Analytical study of the thermodynamic behavior of an antiferromagnetic Heisenberg model

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By introducing a trial action S_0, the thermodynamic properties of the two-dimensional (2D) and 3D quantum and classical antiferromagnetic Heisenberg model are studied and compared analytically with the variational cumulant expansion method. The free energy of the two models are expanded up to the fourth order and the critical temperature T_N is given for each order and for different lattice structures. On the simple cubic lattice and square lattice, the sublattice magnetization M_s and the staggered susceptibility χ_s are calculated.

I. INTRODUCTION

In 1986, Bednorz and Müller[1] discovered the first high-temperature superconductor $La_{2-x}Ba_xCuO_4$ $(x\approx 0.15)$, which has a quasi-two-dimensional Cu-O plane structure. The neutron scattering experiments[2] have indeed revealed a rich magnetic structure. It has been shown that the electron spins of Cu inside a Cu-O plane have a strong antiferromagnetic interaction and the spins in the different planes have a very weak antiferromagnetic coupling. The simplest theoretical model which describes this system is the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model (AFHM). This model has been investigated by many methods [e.g., spin wave theory[3] (SW), renormalization-group approach,[4] high-temperature expansion[5] (HTE), Green function method[6] (Green), and Monte Carlo study[7] (MC)], not only because of its relevance to high-T_c superconductivity, but also because of its theoretical importance in statistical physics. As a quantum model, the commutation relation between spin operators makes the problem difficult to study and the results obtained from these methods are all different.

In order to study the phase transition temperature T_N of the model and its magnetic properties, we adopt the variational cumulant expansion (VCE) method to study the spin-$\frac{1}{2}$ AFHM and compare it with the correspondent classical one.

The VCE method which was first developed in lattice gauge field theory is an improvement of the cumulant expansion method by incorporating variational method into it. Recently, this method has been applied to the quantum ferromagnetic Heisenberg model in which the free energy is expanded to the third order[8] and the results are rather good. In this paper, we introduce a trial action S_0 for the AFHM and expand the free energy to the fourth order and obtain the Néel temperature T_N on the simple cubic (sc), body centered cubic (bcc), and square (sq) lattice. The sublattice magnetization for sc lattice and the staggered susceptibility for the sc and sq lattice are calculated to the fourth order and compared with the classical AFHM.

II. ANTIFERROMAGNETIC HEISENBERG MODEL AND VCE METHOD

The action of the Heisenberg model is

$$S=-\beta\mathscr{H}=\beta J\left(\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\right), \tag{1}$$

where J is the effective exchange coupling constant and Boltzmann's constant k_B has been set to be 1, so we have $\beta=1/T$. When $J>0$, the action describes the ferromagnetic model, when $J<0$, it corresponds to the antiferromagnetic model. In this paper, we take J to be -1. The suffix i runs over all the sites and $\langle ij\rangle$ over all the pairs of site i and j which are the nearest neighbors. The spin operator $\mathbf{S}_i$ satisfies the commutation relation

$$[s_{i\alpha},s_{j\beta}]=i\varepsilon_{\alpha\beta\gamma}\delta_{ij}s_{i\gamma}. \tag{2}$$

For classical model, s equals infinity and the model can be expressed as

$$S_c=-\beta\sum_{\langle ij\rangle}\sigma_i\cdot\sigma_j, \tag{3}$$

where $\sigma_i=\mathbf{S}_i/s$ is a three component unit vector.

In order to calculate the sublattice magnetization, we first divide the whole lattice into two sublattice A and B and introduce a staggered external field H in the direction of z axis. Therefore, the action of the system is

$$S'=-\beta\left(\sum_{\langle i,j\rangle}\mathbf{S}_{iA}\cdot\mathbf{S}_{jB}\right)+H\sum_i(-1)^{\mathbf{r}_i}s_{iAz}+H\sum_j(-1)^{\mathbf{r}_j}s_{jBz}. \tag{4}$$

The partition function of the system can be written as

$$Z=e^{-W}=\mathrm{Tr}[e^{S'}], \tag{5}$$

where W is the free energy of the system. Because of the difficulty of calculating the partition function directly, we introduce an analytically integrable trial action S_0 which is simpler than S' and still has some basic characters of S':

$$S_0=(j+H)\left[\sum_i(-1)^{\mathbf{r}_i}s_{iAz}+\sum_j(-1)^{\mathbf{r}_j}s_{jBz}\right], \tag{6}$$

where j is the variational parameter which will be determined in the following calculation. Therefore, the partition function of the system can be expressed as

$$Z=e^{-W}=\mathrm{Tr}[e^{S'}]=\mathrm{Tr}[e^{S'}\cdot e^{-S_0}\cdot e^{S_0}]. \tag{7}$$

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TABLE I. The Néel temperature of quantum model for different lattices and from different methods.

	1st	2nd	3rd	4th	HTE	SW	Green	MC
sc	1.5	1.5	0.888889	0.863281	0.898 (Ref. 5)	1.105 (Ref. 3)	0.9065 (Ref. 6)	0.8857 (Ref. 7)
bcc	2.0	2.0	1.375	1.46402	1.432 (Ref. 5)	1.455 (Ref. 3)	1.435 (Ref. 6)	
sq	1.0	1.0	0.41667	0.0625		0.91 (Ref. 3)		

When doing cumulant expansion, one should note that $[S',S_0]\neq 0$, so $Z\neq \mathrm{Tr}[e^{S'-S_0}\cdot e^{S_0}]$. Through the cumulant expansion, the free energy can be derived:

$$W=W_0-\sum_{n=1}^{\infty}\frac{1}{n!}\left\langle S'^n+nS'^{(n-1)}(-S_0)+\frac{n(n-1)}{2!}\times S'^{(n-2)}(-S_0)^2+\cdots+\frac{n(n-1)\cdots[n-(k-1)]}{k!}\times S'^{(n-k)}(-S_0)^k+\cdots+(-S_0)^n\right\rangle_c . \quad (8)$$

In general, the free energy can only be expanded to a limited order:

$$W\approx W_0-\sum_{n=1}^{m}\frac{1}{n!}\left\langle S'^n+nS'^{(n-1)}(-S_0)+\frac{n(n-1)}{2!}\times S'^{(n-2)}(-S_0)^2+\cdots+\frac{n(n-1)\cdots[n-(k-1)]}{k!}\times S'^{(n-k)}(-S_0)^k+\cdots+(-S_0)^n\right\rangle_c , \quad (9)$$

where $Z_0=e^{-W_0}=\mathrm{Tr}[e^{S_0}]=z_{00}^N$, N is the total number of the lattice sites, and z_{00} is

$$z_{00}=\sinh\left[\left(s+\frac{1}{2}(j+H)\right)\right]\Big/\sinh\left[\frac{1}{2}(j+H)\right], \quad (10)$$

where s is the spin quantum number. For the classical model,

$$z_{00c}=2\ \sinh[(j+H)]/(j+H). \quad (11)$$

For the quantum model, the first order and second order free energy of each site is

$$w_1=-\ln z_{00}-\beta\frac{L_1^2}{z_{00}^2}+jL_1z_{00}, \quad (12)$$

$$w_2=w_1-\frac{1}{2}\beta^2\frac{d}{z00^2}\left[\frac{1}{2}(s(s+1)z_{00}-L_2)^2+L_2^2+\frac{1}{2}L_1^2\right]+\frac{d}{2}\beta^2\frac{L_1^4}{z_{00}^4}-d(2d-1)\beta^2\left[\frac{1}{z_{00}^3}L_1^2L_2-\frac{L_1^4}{z_{00}^4}\right]+2d\beta j\left[\frac{1}{z_{00}^2}L_1L_2-\frac{L_1^3}{z00^3}\right]-\frac{j^2}{2}\left(\frac{L_2}{z_{00}}-\frac{L_1^2}{z_{00}^2}\right), \quad (13)$$

where $L_1=\partial z_{00}/\partial j$, $L_2=\partial L_1/\partial j$, and d is the dimension. The third order and fourth order free energy can be derived in the same way and we do not give it here because it is too lengthy.

III. CALCULATION AND RESULTS

In the calculation of VCE method, we first determine the variational parameter j as a function of T. According to the minimal condition of the mth order free energy W_m, we obtain the variational condition:

$$\frac{\delta}{\delta j}W_m=0, \quad (14)$$

$$\frac{\delta^2}{\delta j^2}W_m>0, \quad (15)$$

which is called the complete variational condition.[9]

By solving Eq. (14), the variational parameter j is calculated as a function of T. When $T\leq T_N^{(m)}$, j takes a nonzero value; when $T\geq T_N^{(m)}$, j can only be zero. Under this condition, the Néel temperature of every order is determined. The results from the first order to the fourth order for sc, bcc, and sq lattice are given in Table I. For comparison, the results from other methods are also listed. From the second order, every expansion order of $T_N^{(m)}$ has a correction order by order. Compared with the SW result, the $T_N^{(4)}$ is in better agreement with the result of Green function method and the MC result which are generally believed to be comparatively accurate in determining the critical temperature. Especially for the 2D (two-dimensional) square lattice, the $T_N^{(4)}$ is 0.0625, which is very near to the expected value 0.0. In the SW method,[2] the author obtained a phase transition point at $T=0.91$ and simply supposed that the Néel temperature is 0.0.

The sublattice magnetization M_s for the sc lattice and staggered susceptibility χ_s for the sc and sq lattice are also calculated under this condition according to the relation

$$M_s=-T\left(\frac{\partial F}{\partial H}\right)_{T,H=0}, \quad (16)$$

$$\chi_s=\left(\frac{\partial M_s}{\partial H}\right)_{T,H=0}. \quad (17)$$

The χ_s obtained from our calculations are given in Figs. 1 and 2. For comparison, the high-temperature expansion results and MC simulation results are also given. This physical quantity has a diverge character when $T\rightarrow T_N$, but our results are steeper than the HTE and MC results in a very close vicinity of T_N. In the calculation of M_s, the complete varia-

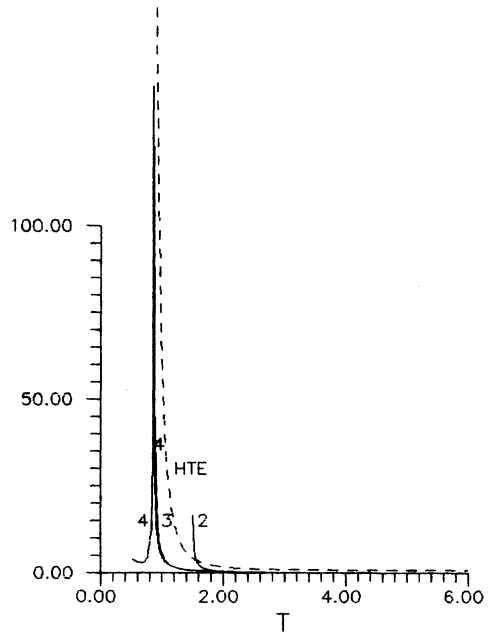

FIG. 1. Staggered susceptibility for $s=1/2$ model on sc lattice. Curves 2, 3, 4 correspond to the 2nd, 3rd, and 4th order approximation in the VCE; the short dashed line is the high-temperature expansion result (Ref. 5).

tional condition makes it diverge when T is very small. In order to solve this problem, we adopt the main value condition to determine the variational parameter.[9] For $T \leq T_N^{(1)}$, considering the jensen inequality

$$Z \geq Z_0 e^{\langle S-S_0\rangle_0}, \tag{18}$$

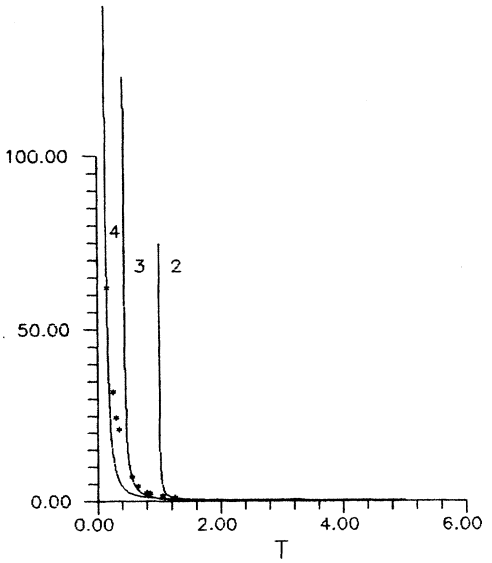

FIG. 2. Staggered susceptibility for $s=1/2$ model on sq lattice. Curves 2, 3, 4 correspond to the 2nd, 3rd, and 4th order approximation in the VCE; the black dots are the MC results (Ref. 7).

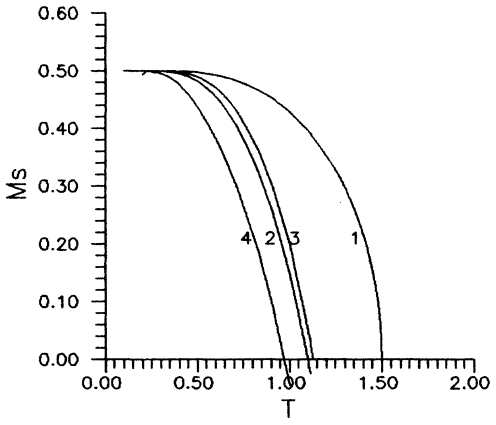

FIG. 3. Spontaneous magnetization for $s=1/2$ model on sc lattice. Curves 1, 2, 3, 4 correspond to the 1st, 2nd, 3rd, and 4th order approximation in the VCE.

we get

$$W \leq W_{\text{eff}} = W_0 - \langle S - S_0\rangle_0 . \tag{19}$$

So we have

$$\frac{\delta}{\delta j} W_{\text{eff}} = 0, \tag{20}$$

$$\frac{\delta^2}{\delta j^2} W_{\text{eff}} > 0. \tag{21}$$

The M_s for the sc lattice from the first to the fourth order are all shown in Fig. 3. Every expansion order of M_s has an intersect point with the horizontal axis, which can also be regarded as the phase transition point according to the definition of order parameter. These points are $T_c^{(1)}=1.5$, $T_c^{(2)}=1.0992$, $T_c^{(3)}=1.125$, and $T_c^{(4)}=0.97$, respectively. Although these values are different from the $T_N^{(m)}$ given in Table I, the fourth order of T_N and T_c are very similar.

The phase transition temperature $T_N^{(m)}$ for the classical antiferromagnetic Heisenberg model are also given with complete variational condition. The results are shown in Table II. From these results, we can see that the quantum effect make the transition temperature much lower than the classical one.

The staggered susceptibility of the classical AFHM on the sc lattice is calculated with the same condition and is given

TABLE II. The Néel temperature of classical model for different lattices and from different methods.

	1st	2nd	3rd	4th	HTE	MC
sc	2.0	1.6667	1.6268	1.5314	1.445 (Ref. 10)	1.443 (Ref. 7)
bcc	2.6667	2.3333	2.3048	2.2218	2.055 (Ref. 10)	2.055 (Ref. 7)
sq	1.333	1.0	0.9333	0.8325		0.0 (Ref. 7)

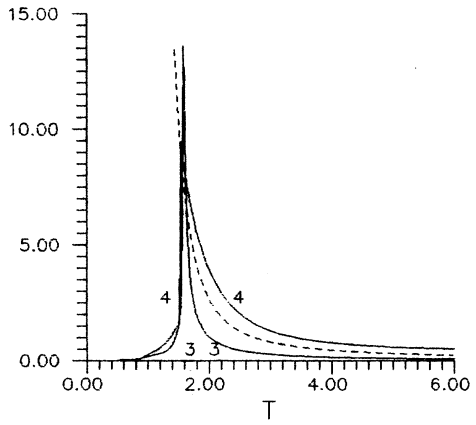

FIG. 4. Staggered susceptibility for classical model on sc lattice. Curves 3, 4 correspond to the 3rd and 4th order approximation in the VCE; the short dashed line is the high-temperature expansion result (Ref. 5).

in Fig. 4. The change of χ_s with the temperature is much softer than the quantum model.

IV. DISCUSSIONS

The Néel temperature and the magnetic characters of the 2D and 3D quantum antiferromagnet over a wide range of temperature are investigated via the VCE method. We propose a trial action S_0 for this model and obtain the Néel temperature which has a correction order by order and the fourth order $T_N^{(4)}$ is in much better agreement with the result of Green function method and the MC result than the SW method.

From the calculation of M_s, we obtained a series of $T_c^{(m)}$ which can also be regarded as the transition point according to the definition. The values of $T_N^{(4)}$ and $T_c^{(4)}$ are very similar, but we think that this is not the intrinsic character of our theory, but only a coincidence. In the classical models, we have not found this phenomena. In other aspects, the values of even-number order $T_c^{(m)}$ are more approaching the MC result than the odd-number order $T_c^{(m)}$.

In the calculation of χ_s, our results are steeper than the HTE and MC result. Whereas, the exact critical behavior of χ_s needs further investigation for the divergence of χ_s near T_N.

At last, it should be emphasized that the trial action S_0 does not commute with the action of this model, that is $[S_0, S'] \neq 0$. This defect causes the divergence of the internal energy and the specific heat. From the principle of effective action, we need to find a trial action S_0 which is more similar to S' and is commutable with S'. With this S_0, the divergence problem would be solved. How to find this kind of S_0 is a very interesting topic to study and we hope to do some research in this direction.

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