SU(N) Heisenberg model with multi-column representations

Tsuyoshi Okubo, Kenji Harada, Jie Lou, and Naoki Kawashima

1 Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan
2 Graduate School of Informatics, Kyoto University, Kyoto 615-8063, Japan
3 Department of Physics, Fudan University, Shanghai 200433, China

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The SU(N) symmetric antiferromagnetic Heisenberg model with multi-column representations on the two-dimensional square lattice is investigated by quantum Monte Carlo simulations. For the representation of Young diagram with two columns, we confirm that a valence-bond solid order appears as soon as the Néel order disappears at \( N = 10 \) indicating no intermediate phase. In the case of the representation with three columns, there is no evidence for both of the Néel and the valence-bond solid ordering for \( N \geq 15 \}. This is actually consistent with the large-\( N \) theory, which predicts that the VBS state immediately follows the Néel state, because the expected spontaneous order is too weak to be detected.

Realization of quantum spin liquid in short-range coupling models has been a popular research target in condensed matter physics for several decades. One approach to obtain a spin-liquid state is to consider a Hamiltonian with higher symmetry. Read and Sachdev generalized antiferromagnetic Heisenberg into SU(N) symmetry\(^{1,2}\). Based on the 1/N expansion they showed that the ground state of the model with sufficiently large \( N \) is a valence-bond-solid (VBS) breaking the lattice rotational or the translational symmetry spontaneously. Recently, in terms of the deconfined quantum criticality\(^{3–5}\), their theory attracts much attention. In particular, the existence of intermediate state was discussed near the boundary of Néel and VBS\(^{6–8}\).

Nature of the ground states of the model can vary depending on the representation of SU(N) algebra. Read and Sachdev suggested that for the model with the representation of \( m \) rows and \( n \) columns Young diagram, the ground state phase diagram on the \( N-n \) plane does not strongly depends on the value of \( m \). Within the 1/N expansion, there are only two types of phases: the small-\( N \) Néel phase and the large-\( N \) VBS phase (see Fig.1(a)). In addition, it was shown that the nature of the VBS state can be classified by the remainder of the division of \( n \) by 4 on the two-dimensional square lattice. For \( n = 1, 3 \) (mod 4), the VBS state is so called columnar VBS where both of translational symmetry and 90\(^\circ\) lattice rotational symmetry are broken (Fig.1(b)). For \( n = 2 \) (mod 4), the VBS state is expected to be a nematic VBS with breaking only lattice rotational symmetry (Fig.1(c)). In the case of \( n = 0 \) (mod 4), there is no spontaneous symmetry breaking, which is an analog of Haldane state in \( S = 1 \) spin chain.

Beyond the 1/N-expansion, it was shown that for \((n, m) = (1, 1)\) the ground state is the SU(N) Néel state for \( N \leq 4 \) while it becomes columnar VBS state for \( N \geq 5 \) by the quantum Monte Carlo (QMC) calculation\(^6\). Related to this case, the SU(N) J-Q model was proposed by Sandvik\(^8\). The SU(N) J-Q model has an additional many-body interaction so that the quantum phase transition between the Néel phase and the columnar VBS phase occurs by continuously changing the Hamiltonian parameter. In order to vary the Hamiltonian continuously, a continuous-\( N \) model was also proposed by Beach \textit{et al.}\(^8\). Because the phase transition might be a realization of deconfined quantum criticality\(^4–5\), nature of these models have attracted much recent interests in condensed matter physics\(^4–5\).

For the case of \( n \geq 2 \), there were a few studies concerning phase boundary between the Néel phase and the

![Fig. 1. (color online) (a): Schematic phase diagram of the SU(N) Heisenberg model on the square lattice with single-row \((m = 1)\) representations. The phase boundaries for the case of \( n = 2, 3 \) are determined in the present study, while that for \( n = 1 \) was from Ref.\(^6\). In the case of \( n = 3, 4 \), we do not see clear evidence of the spontaneous VBS order in the vicinity of the phase boundaries for finite-size QMC simulations. (b,c): Schematic picture of the columnar VBS (b) and the nematic VBS (c) states. Thick solid lines denote larger value of \( \langle \sum_{\alpha,\beta} S_i^{\alpha\beta} S_j^{\beta\alpha} \rangle \) while thin solid and dashed lines indicate smaller values.](https://example.com/figure1.png)
VBS phase. In QMC calculation up to $L = 32$ for $L \times L$ square lattice, no evidence of VBS order was found for $n = 2, 3, 4$ with $m = 12$. This result appeared to suggest an intermediate phase between the Néel phase and the VBS phases. However, whether the missing evidence of the VBS order for $n \geq 2$ is due to an intermediate spin liquid phase or due to the extremely small (but finite) order parameter beyond numerical limitation has not been clarified up to now.

In this paper, we investigate ground state of the SU($N$) Heisenberg model for $n = 2$ and $3$ with $m = 1$ by using QMC simulation. The SU($N$) model we considered is an SU($N$) symmetric antiferromagnetic Heisenberg model on the two-dimensional square lattice with the periodic boundary condition. Hamiltonian of the model is given by

$$\mathcal{H} = \frac{J}{N} \sum_{(i,j), i \in A, \alpha, \beta = 1}^{N} S_i^{\alpha \beta} S_j^{\beta \alpha},$$

(1)

where $S_i^{\alpha \beta}, \bar{S}_i^{\alpha \beta}$ are generators of SU($N$) algebra, and we consider $J > 0$. On one sublattice $A$ of the lattice, the representation of the generators $S_i^{\alpha \beta}$ is characterized by the Young diagram with a single row ($m = 1$) and arbitrary number $n$ of columns, while we use the conjugate representation $\bar{S}_i^{\alpha \beta}$ on the other sublattice. Note that the conjugate representation satisfies the relation $\bar{S}_i^{\alpha \beta} = -S_i^{\beta \alpha}$. We have performed QMC simulation based on the loop algorithm. We modified ALPS/LOOPER code\textsuperscript{16,17} for the present purpose\textsuperscript{18}. We set the inverse temperature $\beta$ as $\beta J = L$ and investigated the zero temperature properties by extrapolating the results to $L \to \infty$.

In order to see the VBS orders, we define two order parameters. The local nematic order parameter is defined as

$$\Phi_j \equiv P_{j,y} - P_{j,x},$$

(2)

where $P_{j,\mu} (\mu = x, y)$ is the nearest-neighbor product of “magnetic” moments

$$P_{j,\mu} \equiv \sum_{\alpha = 1}^{N} S_j^{\alpha \alpha} S_j^{\alpha \mu}.$$  

(3)

The nematic order parameter characterizes the symmetry breaking of 90 degrees lattice rotation. $\langle \Phi_j \rangle$ takes a finite value for both of the nematic VBS and the columnar VBS states in the thermodynamic limit. We also define a local complex order parameter characterizing the columnar VBS order as

$$\Psi_j \equiv (-1)^{j_x} (P_{j,x} - P_{j,-x}) + i(-1)^{j_y} (P_{j,y} - P_{j,-y}),$$

(4)

where $j_x$ and $j_y$ are integers representing the lattice coordinates of site $j$. In the columnar VBS phase $|\langle \Psi_j \rangle| \neq 0$, while $|\langle \Phi_j \rangle| = 0$ for the Néel and the nematic VBS phases. In order to see the phase transition clearly, we examine the two-point correlation functions of an observable $O$: $C_O(R) \equiv \langle O(0)O^\dagger(R) \rangle$. For the Néel order, we use the correlation of a magnetization $S_i^{\alpha \alpha}$: $C_{\text{Mag}}(R) \equiv \sum_{\alpha = 1}^{N} C_{S_{\alpha \alpha}}(R)$. We also consider the nematic VBS correlation $C_{\text{Nem}} \equiv C_{\Phi}(R)$ and the columnar VBS correlation $C_{\text{Col}}(R) \equiv C_{\Psi}(R)$.

First, we examine the case of $n = 2$. In Fig. 2, we show the two-point correlations for $n = 2$ at $|R| = L/4$ for various sizes $L$ and $N$. For the case of the Néel order (Fig. 2(a)), we see that the correlation exponentially decays to zero by increasing $L$ for $N \geq 10$ while it converges to a nonzero value for $N = 9$ indicating that the Néel state is the ground state for $N \leq 9$ and it is not for $N \geq 10$. These observations are consistent with the previous QMC calculation\textsuperscript{19}. For the nematic order parameter (Fig. 2(b)), the two-point correlations tend to
converge to nonzero values for $N \geq 10$, although the situation at $N = 10$ is rather subtle because of larger statistical errors comparable with the correlation function itself. In order to confirm the appearance of the nematic VBS order at $N = 10$, we plot the Binder ratio of the nematic order parameter in Fig. 3. The Binder ratio for the nematic order parameter is given by

$$g_{\text{Nem}} = \frac{1}{2} \left( 3 - \frac{\langle \Phi^4 \rangle}{\langle \Phi^2 \rangle^2} \right),$$

where $\Phi$ is the sum of local nematic order parameters: $\Phi \equiv L^{-2} \sum_j \Phi_j$. $g_{\text{Nem}}$ is normalized so that $g_{\text{Nem}} = 0$ for the Néel phase, while $g_{\text{Nem}} = 1$ for the nematic (or the columnar) VBS phase. The nematic binder ratio at $N = 10$ develops as the system size is increased and, as we see in Fig. 3, the order parameter $\sqrt{\langle \Phi^2 \rangle}$ slightly deviates upward from the power-law decay, $\sqrt{\langle \Phi^2 \rangle}/L \propto 1/L$, which should be obeyed asymptotically when the system is gapped. It indicates the nematic VBS order at $N = 10$ in the thermodynamic limit. We also checked that the order parameter $\Psi$ shows no evidence of long range order for the case of $n = 2$. From these observations, we conclude that for the case of $n = 2$ the ground state is the Néel state for $N \leq 9$, while it is the nematic VBS state for $N \geq 10$. There is no intermediate phase.

Next we move to the case of $n = 3$. We plot two-point correlation functions for $n = 3$ at $| \mathbf{R} | = L/4$ in Fig. 4. The Néel order, we clearly see from the curvature of the curves that the Néel state is the ground state for $N \leq 14$, and it is not for $N \geq 15$. On the other hand, we do not see clear difference among different values of $N$ in the two-point correlation function of the columnar VBS order (see Fig. 4(b)). The behavior of the columnar VBS order parameters indicates that the VBS order is too small to be visible even if it exists for $L \leq 128$ finite systems with the present statistical errors. Indeed, based on the $1/N$ expansion Read and Sachdev proposed that the amplitude of the VBS order parameter becomes exponentially small by increasing $N$ as $|\langle \Psi_j \rangle| \sim \exp(-NE_c)$ with the action of a hedgehog instanton. The constant $E_c$ has been calculated as $E_c = c \ln \xi$ with $c = 0.1245\ldots$ in the limit $N \to \infty$ with the spin correlation length $\xi$ large but fixed.

By using the result of the large $N$ theory, we try to estimate expected amplitude of the VBS order. For the columnar VBS order parameter, more precise expression for our definition of $\Psi_j$ is given by

$$|\langle \Psi_j \rangle| = \frac{N a}{\sqrt{2}} \exp(-NE_c),$$

where $a$ is an unknown constant depending on $n/N$. For the nematic VBS order parameter we also obtain

$$|\langle \Phi_j \rangle| = \frac{N a}{2} \exp(-NE_c).$$

We focus on the expected phase boundary of the columnar VBS phase $N = 15$ with $n = 3$. The spin correlation length at this parameter is calculated as $\xi \approx 5.2$ from a fitting of the correlation function of the Néel order. In the same ratio of $n/N = 0.2$, the spin correlation length at $N = 10$ with $n = 2$ is estimated as $\xi \approx 4.7$. By substituting the values of $\xi$ and $N$ into two equations (16) and (17) with $E_c \approx 0.12459 \ln \xi$, we obtain a relation

$$|\langle \Psi_j \rangle|_{N=15,n=3} \approx 0.67 |\langle \Phi_j \rangle|_{N=10,n=2}. \quad (8)$$

In Fig. 5, we plot the system size dependence of the columnar VBS order parameter $\sqrt{\langle |\Psi|^2 \rangle}$, where $\Psi \equiv L^{-2} \sum_j \Psi_j$, along with that of the nematic VBS order parameter $\sqrt{\langle |\Phi|^2 \rangle}$. These order parameters are expected to converge into $|\langle \Psi_j \rangle|$ and $|\langle \Phi_j \rangle|$, respectively, in the

![FIG. 4. (color online) Log-log plot of the two-point correlation functions at $|\mathbf{R}| = L/4$ for the model with $n = 3$. (a) The correlation function of the Néel order. (b) The correlation function of the columnar VBS order.](image-url)
thermodynamic limit. For the purpose of better comparison, we divide $\sqrt{\langle |\Psi|^2 \rangle}$ by the factor 0.67 which appeared in Eq. 8. In the case of $\sqrt{\langle |\Psi|^2 \rangle}$ it decrease as $L^{-1}$ expected for the case of no long range order, while the $L$ dependence of $\sqrt{\langle \Phi^2 \rangle}$ changes from $L^{-1}$ around $L \simeq 100$ indicating development of a weak long range nematic VBS order. From comparison between $\sqrt{\langle |\Psi|^2 \rangle}$ and $\sqrt{\langle \Phi^2 \rangle}$, we expect that a signature of the columnar VBS order for $n = 3$, $N = 15$ becomes visible for the systems size larger than $L \simeq 400$. Therefore the fact that we did not observe any evidence of the long range VBS order in the present calculation upto $L = 128$ does not necessarily indicate the presence of intermediate phase where both of the Néel and the VBS order disappears. Because the QMC calculation for $L \simeq 400$ needs larger computational cost than the available resources we cannot reach a clear answer for the phase boundary in the case of $n = 3$.

In summary, we have investigated the ground state property of an SU($N$) symmetric antiferromagnetic Heisenberg model on the two-dimensional square lattice for the representations with the $n = 2$ and $n = 3$ columns Young diagrams. For $n = 2$, we conclude that the Néel state is the ground state for $N \leq 9$ while the nematic VBS state becomes the ground state for $N \geq 10$. Thus, there is no intermediate state between them (see Fig. 1(a)). For $n = 3$, the ground state for $N \leq 14$ is the Néel state and it disappears for $N \geq 15$. Although we observed no evidence of the expected columnar VBS order for $N \geq 15$, this observation does not exclude the columnar VBS order in this case, because we estimated that the signature of the VBS order was invisible for smaller sizes $L \lesssim 400$ even if it eventually converges to a finite value. Determining the VBS phase boundary for $n \geq 3$ requires further studies. Our analysis indicates that we need careful extrapolations of the finite-size data into the thermodynamic limit. Naive extrapolations may lead to an incorrect characterization of the intermediate region even if a weak VBS order is eventually stabilized.

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