Vanishing Néel Ordering of SU(n) Heisenberg Model in Three Dimensions

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The SU(n) Heisenberg model represented by exchange operators is studied by means of high-temperature series expansion in three dimensions, where n is an arbitrary positive integer. The spin-spin correlation function and its Fourier transform $S(q)$ is derived up to $O[(\beta J)^{10}]$ with $\beta J$ being the nearest-neighbor antiferromagnetic exchange in units of temperature. The temperature dependence of $S(q)$ and next-nearest-neighbor spin-spin correlation in the large n cases show that dominant correlation deviates from $q = (\pi, \pi, \pi)$ at low temperature, which is qualitatively similar to that of this model in one dimension. The Néel temperature of SU(2) case is precisely estimated by analyzing the divergence of $\langle S(\pi, \pi, \pi) \rangle$. Then, we generalize n of SU(n) to a continuous variable and gradually increases from $n = 2$. We conclude that the Néel ordering disappears for $n > 2$.

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I. INTRODUCTION

It is known that properties of quantum spin systems tend to approach those of their corresponding classical spin systems as the spin magnitude increases. However, this is not necessarily the case for a sequence of models in which the number of multipolar-interaction terms increases as the spin magnitude increases. Consequently the higher-spin systems may have stronger quantum effects in this case. In other words, such additional terms can break a classical correspondence down even in high dimensions. These “large-spin-magnitude” systems mentioned above include systems in which one unit has more than two degrees of freedom, such as orbitally degenerate systems. In such systems, many coupling constants appear in general. However, experimental information about multipolar couplings is limited. As a starting point to explore such systems, understanding of one of the extreme limits must be useful. Therefore in this paper, we investigate an SU(n) symmetric case10,11,12,13,14,15,16,17,18,19,20,21 in three dimensions, where n is the total number of internal degrees of freedom, by means of high-temperature series expansion (HTSE).

We consider a simple cubic lattice. Let each site take one of the n colors denoted by $|\alpha\rangle$ with $\alpha = 1, 2, \cdots, n$. Using the Hubbard operator $X^{\alpha\beta} := |\alpha\rangle \langle \beta|$, the exchange operator is expressed as

$$P_{ij} := \sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} X^{\alpha\beta}_{i} X^{\beta\alpha}_{j}. \quad (1)$$

Colors of sites i and j are exchanged when $P_{ij}$ is applied. Then, an SU(n) symmetric Hamiltonian reads

$$\mathcal{H} := J \sum_{\langle ij \rangle} P_{ij}, \quad (2)$$

where the summation is taken over all the nearest neighbor pairs. We consider the antiferromagnetic case, $J > 0$. Let us show the relations with spin operators explicitly for some of the special cases below.

(i) When $n = 2$, this model is reduced to the ordinary Heisenberg model with $s = 1/2$ by relation $2P_{ij} - 1 = 4s_{i} \cdot s_{j}$.

(ii) The SU(3) case corresponds to $s = 1$, competing quadratic and biquadratic exchange interaction, $\delta J$.

$$1 + P_{ij} = s_{i} \cdot s_{j} + (s_{i} \cdot s_{j})^{2}. \quad (3)$$

(iii) The SU(4) Heisenberg model is related to spin 3/2 systems but more often discussed in the context of orbital- and spin-degenerate systems.10,11,12,13,14,15,16,17,18,19,20,21 The four local states can be represented by $|\{\pm\}^{t}\{\pm\}|$, $|\{\pm\}^{t}\{\mp\}|$, $|\{\mp\}^{t}\{\pm\}|$, $|\{\mp\}^{t}\{\mp\}|$, where $|\{\pm\}|$ and $|\{\mp\}|$ represent an orbital state and a spin state, respectively. The pseudo-spin operators are defined by $t^{z}|\{\pm\}| = \pm\frac{1}{2}|\{\pm\}|$, $t^{x}|\{\pm\}| = |\{\pm\}|$, $s^{z}|\{\pm\}| = \pm\frac{1}{2}|\{\pm\}|$, $s^{x}|\{\pm\}| = |\{\pm\}|$, and the exchange operator for $n = 4$ is rewritten as

$$P_{ij} = t_{i} \cdot t_{j} + s_{i} \cdot s_{j} + 4(t_{i} \cdot t_{j})(s_{i} \cdot s_{j}) + \frac{1}{4}. \quad (4)$$

The Pauli matrices $\tau = 2t$ and $\sigma = 2s$ may simplify this expression, i.e.,

$$4P_{ij} = \tau_{i} \cdot \tau_{j} + \sigma_{i} \cdot \sigma_{j} + (\tau_{i} \cdot \tau_{j})(\sigma_{i} \cdot \sigma_{j}) + 1. \quad (5)$$

Note that there is a different representation of SU(n) Heisenberg model studied in detail using Quantum Monte Carlo method (QMC). However, the QMC for the Hamiltonian (2) suffers from minus sign problems in more than one dimension.

If the number of competing order parameters is large and frustration exists, the transition temperature can greatly be reduced from the mean-field value even in three dimensions. That will be the case with the Hamiltonian (2). First, it is isotropic with respect to $n^{2} - 1$ independent interacting components. Furthermore, it contains frustration as most clearly seen in Eq. (5) of the SU(4) case. Each of the 15 components, $\tau^{a}$, $\sigma^{a}$, $\tau^{a} \sigma^{a}$,
sites

\[ \langle f_{\text{fifteen components in Eq. (5) contribute equally, and thus}} \]

correlation functions is similar to that in one dimension,

temperature. Namely, in Sec. II we show that the behavior of

some unique features of spatial correlation at finite tem-

perature another correlation occurs with \( n \)-site periodicity.12

Such peculiar correlation in one dimension could sug-

gest an exotic ordering in higher dimensions. However,

not much is known about the antiferromagnetic SU(\( n \))

Heisenberg model in three dimensions. In fact, its fer-

romagnetic variant is studied in Ref. 22 by the HTSE

for the uniform susceptibility that needs less effort to

be calculated than susceptibility of other wave-numbers.

To our knowledge, our calculation in this paper is the

first HTSE aiming at antiferromagnetic exchange of this

model. In this study, we investigate the model system-

atically by changing parameter \( n \) of SU(\( n \)), and report

some unique features of spatial correlation at finite tem-

perature. Namely, in Sec. II we show that the behavior of

correlation functions is similar to that in one dimension,

and in Sec. III that the Néel temperature disappears as

\( n \) increases from \( n = 2 \).

II. TEMPERATURE DEPENDENCE OF CORRELATION FUNCTIONS

What should be calculated here is \( \langle P_{ij} \rangle \), which is re-

lated to a correlation function. For example, when \( n = 4 \),

fifteen components in Eq. 5 contribute equally, and thus

\[ \langle \sigma_i^\alpha \sigma_j^\beta \rangle = \langle \gamma_i^\alpha \gamma_j^\beta \rangle \]

\[ = \langle \gamma_i^\alpha \gamma_j^\beta \rangle = 4 \langle P_{ij} - 1 \rangle / 15 \]

For general \( n \), we can define correlation function between

sites \( i \) and \( j \) as

\[ S_{i-j} := \langle X_i^{\alpha \beta} X_j^{\beta \alpha} \rangle = \frac{1}{n^2 - 1} \left( \langle P_{ij} \rangle - \frac{1}{n} \right) \]

for \( i \neq j, \alpha \neq \beta \), which does not depend on \( \alpha \) nor \( \beta \)
because of the SU(\( n \)) symmetry. Its Fourier transform is

denoted by \( S(\mathbf{q}) \).

The high-temperature expansion is performed by ex-

panding the Boltzmann factor \( e^{-\beta \mathcal{H}} \) in \( \beta \). In practice,

the series coefficients in the thermodynamic limit are ex-

actly obtained by a linked-cluster expansion.23 To obtain

the series expansion of \( \langle P_{ij} \rangle \) up to \( O((\beta J)^{10}) \), we need to

calculate \( \text{Tr}[\mathcal{H}_L^m] \) and \( \text{Tr}[P_{ij} \mathcal{H}_L^m] \) for \( 0 \leq m \leq M \),

where \( \mathcal{H}_L \) is the Hamiltonian in a linked cluster. In calcu-
lating the traces, we use a property of the permutation

operator, and calculation of the traces is reduced to a

combinatorial problem to count the number of circular

permutations in a product of permutations.13,22,26 Here,

an important point of our analysis is that the series co-

efficients are obtained as polynomials of \( n \), for example,

\[ S(\pi, \pi, \pi) = \frac{1}{n} + \frac{6}{n^2} (\beta J) + \frac{36}{n^3} (\beta J)^2 + \frac{(216 - 22 n^2)}{n^4} (\beta J)^3 + \ldots \] (7)

Namely, the order of the series for every \( n \) is the same.

We have obtained the series for \( S_{i-j} \) up to \( O((\beta J)^9) \) for

arbitrary \( i - j \), and consequently \( S(\mathbf{q}) \) up to \( O((\beta J)^9) \) for

arbitrary \( \mathbf{q} \). As a special interest, \( S(\pi, \pi, \pi) \) is obtained up to \( O((\beta J)^{10}) \). The series are extrapolated using the

Padé approximation (PA).

First of all, in order to see the temperature-dependent

nature of the spatial correlation, we analyze the next-

nearest-neighbor correlation function \( S_{110} \) as we have done in one dimension in Ref. 12. Figure II shows the results. Both the axes are scaled so that the high-
temperature limit of every \( n \) matches. Here, we have

simultaneously plotted extrapolation from several differ-

ent choices of the PA, and the difference between them

approximately represents an error of the extrapolation.

The lowest order of the series of \( S_{110} \) has a Néel-order-
type correlation in any \( n \). That is, the series of \( S_{110} \)

starts with \( O((\beta J)|\mathbf{x}|)^{2|\mathbf{x}|+|\mathbf{x}_1|+|\mathbf{x}_2|} \) with sign \((-1)^{|\mathbf{x}|+|\mathbf{x}_1|+|\mathbf{x}_2|} \).

Therefore, \( S_{110} > 0 \) at high temperature. However, as

antiferromagnetic correlation of each interacting compo-

nent becomes larger, each short-range order disturbs an-

other because of the frustration. The change of the sign

of \( S_{110} \) suggests that the correlation acquire a longer pe-
rion at low temperature. For \( n \geq 6 \), it is clear that \( S_{110} \) changes the sign at a low temperature that increases with \( n \) in this scale. For smaller \( n \), the relevant temperature range is below the converged region, and it is difficult to conclude from this data.

Such a change of correlation at low temperature also appears in the Fourier transform of the correlation function. A naive extrapolation of the series for \( S(q) \) shows bad convergence for several \( q \). This is probably because information at position \( x \) is lacking when \( \cos(x \cdot q) \approx 0 \). In order to avoid it, we extrapolate the series of a complex function \( \sum_{x \geq 0} (X_{i}^{\beta} X_{j+\pi}^{\alpha}) e^{-ix \cdot q} w(x) \), and after that take the real part of the extrapolated function. Here, the summation is taken for \( x, y, z \) in a diagonal direction in the \( q \)-space, \( S(q, q, q) \) shows. However, with further decrease of temperature, \( S(\pi, \pi, \pi) \) starts decreasing and \( S(q) \) with other \( q \) increases. It is not very clear from Fig. 2 if the maximum of \( S(q) \) starts moving from \( (\pi, \pi, \pi) \). Hence, let us show another quantity. Note that if the second derivative of \( S(q) \) at \( q = (\pi, \pi, \pi) \) changes sign, the position of the maximum clearly moves. Its temperature dependence for the SU(16) model is plotted in Fig. 3. It shows a change of the sign around \( T \sim J \). In fact, this temperature of changing sign seems to hardly depend on \( n \) of SU(\( n \)). The result above suggests that the Néel order disappear at least in the SU(\( n \)) model with large \( n \). Namely, order with wave number \( q \neq (\pi, \pi, \pi) \), or disorder, should appear. Then, the next question is, at which \( n \) the Néel order disappears.

**III. NÉEL TEMPERATURE**

It is known that the SU(2) Heisenberg model has the Néel order at low temperature. Therefore in this section, we gradually increases \( n \) of SU(\( n \)) from \( n = 2 \). As a preparation for that, we find a reliable way to estimate a transition temperature first, using the SU(2) model. The Néel temperature \( T_N \) can be characterized by divergence of \( S(\pi, \pi, \pi) \), namely, by a singularity of \( S(\pi, \pi, \pi) \) as a function of \( \beta J \). In order to analyze such a singularity, we use so-called D-log-Padé approximation (DLPA), i.e., the PA for the logarithmic derivative. In using the DLPA, transformation of the expansion variable may improve the convergence of extrapolation. We choose a transformation

\[
\beta J = \frac{x}{1 - a^{2}x^{2}},
\]

where \( a \) is an adjustable parameter that improves convergence. In fact, the singularity closest to the origin in the original series is near the imaginary axis, while \( T_N \) corresponds to a singularity on the real axis. With this transformation, singularities on the real axis approach to the origin and those near the imaginary axis go away. Since the DLPA can estimate a position of the nearest singularity most accurately, errors of the DLPA can become smaller by this transformation.

In order to find an optimal \( a \), we calculate \( T_N \) as a function of \( a \) for a couple of choices of the DLPA, and we adopt \( a \) at which difference among different DLPAs is the smallest. Figure 4 shows \( T_N \) as a function of \( a \) for three different choices of the DLPA. Here, \([m/n] \) denotes the DLPA with a polynomial of order \( m \) over a polynomial.
of order $n$. Since $[4/4]$ is from the series one-order lower than the others, we choose $a$ at which $[5/4]$ and $[4/5]$ are the closest, namely, $a = 1.04$. Then, $T_N/J$ obtained here is 1.898, which is close to those in the literature, 1.892 by the QMC\textsuperscript{29} and 1.888 by the HTSE\textsuperscript{30}. In addition, we have obtained a critical exponent simultaneously. We assume that the critical exponent does not depend on the spin magnitude, and compare it with that of the classical antiferromagnetic Heisenberg model, in which $S(\pi, \pi, \pi)$ is identical to the staggered susceptibility equivalent to the ‘uniform susceptibility of the ferromagnetic model’. Hence we can compare the critical exponent $\gamma$. The estimation from our calculation above is $\gamma = 1.399$, which is close to 1.396 by a Monte Carlo method\textsuperscript{31}, 1.406 by HTSE\textsuperscript{32}, and 1.388 by a field theory\textsuperscript{33}, of the classical O(3) model. Therefore, we trust this way of analyzing $T_N$, and use it also for the SU($n$) model with $n > 2$. Also for $n > 2$, the variable transformation $S(q)$ should work because the singularity closest to the origin in the original series is near the imaginary axis.

Originally $n$ is an integer because it is the number of internal degrees of freedom. However, after obtaining the series as an analytic function of $n$, we can regard $n$ as a continuous variable that has a physical meaning only when it happens to take integer values. In fact, as $n$ changes continuously, the properties of the series change also continuously. Therefore, we gradually increases $n$ from $n = 2$ and see $n$-dependence of $T_N$. Figure 4 shows the results. Here, we fix $a = 1.04$, and we plot $[5/4]$ and $[4/5]$ together. The optimal $a$ may depend on $n$. However, since the difference between the two curves is very small, we regard it as an optimal $a$. As $n$ increases, $T_N$ decreases almost linearly, and at $n \sim 2.45$ the singularity corresponding to $T_N$ runs away from the real axis to a complex value with a finite imaginary part. For larger $n$, we do not find any singularity on the antiferromagnetic side of the real axis. Therefore, we conclude that the value of $n$ at which Néel order disappears lies in the range $2 < n < 3$.

In addition, we have also analyzed $S(q)$ with $q \neq (\pi, \pi, \pi)$. However, we have not found any symptom of ordering with $q \neq (\pi, \pi, \pi)$ in the temperature region that we can reach by the present order of the series.

IV. SUMMARY

In summary, we have performed high-temperature series expansions for the SU($n$) Heisenberg model in three dimensions with arbitrary $n$. First of all, we have calculated a next-nearest-neighbor correlation function. At least at large $n$, it changes the sign at low temperature, which suggests that the correlation should not be like Néel order, but have a longer period. Analysis of the Fourier transform of the correlation function also supports that the ground state of the large-$n$ SU($n$) Heisenberg model does not have the Néel-order correlation. Then, we have turned to an approach from $n = 2$. Since the SU(2) Heisenberg model has the Néel order, it should disappear at a certain $n$. We have first found a reliable way to estimate a transition temperature by analyzing the divergence of the $(\pi, \pi, \pi)$ component of the correlation function. Next, we generalize $n$ to a continuous variable and increase $n$ gradually from $n = 2$. We have concluded that the Néel ordering disappears for $n > 2$.

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