Lattice Model for the SU(N) Néel to Valence-Bond Solid Quantum Phase Transition at Large N

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A lattice model for the SU(N) Néel-VBS quantum phase transition at large N

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We generalize the SU($N = 2$) $S = 1/2$ square-lattice quantum magnet with nearest-neighbor antiferromagnetic coupling (J_1) and next-nearest-neighbor ferromagnetic coupling (J_2) to arbitrary N. For all $N > 4$, the ground state has valence-bond-solid (VBS) order for $J_2 = 0$ and Néel order for $J_2/J_1 \gg 1$, allowing us access to the transition between these types of states for large N. Using quantum Monte Carlo simulations, we show that both order parameters vanish at a single quantum-critical point, whose universal exponents for large enough N (here up to $N = 12$) approach the values obtained in a $1/N$ expansion of the non-compact CP^{N-1} field theory. These results lend strong support to the deconfined quantum-criticality theory of the Néel–VBS transition.

Just as the destruction of magnetic order by thermal fluctuations is the paradigmatic example of a classical critical point [1], the destruction of magnetic order at $T = 0$ by quantum fluctuations is a prototypical example of a quantum-critical point [2]. Sometimes the quantum case is entirely different due to novel quantum interference effects, which have no natural classical analogues. An important example is that of the square-lattice SU(N) quantum antiferromagnet, where the destruction of SU(N) symmetry-breaking Néel order in the background of uncompensated Berry phases results in a valence-bond-solid (VBS) state with broken translational symmetry [3–5]. Recent work has presented speculative albeit compelling arguments that a direct generically continuous Néel–VBS transition can exist. At such a *deconfined* quantum critical (DQC) point both order parameters are simultaneously critical [6], a striking feature which is not contained in the conventional field-theory description of two independent order parameters (where direct transitions are generically first-order).

Given the major paradigm shift that could be spawned by the DQC idea, it has been of great interest to verify its validity by unbiased numerical studies of lattice spin models (Hamiltonians) that harbor Néel–VBS transitions [7–11]. The weight of evidence from such work indicates that generically continuous Néel–VBS transitions indeed exist in quantum spin systems, with initial skepticism [9, 12] appearing increasingly unfounded [13, 14].

This DQC scenario predicts that the SU(N) Néel–VBS quantum-critical point falls into the universality class of the $(2+1)$-dimensional non-compact CP^{N-1} field theory [15, 16]. The connection between the phase transition in a microscopic Hamiltonian and the low-energy continuum theory description relies on speculative assumptions that are yet to be demonstrated convincingly. In order to provide support for this connection, therefore, one has to compare universal properties arising from these two starting points. Currently, the only technique with which the properties following from the CP^{N-1} action can be studied analytically is the $1/N$ expansion [17], but it is not clear whether the results of this approach are valid down to the most interesting case of $N = 2$. To test the
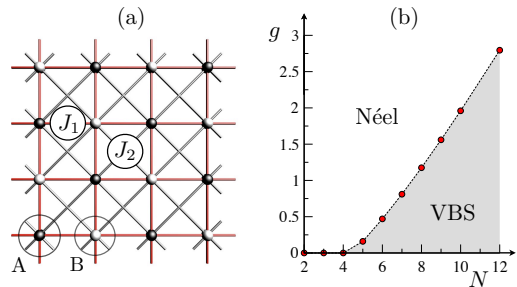

FIG. 1. (Color online) (a) Black (white) lattice sites indicate the A (B) sublattice on which spins of the J_1-J_2 model (1) transform as the fundamental (conjugate) representation of SU(N). J_1 couples nearest neighbors with an SU(N) *singlet projection* and J_2 connects next-nearest neighbors with an SU(N) *permutation*. (b) Phase diagram of the model as a function of N and $g \equiv J_2/J_1$.

DQC theory in an unbiased manner, it is thus of utmost importance to find quantum models in which the SU(N) Néel-VBS transition can be studied for arbitrary large N, to compare the critical exponents with those of the $1/N$ expansion of the continuum field theory. We here provide and study such a model.

Until now, the Néel-VBS transition could be accessed in an unbiased manner only for $N \leq 4$, by quantum Monte Carlo (QMC) simulations of the so-called J-Q model [7–11, 14], in which the $S = 1/2$ Heisenberg (J) model is supplemented by certain multi-spin interactions (Q) favoring a VBS state. It is clear that this model alone cannot access the quantum transition for larger-N, however, simply because for $N \geq 5$ the J model is itself VBS ordered [18, 19] and the Q term only increases the strength of this order. To remedy this problem, we here introduce an SU(N) symmetric generalization of the J_1-J_2 Heisenberg model model, with antiferromagnetic nearest-neighbor coupling J_1 and ferromagnetic next-nearest-neighbor coupling J_2 [illustrated in Fig. 1(a)]. For all $N \geq 5$, this model harbors a VBS phase for $J_2/J_1 = 0$ and a Néel phase for $J_2/J_1 = \infty$. By detailed unbiased QMC studies for $5 \leq N \leq 12$, we find that that the two phases are separated by a single

phase transition, with no signs of discontinuities even on the largest systems sizes studied ($L \times L$ spins with L up to 128). Most remarkably, the anomalous dimensions of the Néel and VBS correlation functions of the model for large-N shows quantitative agreement with the analytically known [20–22] scaling dimensions from the $1/N$ expansions of the non-compact CP^{N-1} model.

The J_1-J_2 model.—Our $SU(N)$ symmetric model is defined with a local Hilbert space of N states on each site of the square lattice illustrated in Fig. 1(a). We adopt the representation used previously in both analytic [4] and numerical [18, 19] works on bipartite lattices, where the sublattice-A states transform under rotations with the fundamental representation of $SU(N)$, and the B sublattice states transform with the conjugate of this representation; $|\alpha\rangle_A \rightarrow U_{\alpha\beta}|\beta\rangle_A$, $|\alpha\rangle_B \rightarrow U^*_{\alpha\beta}|\beta\rangle_B$. The state $\sum_\alpha |\alpha\rangle_A|\alpha\rangle_B$ is, thus, an $SU(N)$ singlet. P_{ij} is defined to be the projector onto this singlet between two sites i and j on *different* sublattices, i.e., $H_{ij} = -P_{ij}/N$ is the $SU(N)$ generalization of the familiar Heisenberg antiferromagnetic exchange (up to a constant). Another simple $SU(N)$ invariant interaction is the permutation operator between two sites on the *same* sublattice, $\Pi_{ij}|\alpha\beta\rangle = |\beta\alpha\rangle$, so that $H_{ij} = -\Pi_{ij}/N$ is the generalization of the the familiar ferromagnetic Heisenberg interaction. The Hamiltonian we study here is given by

$$H = -\frac{J_1}{N} \sum_{\langle ij \rangle} P_{ij} - \frac{J_2}{N} \sum_{\langle\langle ij \rangle\rangle} \Pi_{ij}, \qquad (1)$$

where $\langle ij \rangle$ and $\langle\langle ij \rangle\rangle$ denote first (A-B) and second (A-A and B-B) neighbor sites, respectively.

With $J_2 = 0$ it is now well known that the J_1 model is Néel ordered for $N = 2, 3, 4$ and develops VBS order for $N \geq 5$ [18, 19]. On the other hand, with $J_1 = 0$ each sublattice forms a trivial ferromagnet. A small $J_1 \ll J_2$ will clearly lock the individual sublattice magnetizations into a collective Néel ordered state. Thus, for each $N > 5$ there must be an intermediate value of $g \equiv J_2/J_1$ at which there is a quantum transition between these two phases (as we do not expect any other intervening phase).

QMC simulations.—All off-diagonal matrix elements in Eq. (1) are explicitly negative and, hence, the model is free of QMC sign problems [and it also satisfies Marshall's sign criterion, ensuring an $SU(N)$ singlet ground state]. To obtain exact (within statistical errors) numerical results for its properties on large $L \times L$ lattices, we use the stochastic series expansion QMC method with global loop updates [23–25]. Throughout this work, we set $J_1 = 1$ and the inverse temperature $\beta = L/J_1$ (reflecting the expected [6] dynamic exponent $z = 1$).

We characterize the Néel phase as one with a finite spin stiffness ρ_s (measured by the fluctuations of the winding number W of world lines; $\beta\rho_s = \langle W^2 \rangle$ [25, 26]). In the magnetic phase, the static ($\omega = 0$) Néel order-parameter susceptibility χ_N diverges with the "quantum volume" of
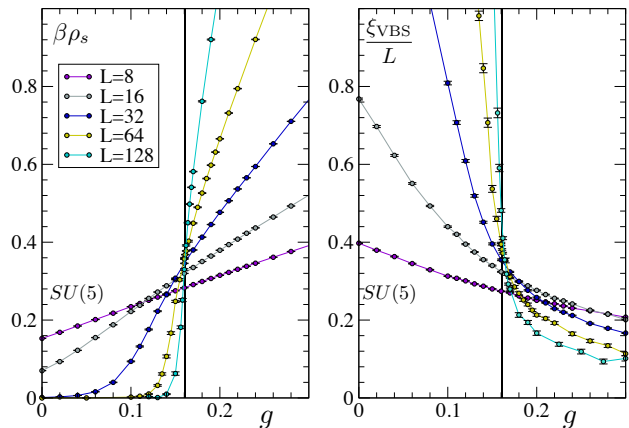

FIG. 2. (Color online) Curve crossings used to locate the critical point for magnetic [VBS] order in the $SU(5)$ J_1-J_2 model are shown in the left [right] panel. The quantity $\beta\rho_s$ [ξ_{VBS}/L] diverges in the magnetic [VBS] phase and goes to zero in the non-magnetic [non-VBS] phase when $\beta = L/J_1$. At a point where magnetic [VBS] fluctuations are critical, $\beta\rho_s$ [ξ_{VBS}/L] becomes L-independent. These properties result in crossings of curves for different L at the critical point. The width of the vertical line shows the range of estimates of the common Néel-VBS critical point; $g_c = 1.615(10)$. Fig. 3 shows the analysis of the crossing points giving this result.

the system according to $\chi_N \sim \beta L^2$. We define the $SU(N)$ VBS correlation function using the operator P defined above in Eq. (1); $N^2 C_V(\mathbf{r}, \tau) = \langle P_{\mathbf{0},\mathbf{0}+\mathbf{x}}(0)P_{\mathbf{r},\mathbf{r}+\mathbf{x}}(\tau)\rangle - \langle P_{\mathbf{0},\mathbf{0}+\mathbf{x}}(0)\rangle^2$. When Fourier transformed at $\omega = 0, \mathbf{q} = (\pi, 0)$ it gives χ_V. This quantity can be used to test for VBS order since it diverges in the VBS phase as $\chi_V \sim \beta L^2$. We also use the standard definition of the correlation length of the VBS order ξ_V as the square root of the second moment of the spatial correlation function C_V. Using these quantities we tested for long-range Néel and VBS order as the ratio $g = J_2/J_1$ is varied for each N and arrived at the phase diagram shown in Fig. 1(b). We elaborate on the quantitative analysis below.

Nature of the phase transition.—Fig. 2 shows QMC results for $\beta\rho_s$ and ξ_{VBS}/L as functions of the coupling ratio g for the $SU(5)$ model on lattices of size $L = 8, 16, 32, 64$, and 128. The quantum-critical point for the magnetic and VBS orders can be located by analysing crossing points versus g in $\beta\rho_s$ and ξ_{VBS}/L, respectively, computed on two different system sizes. As is clearly evidenced directly from this raw data, there are crossing points within a narrow window of g for both Néel and VBS orders, and these crossing points drift toward a common value g_c with increasing L.

In Fig. 3 we have plotted the crossing points between L and $L/2$ curves of $\beta\rho_s$ and ξ_{VBS}/L for $SU(N)$ systems with $N = 5, 6, 10$, and 12. Numerical extrapolations of the crossing data for both Néel and VBS orders in the $SU(5)$ and $SU(6)$ cases (top two panels) provide compelling evidence that in the thermodynamic limit the crossing points for both order-parameters approach
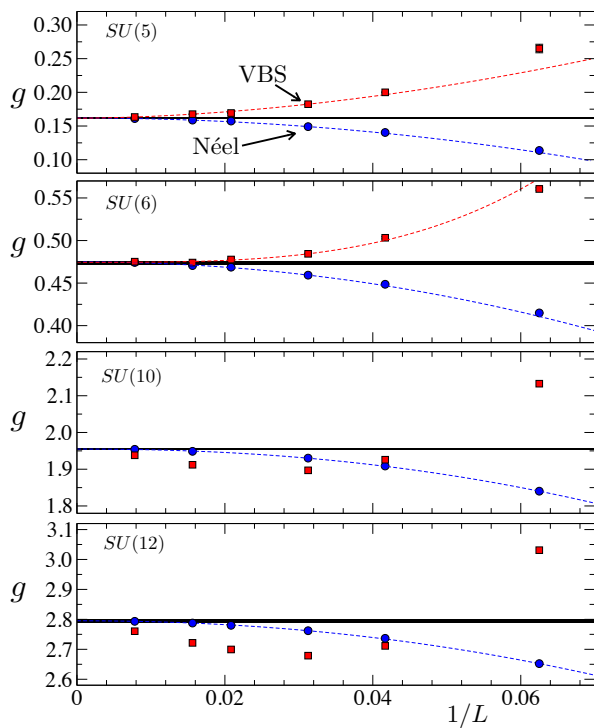
FIG. 3. (Color online) Convergence to a common critical point of the finite-size estimates for the Néel and VBS phase transitions for SU(5), SU(6), SU(10), and SU(12). The crossing points of L and $L/2$ curves for the same quantities as in Fig. 2 are shown for Néel (blue circles) and VBS (red squares) order for $L \leq 128$. For all four cases, the data are consistent, within error bars, with both order parameters becoming critical at the same point when $L \to \infty$. Numerical extrapolations (when reliable) are shown by dashed lines. For SU(10) and SU(12) the VBS correlation function has significant subleading corrections that can be ignored only for the largest sizes (see [27]). The grey lines show our estimates of the critical points (with their widths corresponding to the error bars).

a common critical point. For SU(10) and SU(12) (bottom two panels) there is non-monotonicity in the VBS crossing points, making reliable numerical extrapolations difficult. The source of this behavior is subleading corrections in the VBS correlation function that increasingly dominate the rapidly decaying leading power-law behavior as N increases (see note [27]). However, even for the SU(10) and SU(12) cases, for the largest system sizes the leading behavior still dominates, and the VBS crossings are consistent with the same critical point as obtained from the better-behaved $\beta\rho_s$ crossing in the $L \to \infty$ limit. There is, thus, good reason to believe that both orders go critical at the same point for all N. We have found no evidence for hysteresis or double peaked histograms that would be expected for a first-order transition.

Since a reliable numerical extrapolation of the $\beta\rho_s$ crossing is possible for each N, we use this quantity to extract the quantum-critical points. Note that possible weak corrections to standard scaling behavior in quantities whose scaling from depends only on the dynamic
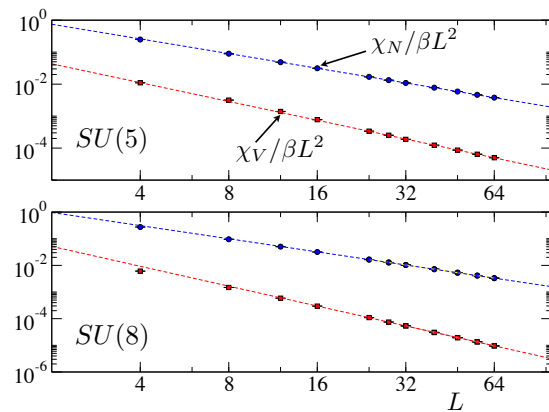

FIG. 4. (Color online) Examples, for the SU(5) and SU(8) models, of power-law scaling of the Néel and VBS order parameters close to the quantum-critical point. According to Eq. (2) and standard finite-size scaling arguments, $\chi_N/\beta L^2 \sim 1/L^{1+\eta_N}$ and $\chi_V/\beta L^2 \sim 1/L^{1+\eta_V}$. The linear regression fits (dashed lines) allow us to extract η_V and η_N, which are shown in Fig. 5 as a function of N.

exponent, such as ρ_s, which have been discussed for the J-Q model [11, 13, 14], would not affect the above analysis of *crossing points* versus g (see Appendix D in [11]). Corrections to scaling of the quantity $\beta\rho_s$ itself will be studied in detail elsewhere.

At a common quantum-critical point, it is expected that the otherwise independent Néel and VBS order parameters will *both* have correlation functions that decay as power laws in space ($\mathbf{r}$) and imaginary time (τ);

$$C_{N,V}(\mathbf{r}, \tau) \sim (\mathbf{r}^2 + c^2\tau^2)^{-(1+\eta_{V,N})/2}. \qquad (2)$$

The exponents η_N and η_V are universal numbers according to standard theory of critical phenomena. Universality implies that they are independent of details of the microscopic interactions of the model from which the correlation functions are extracted, but they do depend on the symmetry of the model, *i.e.*, in our case they should only depend on N of the SU(N) symmetry. To estimate these exponents with QMC simulations, we have studied the $N = 5, 6, 8, 10$, and 12 models at values of the coupling ratio g within the estimated critical points from the analysis shown in Fig. 3. We extract the exponents from the size dependence of the correlation functions, as illustrated for two cases in Fig. 4.

Comparison with large-N results.—The extracted exponents η_N and η_V are shown versus $1/N$ in the main panels of Fig. 5. For SU(10) and SU(12), η_V becomes too large to extract reliably (see note [27]). Our main objective is to compare the results with those of the CP^{N-1} universality predicted by the DQC scenario [6]. Analytic large-N results currently available for these indices are

$$\eta_N = 1 - 32/(\pi^2 N), \qquad 1 + \eta_V = 2\delta_1 N, \qquad (3)$$

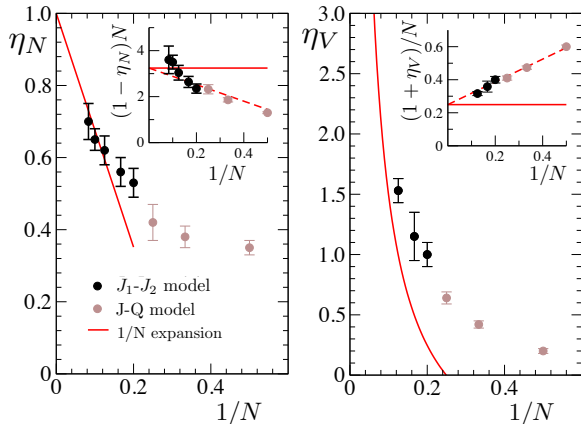where $\delta_1 \approx 0.1246$. It is interesting to note that the

FIG. 5. (Color online) Anomalous dimensions of the Néel (left) and VBS (right) fields extracted from the critical scaling analysis. The main panels show η_N and η_V versus $1/N$. For $N = 2, 3$ and 4, the data are for the J-Q model [10], and the results for $N > 4$ are for our J_1-J_2 model. The analytic results from the $1/N$ expansion of the CP^{N-1} field theory are shown as thick red lines. The left and right insets show $N(1 - \eta_N)$ and $(1 + \eta_V)/N$, respectively. These quantities must be finite in the $N \to \infty$ limit according to the DQC theory and should be given by Eq. (3) (solid straight lines in the insets). The next corrections to the exponents have not been computed analytically yet, but we can estimate them approximately as $1 + \eta_V = 0.2492N + 0.68(4)$, $\eta_N = 1 + 32/(\pi^2 N) - 3.6(5)/N^2$ (shown as dashed lines).

calculations underlying these two results are entirely different. While η_N was obtained from an $1/N$ expansion of the Néel order parameter expressed in terms of the CP^{N-1} fields [20], η_V was computed [21, 22] by exploiting a non-trivial relation, predating the DQC theory, between monopoles in the field theory and the VBS order on the lattice [4].

In Fig. 5 we show the results of the $1/N$ expansion, Eq. (3), as continuous curves. In the insets we plot the same data in such a way that in the $1/N \to 0$ limit we can do a more direct comparison with the two irrational numbers $32/\pi^2$ and $2\delta_1$ that are predicted based on the CP^{N-1} theory. We have also fitted these data to straight lines, which give numerical predictions of the next-higher corrections to the large-N forms in Eq. (3).

The most important features in Fig. 5 that lend support to the DQC scenario are: *(1)* The exponents η_N and η_V for the $N > 4$ J_1-J_2 models are consistent in trend with previous estimates for $N = 2, 3, 4$ based on the entirely different J-Q model [10]. This is line with the concept of universality between different microscopic models, characteristic of a continuous transition. *(2)* The Néel-order exponent η_N connects to the leading $1/N$ behavior, approaching 1 as $N \to \infty$. This large value (in contrast to the normal mean-field value $\eta = 0$ and typically very small values at conventional critical points) was one of the important early "smoking gun" predictions of the DQC scenario [6]. *(3)* The leading $1/N$ correction to

η_N is of the correct sign and within a few percent in magnitude of the analytic result $32/\pi^2$ for the CP^{N-1} theory [20]. *(4)* η_V increases rapidly with N and has a trend that is fully consistent with the very non-trivial large-N result [21, 22].

Conclusions.—We have provided an SU(N) symmetric sign problem free model that allows, for the first time, unbiased studies of the Néel-VBS transition for arbitrary $N > 5$ on large lattices. Our model generalizes to SU(N) the important J_1-J_2 model for SU(2) spins, which has a long history of studies by exact diagonalization and various approximate methods (normally for antiferromagnetic J_2, in which case it has a Néel–VBS transition also for $N = 2$, which, however, is difficult to study reliably due to QMC sign problems) [28]. Our model opens new avenues for detailed connections between large-N theory and unbiased numerical simulations.

In this initial study, we found direct Néel-VBS transitions for $5 \leq N \leq 12$, with no signs of discontinuities up to large system sizes ($L \leq 128$). When analyzed as continuous quantum critical points, we found remarkable agreement for universal exponents with the $1/N$ expansion of the CP^{N-1} field theory. This quantitative comparison lends very strong support to the DQC theory [6].

The SU(N) spin model can be doped with fermions (holes), and it should be possible to carry out QMC studies at least for a small number of mobile holes. This would allow for a comparison with field theoretic predictions for exotic metallic and superconducting states that may arise close to DQC points [29].

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[27] As is apparent from Fig. 5 and Eqs. (2,3), the large corrections to scaling in the VBS correlation function $C_V(r)$ are due to the fact that η_V itself becomes large as N is increased, resulting in a $C_V(r)$ whose leading term decays too quickly to separate it from subleading pieces on moderate-size lattices and with typical QMC errorbars.

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