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Néel and Spin-Peierls Ground States of Two-Dimensional SU(N) Quantum Antiferromagnets

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The two-dimensional SU(N) quantum antiferromagnet, a generalization of the quantum Heisenberg model, is investigated by quantum Monte Carlo simulations. The ground state for $N \leq 4$ is found to be of the Néel type with broken SU(N) symmetry, whereas it is of the Spin-Peierls type for $N \geq 5$ with broken lattice translational invariance. Our computation of the magnetization and the dimerization order parameter shows the absence of the intermediate spin-liquid phase.

The existence of a short-range resonating valence bond (RVB) spin liquid [1] is one of the central problems for low-dimensional quantum spin systems. An RVB spin liquid exhibits a finite gap for spin excitations, has only short-range order, and does not break any lattice symmetry. The search for RVB spin liquid states was motivated by the suggestion that such strongly correlated but quantum disordered states can be turned into a superconducting state upon doping, which may explain the mechanism of the copper-oxide superconductors [2].

An RVB spin liquid is presumably created by strong quantum fluctuations which destroy magnetic ordering. The simplest construction of spin-liquid states is on lattices with an even number of spins per unit cell, such as two spin ladders [3], bilayer [4], or coupled plaquettes [5]. There a strong coupling within the unit cells leads to the formation of weakly coupled spin singlets.

This mechanism does not apply to lattices with an odd number of spins per unit cell, such as the square lattice relevant for the high-T_c cuprates. In the square lattice Heisenberg antiferromagnet quantum fluctuations decrease the Néel order as the spin S is decreased whereas the ground state remains ordered even for $S = 1/2$ [6]. Stronger quantum fluctuations are thus needed and frustrating interactions have been proposed as one route [7]. Since frustrating interactions generally cause a sign problem for quantum Monte Carlo simulations, numerical calculations are usually restricted to small lattices and it is hard to draw definitive conclusions. Still, it could be established that the ground state of the antiferromagnetic Heisenberg model on a triangular lattice is magnetically ordered [8–10]. A disordered ground state was suggested [11] for the fully frustrated model on a kagome lattice, but the nature of this state is not clear. The only clear evidence for an RVB spin liquid in a frustrated system so far is limited to some models with multispin interactions on a triangular lattice [12–14].

The route we follow in this Letter is to increase quantum fluctuations by considering models with higher symmetry than SU(2) and determine the nature of ground state once quantum fluctuations are strong enough to destroy Néel order. Namely, we consider models with the SU(N) symmetry. For small N, the SU(N) models have a long history of research. The SU(3) symmetric points, for instance, occur in spin $S = 1$ Heisenberg antiferromagnets with additional biquadratic interactions [15–20] whereas the SU(4) symmetric models appear as special points in coupled spin-orbital models [21]. However, one such model, i.e., the SU(4)-symmetric Kugel-Khomskii model [21], suffers from a negative sign problem in more than one dimension [22]. While a numerical work [23] based on the exact diagonalization hinted a finite gap, the result is not conclusive due to the system size limitation. For a related antiferromagnetic SU(4) model, there is no negative sign problem. While a mean-field type argument was given [24] for this model in favor of the ordered ground state, an RVB spin-liquid ground state was suggested by previous quantum Monte Carlo simulations [25], as the first example of such a state on a nonfrustrated lattice. These models can be regarded as a generalized Heisenberg antiferromagnet, and belong to a family of SU(N) models employing one of the simplest representations for the symmetry group of the model. In this sense they are "minimal" models for physical systems with higher symmetries than SU(2), and the results are expected to be of relevance as reference models in a wide array of applications.

An SU(N) model is specified by an irreducible representation of the operators, i.e., the Young tableau for the SU(N) algebra. Here we consider the series of models with a single-row Young tableau. In one dimension the ground state of these models is dimerized for any fixed number of columns n_c of the Young tableau as $N \to \infty$ [26]. In two dimensions, in a bosonic representation equivalent to a single-row Young tableau, it was found that for large n_c and N, the ground state is Néel state if $N < \kappa n_c$, where κ is a numerical constant [27]. Read and Sachdev [28] confirmed this result and, by examining the continuous version of the model in the large-N limit, argued that the ground state becomes a spin-Peierls state

as soon as N exceeds the boundary $N^* \equiv \kappa n_c$. Although their approach is less reliable for small N, they conjectured a direct transition with no spin-liquid intermediate phase even for small values of N (i.e., for small n_c)—inconsistent with the conclusion drawn from the numerical evidences for a spin-liquid phase in the SU(4) model [25]. In this Letter, using a new cluster quantum Monte Carlo algorithm, we present conclusive numerical evidence for a direct transition from the Néel state to the spin-Peierls state. No RVB spin-liquid ground state is realized for any N.

Our SU(N)-invariant generalization of the Heisenberg model [26,28] can be formally written as

$$H = \sum_{\langle rr' \rangle} H_{rr'} = \frac{J}{N} \sum_{\langle rr' \rangle} J_\beta^\alpha(\mathbf{r}) J_\alpha^\beta(\mathbf{r}'), \qquad (1)$$

where $\langle rr' \rangle$ runs over all nearest-neighbor pairs on a square lattice, and repeated indices $\alpha, \beta = 1, \ldots, N$ are to be summed over. Throughout this Letter, we set $J = 1$ as the unit of the energy. The symbols $J_\beta^\alpha(\mathbf{r})$ denote the generators of SU(N) algebra, that satisfy $[J_\beta^\alpha(\mathbf{r}), J_\nu^\mu(\mathbf{r}')] = \delta_{r,r'}(\delta_\nu^\alpha J_\beta^\mu(\mathbf{r}) - \delta_\beta^\mu J_\nu^\alpha(\mathbf{r}))$. To uniquely specify the model, we have to choose the representation of the algebra. The model examined in this Letter is the "antiferromagnetic" SU(N) model, in which an operator J_β^α is represented by a N dimensional matrix with the fundamental representation (i.e., a single-box Young tableau) on one sublattice and with the conjugate representation (i.e., the single-column Young tableau with $N - 1$ boxes) on the other sublattice. We note that the Kugel-Khomskii model [21] uses the same representation on both sublattices and that for $N = 2$ both models reduce to the ordinary SU(2) antiferromagnetic Heisenberg model.

In this representation, the model can be conveniently expressed in terms of SU(2) spins with $S = (N-1)/2$. The matrix elements of the pair Hamiltonian $H_{rr'}$ are explicitly given by $\langle \alpha', \beta' | H_{rr'} | \alpha, \beta \rangle = -\frac{J}{N} \delta_{\alpha,-\beta} \delta_{\alpha',-\beta'}$, where $|\alpha, \beta\rangle$ ($\alpha, \beta = -S, -S + 1, \cdots, S$) is the simultaneous eigenstates of the z components of SU(2) spin operators, $S^z(\mathbf{r})$ and $S^z(\mathbf{r}')$. We probe for two types of long-range order. The first is a generalized Néel state with broken SU(N) symmetry characterized by a finite staggered magnetization $M_s \equiv \sum_{\mathbf{r}}(-1)^{\mathbf{r}} S^z(\mathbf{r})$. The second is a dimerized state with broken translational invariance but no broken spin rotation symmetry, characterized by an order parameter such as $D_{\mathbf{k}} \equiv \sum_{\mathbf{r}} e^{-i\mathbf{k}\mathbf{r}} S^z(\mathbf{r}) S^z(\mathbf{r} + \mathbf{e}_x)$ where $\mathbf{e}_x$ is the lattice unit vector in the $\mathbf{x}$ direction. It was argued [28] that $\mathbf{k} = (\pi, 0)$ or $(0, \pi)$ is preferred when the lattice translational symmetry is broken.

Recent developments in quantum Monte Carlo algorithms [29] allow us to perform quantum Monte Carlo (QMC) simulations on larger systems and for a wider range of N than was possible in previous calculations [25]. By splitting each original spin operator into $2S$ Pauli spins with $S = 1/2$ [30], the Hamiltonian of the

SU(N) model in the new extended Hilbert space is expressed [18] as

$$H_{rr'} = -\frac{J}{N}[\Delta_{\text{Horizontal}}^{(N-1)}(\mathbf{r}, \mathbf{r}')]_s, \qquad (2)$$

where the symbol $[\cdots]_s$ denotes the symmetrization with respect to the $2S$ Pauli spins. The symbol $\Delta_{\text{Horizontal}}^{(N-1)}$ denotes the operator whose matrix element is one if the $(N-1)$-fold horizontal graph matches the initial and the final spin states, while it is 0 otherwise (see Fig. 1). This formulation yields the following quantum Monte Carlo algorithm: (i) for a given worldline configuration, distribute the $(N-1)$-fold horizontal graphs with the density J/N, (ii) construct loops by following world lines and horizontal graphs, and (iii) flip each loop independently with probability $1/2$. After a major part of the present work had been done with this algorithm, we found that other algorithms that require a smaller amount of memory could be constructed using the framework of the stochastic series expansion [31] and the idea of coarse graining [32], or directly working with the weight equation (see [33]) in the conventional framework of loop algorithms. This latter algorithm was used in a part of the present calculations. The details of these algorithms will be reported elsewhere [34].

Simulations have been performed at low enough temperatures to be effectively in the ground state. We have measured the spin structure factors at a few different temperatures for each system size to confirm that they exhibit no detectable temperature dependence. The lowest temperature used for $N = 4$ and $L = 128$, for example, is $1/128J$. We explored system sizes L up to $L = 128$ for $N = 3$ and 4, and $L = 64$ for $N = 5, 6, 7$, and 8. The number of Monte Carlo sweeps in a typical set of simulation is 3.4×10^5 for the most time consuming case ($L = 128$ and $N = 4$).

In Fig. 2 we show the spin structure factor, $S_{(\pi,\pi)} = L^{-d}\langle(M_s)^2\rangle$, divided by L^2, which in the SU(N) language reads $S_{(\pi,\pi)} = \frac{N^2(N+1)}{12}\langle(\sum_{\mathbf{r}} J_1^1(\mathbf{r}))^2\rangle$. In the Néel phase, $S_{(\pi,\pi)}/L^2$ converges to the square of the staggered magnetization per spin, m_s, as $L \to \infty$, while it decreases asymptotically to zero, being proportional to L^{-2}, in
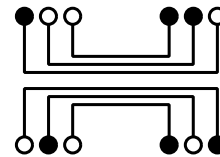

FIG. 1. One of the threefold horizontal graphs for $N = 4$ corresponding to $\Delta_{\text{Horizontal}}^{(3)}(\mathbf{r}, \mathbf{r}')$, with one of its matching spin configurations. [A different choice of the graph does not make any difference because of the symmetrization in Eq. (2).] Open circles denote up-spins and filled circles down-spins. A spin configuration matches a graph if and only if any two connected spins are antiparallel.
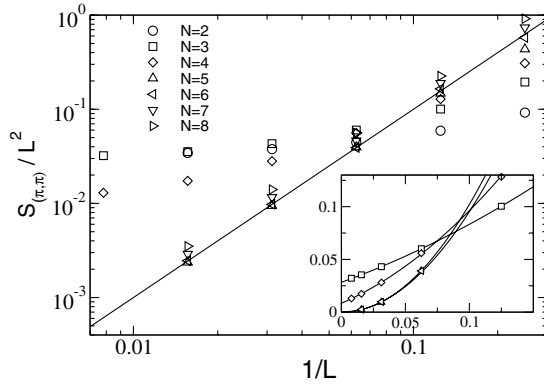
FIG. 2. Static structure factors $S_{(\pi,\pi)}$ for $2 \leq N \leq 8$. The straight line representing the power law, $S_{(\pi,\pi)}L^{-2} \propto L^{-2}$, is drawn for comparison. Estimated statistical errors are not shown because they are equal to or smaller than the symbol size. The inset presents the data for $N = 3, 4, 5, 6$ in the linear scale, together with the best fitting curves obtained by the method of least squares.
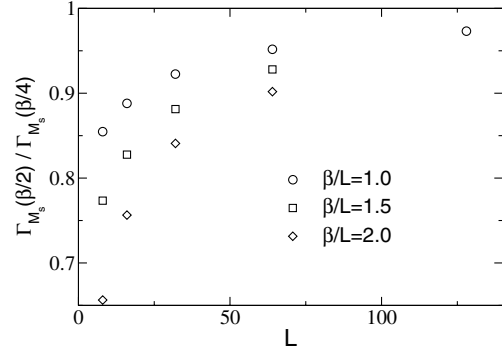

FIG. 3. The ratio of dynamic correlations of staggered magnetization at two imaginary-time intervals, $\beta/2$ and $\beta/4$, for the SU(4) model. As L increases, the value approaches 1, regardless of the aspect ratio β/L.

the absence of Néel order. Our results in Fig. 2 show clear evidence for Néel order for $N \leq 4$ and the absence of Néel order for $N \geq 5$, indicating that the phase boundary of the Néel ground state lies between $N = 4$ and 5.

For $N \leq 4$ the staggered magnetization in the thermodynamic limit is calculated from a finite size extrapolation using a second order polynomial in $1/L$. A least-squares fit based on the data for $L \geq 8$, gives

$$m_s = 0.1682(6) \qquad \text{for } N = 3, \qquad (3)$$

$$m_s = 0.091(3) \qquad \text{for } N = 4, \qquad (4)$$

where the numbers in the parentheses indicate the estimated statistical error (of 1 standard deviation) in the last digit. For $N = 5$ and $N = 6$, the estimated m_s^2 agrees with zero within the statistical error ($m_s^2 = -0.0003(6)$ for $N = 5$ and $m_s^2 = 0.0004(5)$ for $N = 6$).

The existence of Néel order at $N = 4$ is further confirmed by the correlation ratio, which eliminates contributions from short-range correlations [35]. While the structure factor $S_{(\pi,\pi)}$ is a sum of two-point correlation functions with all distances and therefore contains short-range correlations, the quantity $\Gamma_{M_s}(\tau) \equiv \langle M_s(\tau)M_s(0) \rangle \equiv \langle e^{\tau H} M_s e^{-\tau H} M_s \rangle$ does not if τ is sufficiently large. We measure this quantity at a fixed aspect ratio, β/L, and compute the ratio $\Gamma_{M_s}(a'\beta)/\Gamma_{M_s}(a\beta)$ with $a < a'$ for various system sizes. As L is increased, this ratio converges to 1 if the system has long-range order. If, on the other hand, the system is disordered with a finite gap and therefore has a finite correlation length in the imaginary-time direction, it will converge to 0. Hence this ratio serves as a good indicator of the existence of a long-range order, similar to the well-known Binder parameter. In Fig. 3, we plot the correlation ratio for various aspect

ratios $\beta/L = 1.0, 1.5$, and 2.0 for $N = 4$. We can see that the correlation ratio approaches 1 and thus establish long-range Néel order.

The disagreement of our conclusion (Néel order for $N = 4$) with that of Ref. [25] is not in the raw numerical data. Their estimates of $S_{(\pi,\pi)}$ agree with ours shown in Fig. 2 within the statistical errors. The disagreement is solely due to the small system sizes studied in Ref. [25]. The convergence of the magnetization to a finite value in Fig. 2 can be seen only for system sizes $L \geq 32$, whereas the previous simulations were limited to $L = 12$.

In order to fully answer the question of whether an intermediate spin-liquid phase exists, we next determine at which value of N the ground state starts being dimerized. Figure 4 shows the dimer structure factor, $S_{\boldsymbol{k}}^D \equiv L^{-d} \langle D_{-\boldsymbol{k}} D_{\boldsymbol{k}} \rangle$, for $\boldsymbol{k} = (\pi, 0)$ divided by L^2 at $N = 4, 5$, and 6. In the thermodynamic limit, $S_{\boldsymbol{k}}^D/L^d$ should converge to the squared dimerization per spin. In Fig. 4 we see a clear power law decay of $S_{\boldsymbol{k}}^D/L^2$ following L^{-2} and thus the absence of dimerization for $N = 4$, but a slower decay and upward bending for $N = 5$ and 6. This suggests convergence to finite values, although the examined systems are not large enough to cover the region where $S_{(\pi,0)}^D$ shows no size dependence. For a more systematic analysis, we once more perform a least-squares fit of the data of $S_{(\pi,0)}^D$ for $L \geq 8$, using a second order polynomial in $1/L$. Our results for the spontaneous dimerization per site are 0.103(3) for $N = 5$ and 0.18(5) for $N = 6$ (see the inset of Fig. 4). For $N = 4$, the same analysis yields $[D_{(\pi,0)}/L^d]^2 = -0.00002(2)$, consistent with absence of dimerization.

We also compute $S_{\boldsymbol{k}}^D$ at $\boldsymbol{k} = (\pi, \pi)$ and find $S_{(\pi,\pi)}^D/L^2 \propto L^{-2}$, for $N = 4, 5$, and 6, indicating the absence of dimerization at this wave vector, consistent with the previous suggestion [28].

In conclusion, our high-accuracy QMC simulations using new loop-type QMC algorithms have shown that the ground state of the SU(N) square lattice antiferromagnet is the Néel state for $N \leq 4$, whereas it
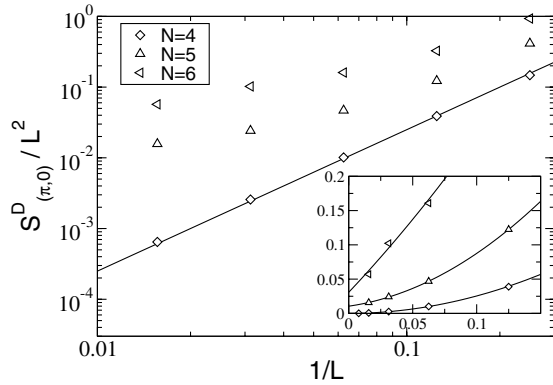
FIG. 4.   The $k = (\pi, 0)$ dimer structure factors $S^D_{(\pi,0)}$ for $N = 4, 5, 6$ in logarithmic scale. The inset is the linear-scale plot. The solid lines in the inset are the best fitting curves of least squares based on the $L \geq 8$ data.

is the dimerized or Spin-Peierls state for $N \geq 5$. No intermediate spin liquid has been observed, consistent with analytical arguments [28], but inconsistent with the conclusion drawn, naturally, from previous numerical simulations on smaller lattices [25].

It is interesting to compare the present result with the analytical estimate of the phase boundary [27]: $n_c \sim 0.19 N^*$ where n_c is the number of the columns of the Young tableau. This estimate is supposed to be accurate for large N, and is not necessarily justified for the present case where $n_c = 1$ but is still surprisingly accurate. For our model it would indicate Néel order up to $N = 5$, while we find Néel order only up to $N = 4$.

Concerning the existence of true RVB spin-liquid states without any broken symmetry, our results are essentially negative. By showing that the proposed spin-liquid state in an SU(4) model exhibits Néel order, we are left with only a few models with multispin interactions on a triangular lattice as the models with clearly established spin-liquid ground state [12–14]. Since the hardcore dimer model on the square lattice does not show any gapped spin-liquid phase [36], and in numerical simulations only symmetry broken phases were found so far for frustrated lattices, we are led to conjecture that a spin-liquid state without any broken symmetry seems to be impossible to obtain on a bipartite lattice with an odd number of spins in the unit cell.

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