_s$ is discontinuous for other reason (except in the case of a real level crossing).

The dynamic exponent can also be extracted from the temperature dependence of the uniform susceptibility; $\chi_u = J T^{-\eta} (\sum_i S_i^2)^2 / N$. For a 2D quantum-critical system it should scale as

$$\chi_u = a + b T^{2z - 1},$$

(10)

where $b$ is a constant related to the spin-wave velocity and $a = 0$ at the critical coupling. Away from the critical coupling $a \neq 0$ and there is low-$T$ cross-over to a different form. The earlier results were consistent with $a = 0$ and an expected cross-over to a different form. The behaviors are typical of quantum-critical scaling.

We observe a linear behavior over an extended range of temperatures, but a line fitted to the data has a small but clearly non-zero intercept, suggesting AF order up to very large lattices we would eventually find $\Delta = 0$. We therefore believe that the stiffness of the J-K model in Fig. 1(a). This shows that a discontinuity in the thermodynamic limit can easily be mistaken for a continuous transition with an anomalously small $z$—going to very large lattices we would eventually find $z = 0$. We therefore believe that the stiffness of the J-K model is also discontinuous. This does not have to imply

![FIG. 1: (Color online) (a) Dependence of the size-scaled stiffness on the coupling $K/J$ of the J-K model, using $z = 0.4$. (b) The size-scaled stiffness of the anisotropic Heisenberg model versus the Ising anisotropy $\Delta$, using $z = 0.3$.](image1)

![FIG. 2: (Color online) Temperature dependence of the spin susceptibility for values of $K/J$ in the vicinity of the $T = 0$ AF-VBS transition. Error bars are not shown but are at most the same size as the symbols.](image2)
From the slope of \( \langle m_p^2 \rangle \) we get \( z + \eta \approx 0.98 \pm 0.04 \) (taking into account our estimated accuracy of \( K_c \)) using \( z \). The uncertainty in \( \eta \) extracted from \( z \) is much higher, however, due to the significant changes in \( \chi_P \) close to \( K_c \). We can only give a rough estimate, \( \eta \in (-0.5, 1.0) \), which gives \( z \in (1.5, 2.0) \). Since \( z \) is normally integer, this would suggest \( z = 2 \), but clearly further work is needed to confirm this. A negative \( \eta \) is unusual, but the combination \( z + \eta \approx 1 \), corresponding to \( \sim 1/L \) VBS correlations, is not unusual. We note that unusually large lattices, \( L \approx 40 \), are required before the (likely) asymptotic behavior of \( \langle m_p^2 \rangle \) and \( \chi_P \) commences. This could be explained as a cross-over away from another critical point, located nearby in an extended parameter space, which we have already argued for above. For a first-order transition, one might expect such a cross-over for \( K < K_c \) to be followed by a rather sharp change to an \( 1/L^2 \) behavior for both \( \langle m_p^2 \rangle \) and \( \chi_P \) (reflecting short-range correlations), because the cross-over should then correspond the size of a typical VBS droplet. Instead, \( \langle m_p^2 \rangle \) for both \( K < K_c \) and \( K > K_c \) approaches an \( \sim 1/L \) scaling, and the drop in \( \chi_P \) occurs only for much larger \( L \), well inside the AF phase. Although we can still not completely exclude a first-order transition, the intriguing possibility of critical VBS fluctuations but discontinuities in the spin sector at the same point deserves further analysis.

A discontinuous \( \rho_s \) can be accounted for if the VBS would be associated with a continuously opening spin gap, as illustrated in Fig. 3(a)—the stiffness must vanish once an infinitesimal gap opens. In this scenario the spin correlations would still change continuously, in a non-critical manner, from long-ranged to exponentially decaying. To argue for the possibility of such an exotic transition, we first discuss the conditions for symmetry breaking in the AF and VBS phases in terms of quantum levels for finite system size \( N \). We then assume a continuous onset of VBS order and investigate the consequences of this on the relevant quantum states.

AF order is associated with a “tower” of quantum-rotor states (global spin-rotation excitations) that become degenerate with the ground state as \( 1/N \) when \( N \to \infty \). In a spin-isotropic system the ground state has spin \( S = 0 \) and the rotor states \( S = 1, 2, ... \) \[10\]. The XY model does not conserve total spin, but we will use the notation \( S = 0, 1, ... \) also for its rotor states. For simplicity we restrict the discussion to the \( S^z = 0 \) sector. The ground state has momentum \( k = 0 \) and the \( k > 0 \) spin wave excitations all have their own rotor towers.

A columnar VBS state is a quadruplet corresponding to the \( Z_4 \) symmetry of a columnar dimer pattern. We refer to the lattice-symmetry related quantum numbers with a single label, \( p = 0, 1, 2, 3 \), and call the states with \( p = 1, 2, 3 \) VBS states. Like the ground state \( |00\rangle \), the VBS states have \( S = 0 \), and, due to the discrete VBS order parameter, the level spacing within the quadruplet vanishes exponentially with \( N \).

We now explore an AF-VBS transition involving only the states discussed above, i.e., those states are assumed to stay at low energy and no other states descend from higher energies. We will follow the evolution of the levels \( |S^z_p\rangle \) \( (S = 0, 1, ..., p = 0, 1, 2, 3) \) as we vary \( K \). Although the character of the states changes as they evolve, we continue to call them rotor and VBS states also in their “wrong” phase. We assume that the ground state \( |00\rangle \) evolves continuously and is not crossed by any other level.

For \( \delta = K_c - K > 0 \) the VBS correlation length grows as \( \delta^{-\nu} \), corresponding to a gap \( \Delta \sim \delta^{-\nu} \) between \( |00\rangle \) and \( |01\rangle \). Thus, for all \( K < K_c \) there is some \( N \) above which there are rotor states \( |1, 2, ..., N\rangle \) below the first VBS state \( |01\rangle \). As \( N \to \infty \) a tower builds up and AF order can form. There is no apparent reason why the AF order has to vanish as \( K \to K_c^- \). Accounting for a generic critical point at which both the AF and VBS orders vanish is in fact highly non-trivial—accomplished in the theory of deconfined quantum-criticality \[1\]. For the J-K model, our QMC results suggest instead that the spin stiffness remains non-zero as \( K \to K_c^- \), and hence that AF order is robust in the presence of diverging VBS correlations.

For \( K > K_c \), the VBS states \( |0123\rangle \) approach the ground state exponentially as \( N \to \infty \). There is thus an \( N \) above which the VBS quadruplet falls below the lowest rotor state \( |1\rangle \). The rotor states \( |1, 2, ..., N\rangle \) should also develop VBS correlations as \( K \to K_c^- \), breaking the \( Z_4 \) symmetry for \( K > K_c \). Therefore, the rotor states should be approached by VBS-like states \( |1, 2, ..., N\rangle \), which become degenerate at \( K_c \). The tower of rotor states, along

**FIG. 3:** (Color online) Finite-size scaling of the squared VBS order parameter (a), and susceptibility (b). In (a) the line has slope \(-1\), and the ones in (b) have slopes \(1/2\) and 1.
with the states joining them in quadruplets, thus evolve into a series of VBS-like states. This will also apply to the \( k \neq 0 \) towers. What we propose is that these are the elementary excitations of the VBS, which hence cannot be regarded as “pure VBS” excitations but involve spin as well. Clearly there will also be \( S = 0 \) excitations of the VBS—these are the pure VBS excitations, which in our scenario would be at higher energy and irrelevant at the transition [in contrast to deconfined quantum-criticality, where there are gapless \( S = 0 \) excitations due to an emergent \( U(1) \) symmetry]. The key aspect of our scenario is that all the rotor states change qualitatively (but continuously) in a manner similar to the ground state, turning into gapped VBS/spin excitations. No other low-energy states emerge. With no tower of degenerate rotor states as \( N \to \infty \) there can be no long-range AF order and hence the stiffness jumps to zero when the gap opens.

What is the nature of such spinful gapped VBS excitations and, specifically, why should they be gapped? Regarding a VBS dimer as two spins \( i, j \) in a singlet \( (|\uparrow_i \downarrow_j - |\downarrow_i \uparrow_j) \), the state \( |1\rangle_0 \) can be obtained by exciting a dimer into a state \( (|\uparrow_i \downarrow_j + |\downarrow_i \uparrow_j) \). This pair state can separate spatially into two spin-\( \frac{1}{2} \) degrees of freedom—spinons—between which a string of out-of-phase dimers forms \( |\uparrow_i \downarrow_j \downarrow_i \uparrow_j \rangle \). The string provides a linear confining potential for the spinons and hence there should be a discrete set of gapped excitations. This singlet-triplet picture is strictly based on \( SU(2) \) symmetry, but even in the XY case, where an excited dimer is not a triplet state, there should be analogous confining string states. At the critical point the spinons will become deconfined, and hence our scenario shares some features with deconfined quantum-criticality. There are major differences, however; the absence of emergent \( U(1) \) symmetry and AF correlations that are not critical but \( \sim e^{-\Delta r} \), where \( \Delta \) is the gap and \( a \) is a constant. The AF correlation length is thus divergent as \( K \to K_c \) from above, but at \( K_c \) the correlations are long-ranged, not power-law.

We have not explained why the VBS forms, but we have argued that if it does form continuously a simultaneous AF transition of the type we have found numerically is not an unlikely consequence. We also cannot predict the universality class, because our mechanism does not require a particular scaling of the gap at the critical point (related to the dynamic exponent).

We have argued for the existence, in an extended parameter space, of an AF-VBS transition in which also the spin stiffness vanishes continuously. In Fig. 4(b) we consider the evolution of the transition point when a suitable coupling \( V \) is added to the J-K model. A line of critical points—which would presumably be in the deconfined class—could extend from the point at which the stiffness first becomes continuous. Another possibility is that the transition is first-order beyond this point. Fig. 4(b) shows a scenario where there is coexisting AF and VBS order, which requires a different mechanism than the one we have discussed.

In principle we cannot rule out a weakly first-order AF-VBS transition \( |\uparrow\rangle |\uparrow\rangle \) in the J-K model, but our results do not require this. Our simulations, in combination with general arguments of symmetry-breaking and adiabatic evolution of quantum states, instead point to a new potential route to quantum phase transitions beyond the Ginzburg-Landau-Wilson framework. To confirm this scenario, it would clearly be important to identify a field theory exhibiting this type of transition.

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\[ \text{(a)} \quad \text{FIG. 4: (Color online) (a) Conjectured behavior of the spin stiffness and the spin gap at the AF-VBS transition. (b),(c) Possible phase diagrams in an extended parameter space where a point with continuous } \rho_s \text{ can be reached. On the solid (blue) curves, the transition is of the type shown in (a), with a stiffness jump. The dashed (red) curve in (b) could be a line of deconfined quantum-critical points. In (c) there is an intervening coexistence phase.} \]

\[ \text{(b)} \quad \text{\textbf{Δ}} \]

\[ \text{(c)} \quad \text{SF, SF+VBS} \]

\[ \text{SF, SF+VBS} \]
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