Ground States of the SU(N) Heisenberg Model

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(Received 29 September 2006; published 29 January 2007)

The SU(N) Heisenberg model with various single-row representations is investigated by quantum Monte Carlo simulations. While the zero-temperature phase boundary agrees qualitatively with the theoretical predictions based on the $1/N$ expansion, some unexpected features are also observed. For $N \geq 5$ with the fundamental representation, for example, it is suggested that the ground states possess exact or approximate U(1) degeneracy. In addition, for the representation of Young tableau with more than one column, the ground state shows no valence-bond-solid order even at N greater than the threshold value.

DOI: 10.1103/PhysRevLett.98.057202 PACS numbers: 75.10.Jm, 75.40.Mg

Since the resonating-valence-bond state was proposed [1] as a possible mechanism that supports novel superconductivity in cuprates, it has been a major target of condensed matter theory to find a short-range interaction model that realizes a spin-liquid state at zero temperature. Introducing frustrations into the model that otherwise has a magnetic ground state is one of promising directions to achieve this goal. Numerical verification for such models is, however, technically very difficult, and conclusive results are still missing for geometrically frustrated systems such as the antiferromagnet on a triangular lattice. Another approach was taken in [2,3], where the authors generalized the Heisenberg antiferromagnet to higher symmetries, thereby increasing the model's degrees of freedom and enhancing quantum fluctuations. Based on the $1/N$ expansion treatment, they predicted that the model with sufficiently large N has a valence-bond-solid (VBS) ground state with spontaneously broken lattice symmetry. The nature of the ground states may depend on the representation, somewhat analogous to what happens in the SU(2) models in one dimension though the underlying mechanisms may be rather different.

More specifically, it was suggested [2,3] that, for the model with the Young tableaux with m rows and n columns, the N-n phase diagram does not strongly depend on m, and has a line of phase transition separating the small-N Néel region from the large-N VBS region. It was also argued that the nature of the VBS ground state can be classified according to the quotient of the division of n by 4. If $n \equiv 1$ or 3 (mod 4), the ground state has a columnar ordering [Fig. 1(a)] with the translational symmetry and the 90° rotational symmetry both broken, whereas if $n \equiv 2$ (mod 4) it has a "nematic" VBS ordering [Fig. 1(b)] with only the lattice-rotational-symmetry broken. Finally, if n is a multiple of 4, there is no spontaneous breaking of the lattice symmetry.

They also showed that the $O(1/N)$ effective Hamiltonian with the fundamental representation is exactly the same as the quantum dimer model [4] at $V = 0$. For the quantum dimer model, it was shown by a numerical calculation [5] that the ground state is a VBS state with columnar arrangement of dimers. This is in agreement with the above conjecture that the degeneracy is 4 for $n = 1$. A direct check of the spontaneous breaking down of the translational symmetry for $m = n = 1$ was carried out in a previous Letter [6], which yielded the transition value of N, namely, $4 < N^*(m = n = 1) < 5$.

The model Hamiltonian we discuss is defined as

$$H = J \sum_{(\boldsymbol{R},\boldsymbol{R}')} \sum_{\alpha,\beta=1}^{N} S^{\alpha\beta}(\boldsymbol{R}) S^{\beta\alpha}(\boldsymbol{R}'), \tag{1}$$

where the operator $S^{\alpha\beta}$ is the generator of the SU(N) algebra. Here we consider the simple square lattice with the periodic boundary condition. We divide the whole lattice into two sublattices, say, A and B. The representation of the generators on sublattice A is characterized by the Young tableau with a single raw ($m = 1$) and varying number of columns. The representation on sublattice B is the conjugate of that on sublattice A. We have performed quantum Monte Carlo simulations by the directed loop algorithm [7] and extrapolated the results to the zero-temperature limit. The algorithm can be obtained by generalizing the idea of the coarse-grained algorithm for $N = 2$ [8] to the present general N case. The technical details will be published elsewhere [9].

Our principal findings are as follows. (i) For $n = 1$, the ground state in the large-N region adjacent to the Néel

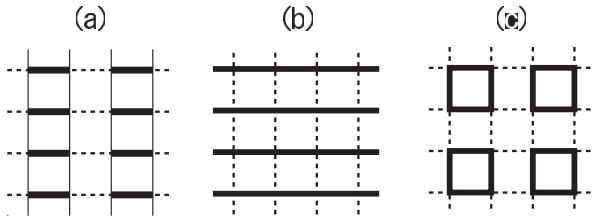

FIG. 1. Three types of VBS states: (a) columnar ($\bar{D}_x \neq 0$ and $\bar{D}_y = 0$), (b) nematic ($\bar{D}_x = \bar{D}_y = 0$), and (c) plaquette ($\bar{D}_x = \bar{D}_y \neq 0$). The quantities $\bar{D}_x$ and $\bar{D}_y$ characterize spontaneous translational-symmetry-breaking in the x and y directions, respectively. [See Eq. (4) for the definition.]

region is the columnar VBS state as the previous works suggested. However, up to $L = 32$, it appears to have infinite degeneracy corresponding to a continuous U(1) symmetry that does not exist in the original microscopic Hamiltonian but may emerge asymptotically. Accordingly, the resonons [4] are gapless. (ii) The ground state in the large-N region for $n > 1$ shows no evidence of break down of any lattice translational symmetry, in particular, the ones predicted in Read and Sachdev [2,3]. The distance dependence of the energy-energy correlation function is consistent with the algebraic decay.

In the present Letter, we start by showing some results that confirm the conclusions of the previous numerical work on the SU(N) model, and then discuss the new findings. We first look at the case of the fundamental representation ($n = 1$). It was found [6] that for $N \leq 4$ the ground state is a Néel state whereas it does not have a spontaneous staggered magnetization for $N \geq 5$. Instead the ground state for $N = 5$ and 6 was found to possess the spontaneous dimerization. Although a macroscopic quantity is often used as a probe for detecting the transition, here we examine two-point correlation functions in order to see the transition more clearly: $C_Q(R; L) \equiv \langle Q(R\boldsymbol{e}_\mu)Q(0)\rangle_L - \langle Q(R\boldsymbol{e}_\mu)\rangle\langle Q(0)\rangle_L$, where L is the system size, $\boldsymbol{e}_\mu$ ($\mu = x, y$) a lattice unit vector, and $Q(\boldsymbol{R})$ an arbitrary quantity locally defined around the position $\boldsymbol{R}$. We also use the correlation ratio [10] defined simply as $R_Q(L) = C_Q(L/2; L)/C_Q(L/4; L)$. Similar to the Binder parameter, the correlation ratio is a dimensionless quantity and, when plotted against a relevant physical parameter, the common crossing point of curves with various system sizes marks the transition point. In Fig. 2, the correlation ratio for the ''magnetic'' moment is plotted against N for various system sizes for $m = 1$. Here, the magnetic moment is defined as

$$\Sigma(\boldsymbol{R}) \equiv S^{11}(\boldsymbol{R}) - S^{22}(\boldsymbol{R}).$$

While the ratio tends to converge to unity for $N = 2, 3, 4$, indicating the existence of the Néel ordering, it rapidly decreases for $N \geq 5$. Based on this figure, we can estimate the transition point as $N^*(n = 1) \sim 4.3$.

While Fig. 2 establishes the absence of the magnetic ordering for $N = 5, 6, 7$, it does not tell us much about the nature of the ground state. It was shown in [6] that in the ground state the lattice translational invariance is broken. Here we reconfirm the presence of the VBS order by detecting the long-range correlation in $C_A(\boldsymbol{R}; L)$, where A is defined as

$$A(\boldsymbol{R}) \equiv P_x(\boldsymbol{R}) - P_y(\boldsymbol{R}), \tag{2}$$

and $P_\mu(\boldsymbol{R})$ is the nearest-neighbor product of the magnetic moments, i.e.,

$$P_\mu(\boldsymbol{R}) \equiv \Sigma(\boldsymbol{R})\Sigma(\boldsymbol{R} + \boldsymbol{e}_\mu). \tag{3}$$

In Fig. 3, $C_A(L/2; L)$ is plotted. It is expected that the correlation must decay down to zero in the large L limit for a Néel state, whereas for any type of the VBS states in Fig. 1 it must converge to a nonzero value. Figure 3 clearly shows that the large-N phase for the fundamental representation is the VBS phase.

These observations are consistent with the columnar VBS states [such as Fig. 1(a)] as is conjectured for $N > N^*$ [2,3]. However, the above-mentioned probe A only is not sufficient to rule out the plaquette VBS state [Fig. 1(c)]. Since the columnar VBS states do not possess the 90° rotational symmetry while the plaquette VBS state does, one may naively expect that measuring the difference between the average bond strength in the x direction and that in the y direction can distinguish the two. Therefore, we have computed the quantity $B \equiv \langle(\bar{P}_x - \bar{P}_y)^2\rangle$, where an overline indicates the average over the volume, i.e., $\bar{P}_\mu \equiv V^{-1}\sum_{\boldsymbol{R}} P_\mu(\boldsymbol{R})$. The quantity B is plotted in Fig. 4 against the system size.

Instead of distinguishing the two types of states, the quantity B turns out to reveal an interesting property. The quantity B is proportional to $1/L^2$ not only for $N = 3$ and 4 but also for $N = 5$ and 6, indicating that the average bond strength in the x direction is the same as that in the y

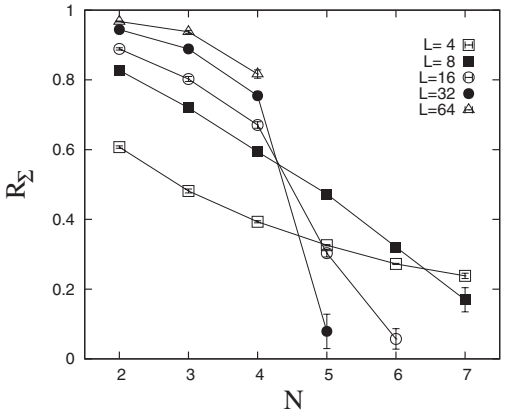

FIG. 2. The correlation ratio, $R_\Sigma(L)$, of the magnetization for the fundamental representation ($n = 1$).

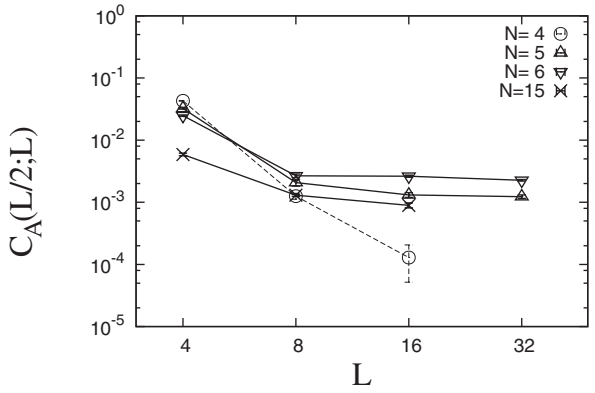

FIG. 3. The two-point correlation function the rotational-symmetry-breaking order parameter, A, for the model with the fundamental representation ($n = 1$).

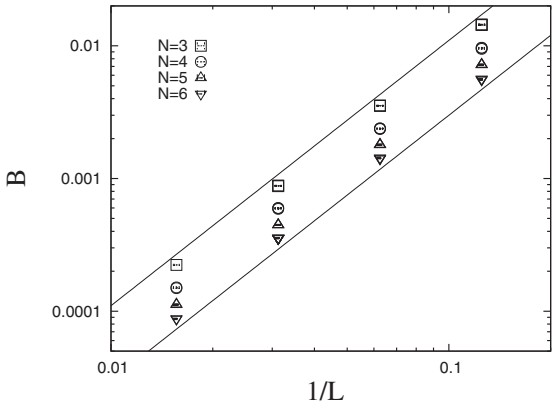

FIG. 4. The squared difference of the average bond strengths in the x and y directions for the fundamental representation. The straight lines that correspond to $B \propto 1/L^2$ are drawn for comparison.

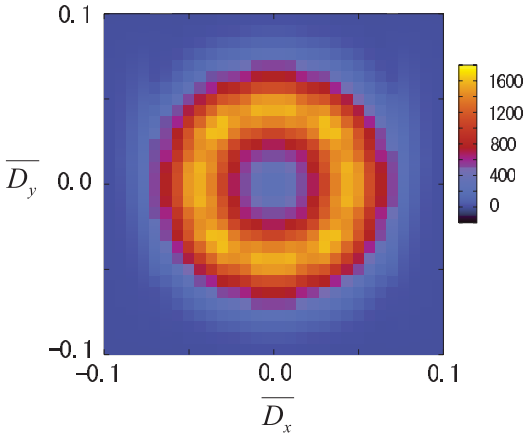

FIG. 5 (color). The frequency of observing a pair of values $(\bar{D}_x, \bar{D}_y)$ during the Monte Carlo simulation for $N = 6$ at $L = 32$ and $\beta = 16$. The value at each pixel is the average over eight symmetrically equivalent points, $(\pm\bar{D}_x, \pm\bar{D}_y)$ and $(\pm\bar{D}_y, \pm\bar{D}_x)$.

direction even in the VBS state. It follows that the expectation value of the nearest-neighbor correlation $P_\mu(\boldsymbol{R})$ in a single (pure) VBS ground state has the form

$$\langle P_\mu(\boldsymbol{R})\rangle_{\text{single}} = \bar{P} + \bar{D}_\mu \times (-1)^{R_\mu} \quad (\mu = x, y) \qquad (4)$$

with the direction-independent average value $\bar{P}$ and some direction-dependent constant $\bar{D}_\mu$ that characterizes the dimerization order. The constants $\bar{D}_x$ and $\bar{D}_y$ are expressed by the local quantities $D_\mu(\boldsymbol{R})$ as $\bar{D}_\mu = V^{-1}\sum_{\boldsymbol{R}} D_\mu(\boldsymbol{R})$, where $D_\mu(\boldsymbol{R}) \equiv [P_\mu(\boldsymbol{R} + \boldsymbol{e}_\mu) - P_\mu(\boldsymbol{R})]/2$.

In order to distinguish the columnar state from the plaquette state, we have to examine the joint distribution function, Prob$(\bar{D}_x, \bar{D}_y)$. For small systems, it consists of a single broad peak at the center, $(\bar{D}_x, \bar{D}_y) = (0, 0)$, even for $N \geq 5$. However, as the system grows the weight at center should diminish and peaks must appear according to the structure of the VBS phase. If the columnar VBS states are the true ground state, four peaks must develop at symmetric positions on the x and y axes $[(\bar{D}_x, \bar{D}_y) = (\pm D, 0), (0, \pm D)]$, whereas if the plaquette VBS states are the ground states, the peaks must appear at diagonal positions $[(\bar{D}_x, \bar{D}_y) = \pm(D, D), \pm(D, -D)]$.

As we see in Fig. 5, the distribution obtained from our computation shows neither feature. The distribution is circularly symmetric. This feature does not depend on N, the temperature, or the system size (at least up to $L = 32$), whenever a finite VBS order is observed. This suggests that the ground state is not only fourfold degenerate but also infinitely degenerate. The ground state manifold possesses the U(1) invariance, although it is not obvious from the microscopic Hamiltonian Eq. (1). Since each ground state breaks this U(1) symmetry, there must be a Goldstone mode associated with it, which may correspond to "resonons" mentioned in [4], though its gapless nature was predicted only for an isolated critical point. If the apparent U(1) symmetry persists to the thermodynamic limit, the resonons must be gapless not only at the isolated critical point $N = N^*$ but also in the whole region of the VBS phase. However, another possibility cannot be excluded by the present numerical calculation, i.e., the possibility that this apparent U(1) symmetry may be a transient behavior that applies only to certain intermediate length scales and the discrete symmetry of the original microscopic Hamiltonian is recovered for larger length scales. If this is the case, there should be a finite number of preferred angles in the two-component order-parameter space to which the true ground states correspond, and the resonon modes have a small but finite excitation gap.

Next we consider the model with the representation of Young's tableaux with two or more columns ($n \geq 2$). In order to determine the critical value of N, we have computed the correlation ratio for the magnetization as described above. For $n = 2$, the correlation ratio for the magnetization is plotted in Fig. 6. The Néel state is the ground state for $N \leq 9$, whereas it is not for $N = 10$ and larger. We can see the trend changes around $N^*(n = 2) \sim 9.5$, at which curves cross each other. This is again in a good agreement with the $1/N$ expansion result, $N^* \sim 5.3n$

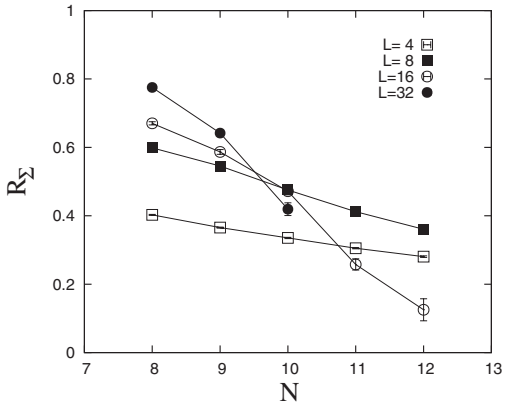

FIG. 6. The correlation ratio of the magnetization for the representation of two-box Young tableau ($n = 2$).

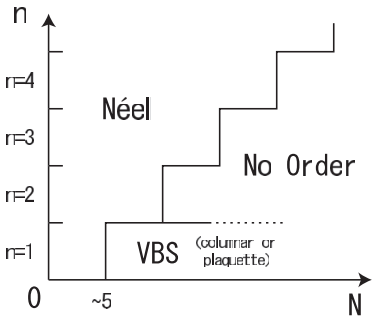

FIG. 7. The zero-temperature phase diagram of the SU(N) model on a square lattice with single-row ($m = 1$) representations.

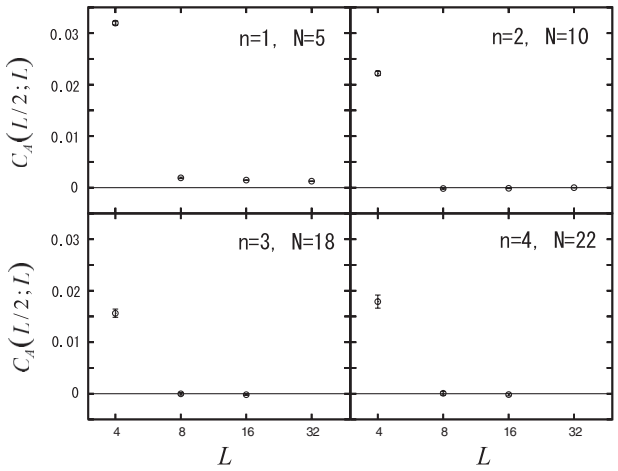

FIG. 8. The correlation function of the rotational-symmetry-breaking order-parameter A at the largest distance for $n = 1$, 2, 3, 4. The value of N for each n is close to but larger than the threshold value, $N_c(n)$.

[2,11]. For $n = 3$ and $n = 4$ we have performed similar computation and located the phase boundary as $N^*(n = 3) \sim 14$ and $N^*(n = 4) \sim 20$, respectively. These results are summarized in the schematic phase diagram (Fig. 7).

Lastly, we turn our attention to the nature of the nonmagnetic ground states for $n \geq 2$. As mentioned above, any type of the VBS states in Fig. 1 can be characterized by a nonzero value of $C_A(L/2; L)$ in the $L \to \infty$ limit. This correlation function is plotted in Fig. 8 for $n = 1$, 2, 3, 4. Characteristic features do not depend on N for each n. We show only the data for a single value of N for the sake of readability of the figure. (The value of N shown in Fig. 8 is chosen so that it is close to but definitely above the estimated threshold value.) The top left panel for $n = 1$, $N = 5$ is shown for comparison. As is clear from the figure, the system possesses the VBS ordering only for $n = 1$, but not for $n = 2$, 3, 4.

To obtain some information as to whether the large-N phase at $n \geq 2$ is gapless or not, we have also computed the correlation function of $P_\mu(\boldsymbol{R})$ itself, which is proportional to the energy-energy correlation. In a clear contrast to the case of $n = 1$, we have seen monotonic decrease to zero for $n = 2$, 3, 4, which is consistent with the absence of the rotational-symmetry breaking for $n = 2$, 3, 4 mentioned above. We do not clearly observe exponential decay in any of the disordered cases. The decay in the correlation up to the length scale of $L \sim 32$ is consistent with the power law with the decay exponent between 2 and 3. However, the correlation function for large L is very small and the relative error is too large to obtain a definite answer to the question whether this phase is gapless or not.

To summarize, in addition to the confirmation of the previous result [6], we have found evidence of an emergent (exact or approximate) U(1) symmetry of the ground state space of the SU(N) model with the fundamental representation, and also found no VBS order in the large-N region adjacent to the phase boundary to the Néel region. The latter finding is the first strong evidence for the spin-liquid (disordered) ground state in the present model that does not have geometrical frustrations in contrast to the models studied previously in search for the quantum disordered states. As for the first finding, it is appropriate to mention the recent works on the deconfinement critical phenomena (DCP). The present SU(N) model is the model that was discussed in previous works [12–14] related to DCP, where the authors argued that some unconventional type of the second-order phase transition is possible between two phases with apparently unrelated symmetries (e.g., the VBS phase and the Néel phase). Also discussed there was the emergent U(1) symmetry at (or near [14]) the critical point. We suspect that the U(1) structure that we have observed reflects validity or approximate validity of the DCP scenario in the present model at zero temperature.

The author would like to thank Cristian Batista and Anders Sandvik for useful comments. The computation presented here was performed on SGI Altix 3700/1280 at Supercomputer Center, Institute of Solid State Physics, University of Tokyo.

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