Néel to valence-bond solid transition on the honeycomb lattice: Evidence for deconfined criticality

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We study a spin-1/2 SU(2) model on the honeycomb lattice with nearest-neighbor antiferromagnetic exchange \( J \) that favors Néel order, and competing 6-spin interactions \( Q \) which favor a valence bond solid (VBS) state in which the bond-energies order at the “columnar” wavevector \( K = (2\pi/3, -2\pi/3) \). We present quantum Monte-Carlo evidence for a direct continuous quantum phase transition between Néel and VBS states, with exponents and logarithmic violations of scaling consistent with those at analogous deconfined critical points on the square lattice. Although this strongly suggests a description in terms of deconfined criticality, the measured three-fold anisotropy of the phase of the VBS order parameter shows unusual near-marginal behaviour at the critical point.

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Many interesting materials at low temperature appear to be on the verge of a quantum phase transition involving a qualitative change in the nature of the ground state[1]. When one of the two competing \( T = 0 \) phases spontaneously breaks a symmetry, the transition can be studied using a path integral representation with a Landau-Ginzburg action[2] written in terms of the order parameter that characterizes the broken symmetry phase[1]. If phases on two sides of the critical point break different symmetries, Landau-Ginzburg theory generically predicts a direct first-order transition or a two-step transition with an intermediate phase. However, this path integral description in terms of order-parameter variables can sometimes involve Berry phases in a non-trivial way[3–5]. The presence of Berry phases, which correspond to complex Boltzmann weights for the corresponding classical statistical mechanics problem in one higher dimension[1], can invalidate the conclusions reached by the Landau-Ginzburg approach.

In some of these cases, it is useful[6] to think in terms of topological defects in one of the ordered states, and view the competing ordered state as being the result of the condensation of these topological defects — this description[6] makes sense only if the quantum numbers carried by defects in one phase match those of the order parameter variable in the other phase. Under certain conditions, this alternate “non-Landau” description generically predicts a direct continuous transition[7,8] between the two ordered states, in contrast to predictions of classical Landau-Ginzburg theory. Square lattice \( S = 1/2 \) antiferromagnets undergoing a transition from a ground state with non-zero Néel order parameter \( M_n \) to a valence-bond solid (VBS) ordered state, in which the “bond-energies” (singlet projectors) \( P_{\langle ij \rangle} = \frac{1}{2} - \hat{S}_i \cdot \hat{S}_j \) on nearest-neighbour bonds \( \langle ij \rangle \) in the \( \hat{x} \) (\( \hat{y} \)) direction develop long-range order at the “columnar” wavevectors \( K_1 = (\pi, 0) \) \( (K_2 = (0, \pi)) \), provide the best-studied example of such “deconfined critical points” [7,8]. In this case, \( Z_4 \) vortices in the complex VBS order parameter \( \Psi \) carry a net spin \( S = 1/2 \) in their core, suggesting that the onset of Néel order can be studied using a CP\(^1\) description of \( M_\alpha \). \( \bar{M}_\alpha = z_\alpha^* \bar{d}_\alpha z_\beta \), where \( \bar{d} \) are Pauli matrices and the \( Z_4 \) vortices are represented by a two-component complex bosonic field \( z_\alpha \) coupled to a compact \( U(1) \) gauge field \( A_\alpha \)[6,8], whose space-time monopoles correspond to hedgehog defects in the Néel order. Only quadrupled hedgehog defects (corresponding to four-fold anisotropy in the phase of \( \Psi \)) survive the destructive interference of Berry phases on the square lattice[3,5,9], and their irrelevance at criticality[7,8] leads to a non-compact (monopole-free [10,12]) CP\(^1\) (NCCP\(^1\)) description of this transition.

Here, we use Quantum Monte Carlo (QMC) simulations[13–15] to study a spin-1/2 Heisenberg model on the honeycomb lattice with nearest-neighbor antiferromagnetic exchange \( J \) that favors Néel order, and competing 6-spin interactions \( Q \) which favor VBS order at the columnar wavevector \( K = (2\pi/3, -2\pi/3) \):

\[
H = -J \sum_{\langle ij \rangle} P_{\langle ij \rangle} - Q \sum_{\langle iijklmn \rangle} P_{\langle ij \rangle} P_{\langle kl \rangle} P_{\langle mn \rangle} + P_{\langle jk \rangle} P_{\langle lm \rangle} P_{\langle ni \rangle},
\]

where \( \langle \langle iijklmn \rangle \rangle \) denotes hexagonal plaquettes (Fig[1]). We find evidence for a direct continuous Néel-VBS transition at \( (Q/J)c \equiv q_c \approx 1.190(6) \), with correlation length exponent \( \nu \approx 0.54(5) \), and anomalous exponents \( \eta_{\text{Néel}} \approx 0.30(5) \), and \( \eta_{\text{VBS}} \approx 0.28(8) \); within errors, these values match corresponding results at the Néel-columnar VBS transition on the square lattice[16,18]. In addition, we find evidence for apparently logarithmic violations of finite-temperature scaling of the uniform spin susceptibility \( \chi_\alpha \) and stiffness \( \rho_\alpha \), analogous to the square-lattice case[17]. However, in sharp contrast to the square-lattice transition at which the four-fold anisotropy vanishes for large systems[18,20], a careful study of the three-fold anisotropy in the phase of \( \Psi \) reveals surprising near-marginal behaviour on the honeycomb lattice.
On the square lattice, only proceed in two steps with an intermediate phase [7, 8].

transition to be first-order in the simplest scenario, or allowed in the CP

description of the transition to be a conventional Landau-

triple anisotropy at criticality suggests that three-

hand, our observation of near-marginal behaviour of the three-fold anisotropy felt by the phase of Ψ. If

vortices in staggered VBS states [6]. Indeed, most of our results on universal critical properties are very similar to previous QMC simulations of computationally tractable spin models exhibiting Néel-columnar VBS transitions on the square lattice [16–18, 20–23]. While some of these studies [16–18, 20, 31, 35] have interpreted these square-lattice re-
In the vicinity of such a transition, we also expect the g ⃗Ms is lost, we compute the “dimensionless” Binder cumulant g ⃗Ms/D ⃗r of the universal scaling function Ψ = Ψ(∆qD) if there is a continuous transition at ∆qD and Ψ = 0 results. Bottom inset: Temperature dependence of χu/T close to criticality. In the Néel phase (q = 1.18), QMC data (symbols) are well-fit by χu/T = a + b/T, whereas on the VBS side (q = 1.2), a sharp drop is observed as expected. Close to criticality (q = 1.19), QMC data are better fit by χu/T = c + d log(J/T). Lines are fits to the above forms with a = 0.024, b = 0.0005, c = 0.022 and d = 0.0024.

columnar wavevector K. This is characterized by the VBS order parameter Ψ = ∑⃗rP⃗r/3 = (∑⃗rP⃗r/3)πi/3 = (Ψ2). This is characterized by the (basis-dependent) Binder cumulant of the universal scaling function Ψ = Ψ(∆qD) if there is a continuous transition at ∆qD and Ψ = 0 results. Bottom inset: Temperature dependence of χu/T close to criticality. In the Néel phase (q = 1.18), QMC data (symbols) are well-fit by χu/T = a + b/T, whereas on the VBS side (q = 1.2), a sharp drop is observed as expected. Close to criticality (q = 1.19), QMC data are better fit by χu/T = c + d log(J/T). Lines are fits to the above forms with a = 0.024, b = 0.0005, c = 0.022 and d = 0.0024.

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FIG. 5: (Color online) The dimensionless $Z_3$-anisotropy parameter $W_3$ scales to zero with increasing $L$ in the Néel phase, but grows with size in the columnar VBS phase. Top inset zooms in on behaviour of near-critical systems which display nearly scale-independent behaviour. Bottom inset: Histogram of $E\Psi$ for $L = 36$ at $q = 1.184$ close to $q_c$. Brightness of each color patch reflects the weight.

transition, we also expect the corresponding scaling form \[
\langle |\Psi|^2 \rangle = L^{-(1+\eta_{\text{VBS}})} G_\Psi (\Delta q_D)
\]
for the dimensionful observable.

We pinpoint the $T = 0$ Néel and VBS transitions from the crossings of the Binder ratios $g_{\text{N}}, g_{\text{E}}$ as a function of $q$ for various $L$—at this stage, we do not assume that the two transitions coincide. Given the relatively sharp nature of the crossings and the monotonic nature of their $q$ dependence for fixed $L$ (Fig. 2), we are confident that the transition(s) is (are) continuous. We fit data for each dimensionless ($g_{\text{N}}, g_{\text{E}}$) and (appropriately scaled) dimensionful quantity $\langle M_0^2 \rangle, L^{1+\eta_{\text{N}}}, \langle |\Psi|^2 \rangle, L^{1+\eta_{\text{VBS}}}$ in the critical range to a polynomial function of $(q-q_c)L^\nu$ (corresponding to a polynomial approximation of scaling functions), with the corresponding $q_c, \nu, \eta$ and polynomial coefficients being fitting parameters. For each dimensionless quantity, the best-fit values vary somewhat depending on the range of $L$ and $q$ studied. Results of such fits for one choice of data-set for the dimensionless quantities are displayed as lines in Fig. 2 with the corresponding scaling collapse displayed in Fig. 3. Similar results for Néel and VBS correlators [11] confirm this.

Based on a detailed study of such fits, we estimate $q_{c,N} \approx 1.1936(24), q_{c,D} \approx 1.1864(28), \nu_N = 0.51(3), \nu_D = 0.55(4), \eta_{\text{N}} = 0.30(5)$ and $\eta_{\text{VBS}} = 0.28(8)$. The error bars quoted here reflect not just the error in determining best-fit values for a given data-set for each quantity, and variation in these best-fit values from quantity to quantity, but also the dependence of these best-fit values on the data set used, i.e. the size of the critical window in $q$, and the range of $L$ used in the fits. We also emphasize that our estimates of $\eta_{\text{VBS}}$ and $\eta_{\text{N}}$ depend sensitively on the value of $q_c$, resulting in the relatively large error bars quoted here. Nevertheless, we are in a position to exclude the relatively tiny values of $\eta$ that characterize conventional second-order critical points in 2+1 dimensions. Since $\nu_N$ coincides with $\nu_D$ within error bars, and the allowed ranges of $q_{c,N}$ and $q_{c,D}$ almost touch at the one-sigma level, the simplest interpretation of our data is that Néel order is lost and VBS order sets in at a single continuous $T = 0$ transition whose location is estimated to be $q_c \approx 1.190(6)$, with correlation exponent $\nu = 0.54(5)$, and anomalous exponents $\eta_{\text{N}} = 0.30(5)$ and $\eta_{\text{VBS}} = 0.28(8)$. This, taken together with the relatively large values of $\eta_{\text{N}}$ and $\eta_{\text{VBS}}$ characteristic of deconfined critical points, suggests an interpretation in terms of deconfined criticality.

Indeed, our estimates of $\eta_{\text{VBS}}, \eta_{\text{N}}$, and $\nu$, as well as of the universal critical value $g^* = 1.42(1)$ of the Néel Binder ratio at the $T = 0$ transition are consistent within errors with values for the analogous transition on the square lattice [16–18]. We also study the temperature dependence of the uniform spin susceptibility $\chi_u$ and the antiferromagnetic spin stiffness $\rho_s$ using finite-$T$ QMC methods [15] at low temperatures in the vicinity of this $T = 0$ transition. As is clear from Fig. 4, data for these quantities do not fit well to standard scaling predictions. However, excellent data collapse is obtained upon inclusion of logarithmic violations of scaling, using the same functional forms employed earlier on the square lattice [17]. These logarithmic violations may be related to (near) marginal operators in the NCCP theory [12, 14, 44].

Finally, we turn to a study of the effective three-fold anisotropy felt by the phase of $\Psi$ at criticality, as seen in histograms of $E\Psi$ near $q_c$. The phase $\theta$ of $E\Psi$ (inset of Fig. 5) appears to feel significant anisotropy near the $T = 0$ transition on the honeycomb lattice. To quantify this anisotropy in the distribution $P(E\Psi)$ near the critical point, we use a (dimensionless) estimator $W_3 = \int dE\Psi P(E\Psi) \cos(3\theta)$, designed to be 0 for a $U(1)$-symmetric distribution and 1 ($-1$) for ideal columnar (plaquette) VBS states (Fig. 1). In Fig. 5, we see that $W_3$ appears to saturate to a scale-independent constant at large $L$ as the transition is approached from the Néel phase, before growing with size as one moves into a columnar VBS state. This near-marginal behaviour of the anisotropy in $P(E\Psi)$ at the largest scales accessible to our simulations is very different from the $U(1)$ symmetric probability distribution of $E\Psi$ near the square lattice critical point [18, 19]. A more refined scaling analysis [11] yields the same result, leading us to our earlier suggestion that three-fold monopole insertions are (very close to) marginal at the NCCP critical point—this is consistent with recent parallel work that discusses relevance of $q$-fold monopoles in SU($N$) spin models [44, 45].

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