# Variational cumulant expansion for the Heisenberg model with the critical temperature determined to third order

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The variational-cumulant-expansion (VCE) method is adopted to calculate the Heisenberg model. The free energy of the model is expanded to the third order, and the analytical formulas for the critical temperature $T_c$ are given for each order. The first order of VCE corresponds to the mean-field theory, the second order gives the same result for $T_c$ as the $1/z$ expansion, and the third order gives a more complicated correction. As a comparison, the results of the two-dimensional (2D) Ising model for VCE to the seventh order are shown. We carry out a trial to predict the critical temperature of the infinite order of the VCE, and get a very accurate result for the 2D Ising model. A prediction of $T_c$ for the Heisenberg model is also made.

## I. INTRODUCTION

Expansion methods are often used in the study of the Heisenberg model. The conventional method is mean-field (MF) theory, which ignores the coupling of spin fluctuations on neighboring sites. The cluster-expansion techniques[1] overcomes the shortcomings of MF theory to some degree and gets better results. Recently, Fishman and co-workers applied the $1/z$ expansion,[2] where $z$ is the number of the nearest neighbors, to Heisenberg models for varied spins, exchange constants, etc., and got fairly good results.

This paper uses the variational-cumulant-expansion (VCE) approach to study the Heisenberg model. VCE is an effective analytical method which originated in the study of lattice gauge theory[3] and has been widely used in statistical physics to study classical statistical models.[4,5] It shows good convergence at high and low temperatures simultaneously. The preliminary results are all fairly good. The VCE method is applied here to quantum spin models. We expand the free energy of the Heisenberg model to third order and give the critical temperature $T_c$ to first, second, and third order with varied spins on square and cubic lattices. The result shows that the first and second orders correspond to the zero and first orders of the $1/z$ expansion, respectively, and the third order gives more a complicated and accurate correction of $T_c$. In comparison, the spin-$\frac{1}{2}$ Ising model on a square lattice is calculated with the VCE method to the seventh order. The two-dimensional (2D) Ising model is simple and soluble; therefore, it can be calculated to high order and compared with the exact result,[6] which may reveal some properties of the VCE method.

Finite-order expansion usually has an obvious deviation from the exact value, especially when the order is low. The effective way to overcome it has never been found in previous work on the VCE method. We think there are two ways to deal with it: First, make an effort to evaluate the order as high as possible; second, try to find an extrapolating method to predict the critical-point behavior at infinite expansion with information obtained from finite series. In most cases high order is difficult to reach; one must seek help from the extrapolating method. We use the weighted fitting method of statistical mathematics and obtained stable and accurate predictions of the critical temperature of the 2D Ising model with deviations of 0.04%. The prediction is also made for the Heisenberg model in varied cases.

## II. MODELS AND THE VCE METHOD

The actions corresponding to the spin-$\frac{1}{2}$ Ising and spin-$s$ Heisenberg models are

$$S_I=-\beta H_I=\beta\sum_{\langle ij\rangle}\sigma_i\sigma_j\ , \tag{1}$$

$$S_H=-\beta H_H=\beta\sum_{\langle ij\rangle}\mathbf{s}_i\cdot\mathbf{s}_j\ , \tag{2}$$

where we let the coupling constant and Boltzmann's constant $k_B$ be 1, and therefore $\beta=1/T$, with $T$ as the temperature of the system and $\sigma_i$ taking a value of $\pm1$. The suffix $i$ runs over all the sites and $\langle ij\rangle$ over all the pairs of sites $i$ and $j$ which are nearest neighbors. In Eq. (2), the spin operators $\mathbf{s}_i$ obey the commutation relations

$$[s_{i\alpha},s_{j\beta}]=i\varepsilon_{\alpha\beta\gamma}\delta_{ij}s_{i\gamma}\ . \tag{3}$$

The trial action $S_0$ is chosen as

$$S_{0I}=J_I\sum_i\sigma_i\ , \tag{4}$$

$$S_{0H}=J_H\sum_i s_{iz}\ , \tag{5}$$

where $J_I$ and $J_H$ are the variational parameters.

The partition function is written as

$$Z=\mathrm{Tr}[e^{S}]=\mathrm{Tr}[e^{S-S_0}e^{S_0}]=Z_0\langle e^{S-S_0}\rangle_0\ , \tag{6}$$

where $Z_0\equiv e^{-F_0}=\mathrm{Tr}[e^{S_0}]$ and $\langle\cdots\rangle_0\equiv Z_0^{-1}\mathrm{Tr}[e^{S_0}(\cdots)]$. From Eq. (6), we get

 

$$F=F_0-\sum_{n=1}^{\infty}\frac{1}{n!}\langle (S-S_0)^n\rangle_c \qquad (7)$$

or

$$F\approx F_m=F_0-\sum_{n=1}^{m}\frac{1}{n!}\langle (S-S_0)^n\rangle_c \;, \qquad (8)$$

where $\langle \cdots \rangle_c$ indicates an average value for the cumulant expansion.[7]

The detailed VCE results of the Ising model can be seen in the previous work;[4] therefore, we only display the detailed results of the Heisenberg model. For the Heisenberg model, one can draw easily $Z_0=Z_{00}^N$, where

$$Z_{00}=\sinh[(s+\tfrac{1}{2})J]/\sinh[\tfrac{1}{2}J] \;, \qquad (9)$$

and $N$ is the number of the lattice sites. The first-order free energy of the VCE of each site is

$$f_1=\frac{1}{N}F_1=-\ln Z_{00}-\beta d L_1^2/Z_{00}^2+JL_1Z_{00} \;, \qquad (10)$$

where $L_1=\partial Z_{00}/\partial J$ and $d$ is the dimension. The second-order free energy is

$$f_2=f_1-\frac{1}{2}\beta^2\frac{d}{Z_{00}^2}\left[\frac{1}{2}[s(s+1)Z_{00}-L_2]^2+L_2^2-\frac{1}{2}L_1^2\right] +\frac{d}{2}\beta^2\frac{L_1^4}{Z_{00}^4}-d(2d-1)\beta^2\left[\frac{1}{Z_{00}^3}L_1^2L_2-\frac{L_1^4}{Z_{00}^4}\right] +2d\beta J\left[\frac{1}{Z_{00}^2}L_1L_2-\frac{L_1^3}{Z_{00}^3}\right]-\frac{J^2}{2}\left[\frac{L_2}{Z_{00}}-\frac{L_1^2}{Z_{00}^2}\right] , \qquad (11)$$

where $L_2=\partial L_1/\partial J$. The third-order free energy is carried out in the same way; because it is very long and complicated, we do not display it, but the determined critical temperature is shown in the following section.

## III. CRITICAL TEMPERATURES OBTAINED FROM THE VCE METHOD

In the involved problem, the $m$th modified free energy $F_m(J,T)$ versus $J$ has the general quality as shown in Fig. 1(a) for low temperature $T$, which has two minimum points mirrored by the $j=0$ line. As $T$ increases, both of the minimum points are close to $J=0$, and after a definite temperature $T_c^{(m)}$, there is only one minimum point at $J=0$ as shown in Fig. 1(b). $T_c^{(m)}$ is the critical temperature determined by the $m$th order of the VCE approach. The above description can be expressed as[5]

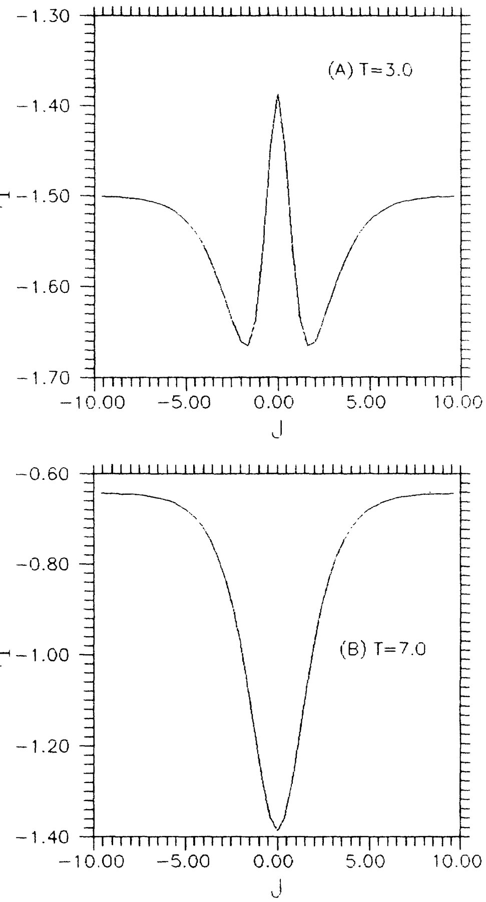


FIG. 1. First-order free energy of the Heisenberg model $f_1$ vs the variational parameter $J$ at temperature $T$: (a) $T=3.0$, (b) $T=7.0$. The critical temperature is $T_c^{(1)}=5.0$.

$$\left.\frac{\delta^2 F_m}{\delta J^2}\right|_{T=T_c^{(m)},J=0}=0 \;; \qquad (12)$$

then, one can derive $T_c^{(m)}$ from Eq. (12).

The critical temperature $T_c^{(m)}$ of the Ising model is displayed from the first to seventh order:

$$\begin{aligned}
&T_c^{(1)}=2d \;,\\
&T_c^{(2)}=2d-1 \;,\\
&T_c^{(3)}=(12d^2-12d+2)/(6d-3) \;,\\
&T_c^{(4)}=(24d^3-36d^2+8d+5)/(12d^2-12d+2) \;,\\
&T_c^{(5)}=(240d^4-480d^3+180d^2+120d-58)/(120d^3-1080d^2+40d+25) \;,\\
&T_c^{(6)}=(720d^5-1800d^4+1020d^3+270d^2+167d-376)/(360d^4-720d^3+270d^2+180d-87) \;,\\
&T_c^{(7)}=(10\,080d^6-30\,240d^5+23\,520d^4-1680d^3+17\,052d^2-29\,232d+10\,502)/\\
&\qquad (5040d^5-12\,600d^4+7140d^3+1890d^2+1169d-2632) \;.
\end{aligned} \qquad (13)$$

TABLE I. Critical temperatures of the 2D Ising model given by the VCE approach with the non-weighting and $1/D(m)$-weighting fit method. For comparison, the exact result is also given.

| Order $(m)$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| VCE | 4.00000 | 3.00000 | 2.88889 | 2.65384 | 2.61449 | 2.54102 | 2.51666 |
| No weight | | | 2.23077 | 2.22222 | 2.24208 | 2.24607 | 2.25329 |
| $1/D(m)$ weight | | | 2.26912 | 2.23768 | 2.26068 | 2.26091 | 2.26834 |
| Exact result | | | | | | | 2.26920 |

The critical temperatures $T_c^{(m)}$ of Heisenberg model from the first to third order are

$$T_c^{(1)}=2ds(s+1)/3 ,$$
$$T_c^{(2)}=T_c^{(1)}-s(s+1)/3-1/4 , \tag{14}$$
$$T_c^{(3)}=T_c^{(2)}-(1-16s-32s^2-32s^3-16s^4)/[20(-3-4s+8ds-4s^2+8ds^2)] ,$$

where $s$ is the spin quantum number and $s(s+1)$ is the eigenvalue of spin operator $s^2$. One can see that $T_c^{(1)}$ and $T_c^{(2)}$ are the same as the results given by the zero and first orders of the $1/z$ expansion,[2] respectively.

## IV. EXTRAPOLATING METHOD AND PREDICTION OF THE CRITICAL TEMPERATURE

The numerical results of the critical temperature of the Ising model in a square lattice, where $d=2$, are shown in Table I. The values approach the exact value order by order, but have fairly large deviations. The numerical results of the Heisenberg model are also shown for square and cubic lattices with different spins; see Table II.

Figure 2 shows the plots of the critical points $T_c^{(m)}$ of the 2D Ising model against $1/m$; we find that the trend of points $(1/m, T_c^{(m)})$ shows good linearity, where $m=1,\ldots,7$. It is reasonable to fit these points with

$$T=a+b/m . \tag{15}$$

We attempt to find a good fitting such that the estimated $a$ is as close to $T_c^{(\infty)}$, the critical temperature of infinite expansion, as possible.

In general, high-order expansion is more accurate than the lower one. Since information given by the higher-order expansion is more important, one should add larger weight to it to fit the straight line [Eq. (15)]. The weighting is a basic approach to dealing with such kinds of problems. Because information of involved deviation is very limited, we were unable to determine the weights theoretically. One thing that can be done is to try to find some weighting method which can estimate the exact value stably and accurately. Several natural and reasonable ways have been tried, and the best one found by far for the 2D Ising model is adding the weight

$$W(m)=1/D(m) \tag{16}$$

to $(T_c^{(m)}-a-b/m)^2$, where $D(m)$ is the distance between the points $(0,a)$ and $(1/m, T_c^{(m)})$, and

$$D(m)=\sqrt{(1/m)^2+(a-T_c^{(m)})^2} . \tag{17}$$

This can be explained geometrically: The accuracy of $a$ is emphasized by adding larger weight to the point which is nearer to the point $(0,a)$, and the weight is inversely proportional to the distance between $(0,a)$ and $(1/m, T_c^{(m)})$.

One can obtain the estimated $a$ and $b$ by minimizing the value of

$$\sum_{n=1}^{m} W(n)(T_c^{(n)}-a-b/n)^2 \tag{18}$$

with fixed $W(n)$. In matrix form, one gets

$$B=(X^TWX)^{-1}X^TWT , \tag{19}$$

where

$$B=\begin{bmatrix} a \\ b \end{bmatrix}, \quad X=\begin{bmatrix} 1 & 1 \\ 1 & \frac{1}{2} \\ \vdots & \vdots \\ 1 & 1/m \end{bmatrix}, \quad T=\begin{bmatrix} T_c^{(1)} \\ T_c^{(2)} \\ \vdots \\ T_c^{(m)} \end{bmatrix},$$

TABLE II. Critical temperatures of the Heisenberg model given by the VCE approach with the $1/D(m)$-weighting fit method for varied dimensions and spins.

| $d$ | $s$ | First order | Second order | Third order | Prediction of $1/D$ weighting |
|---|---|---|---|---|---|
| 2 | $\frac{1}{2}$ | 1.0000 | 0.5000 | 0.3333 | 0 |
| 2 | 1 | 2.6667 | 1.7500 | 1.5238 | 0.9315 |
| 2 | $\frac{3}{2}$ | 5.0000 | 3.5000 | 3.1619 | 2.1992 |
| 3 | $\frac{1}{2}$ | 1.5000 | 1.0000 | 0.9167 | 0.6029 |
| 3 | 1 | 4.0000 | 3.0833 | 2.9550 | 2.3826 |
| 3 | $\frac{3}{2}$ | 7.5000 | 6.0000 | 5.8028 | 4.8660 |

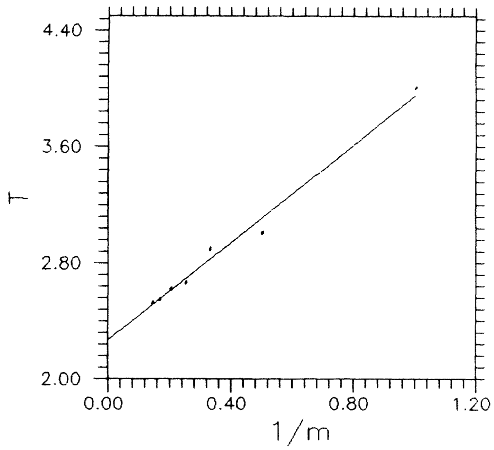


FIG. 2. For the 2D spin-$\frac{1}{2}$ Ising model, the fitting straight line $T-1/m$ of points $(1/m, T_c^{(m)})$, where $T_c^{(m)}$ denotes the critical temperature determined by the $m$th-order VCE.

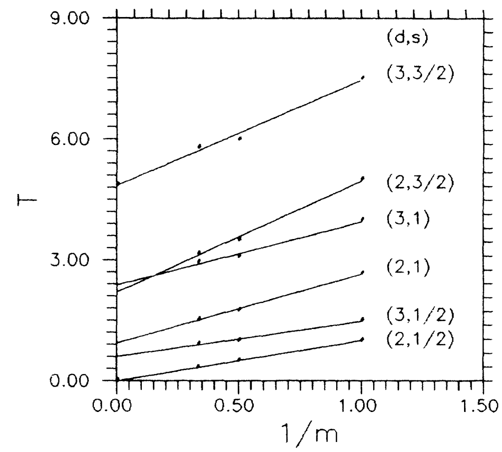


FIG. 3. For the Heisenberg model with varied $(d,s)$, where $d$ is the lattice dimension and $s$ is the spin quantum number, the fitting straight line $T-1/m$ of points $(1/m, T_c^{(m)})$, where $T_c^{(m)}$ denotes the critical temperature determined by the $m$th-order VCE.

and

$$W=\begin{bmatrix} W(1) & 0 & \cdots & 0 \\ 0 & W(2) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & W(m) \end{bmatrix}.$$

One can get $a$ and $b$ by solving Eq. (19), noting that $W$ depends on $a$ and $b$.

With the above method, the results of the 2D Ising model are carried out and displayed in Table I, labeled "$1/D(m)$ weight," where the value for the $m$th order means that a fitting is made among the figures of the first $m$ orders of the VCE. The predictions are fairly stable among different orders, and the prediction of higher order is more accurate, for example, the seventh order estimates $T_c=2.268\,34$ with deviation of 0.038% from the exact result. For comparison, the results of the nonweighted fitting method are also given in Table I. The predictions are also very good, which means linearity is the main property of the points $(1/m, T_c^{(m)})$, but they are not as accurate and stable as the weighting ones. In fact, "$1/D(m)$ weight" means modifying the linear fitting by considering unlinear factors; it is more complicated and detailed. Therefore one gets more accurate predictions with this method.

The Heisenberg model is studied in the same way. We plot the points $(1/m, T_c^{(m)})$, where $m=1,2,3$ for different $(d,s)$ in Fig. 3, where $(d,s)$ indicates the system with dimension $d$ and spin $s$, and find that the points also show linearity. We fit them with the $1/D(m)$ weighting method and make a prediction of the infinite series. Because there are only three points to fit one line, the prediction is not so reliable as in the Ising model. However, it gives some information of the actual $T_c$ at least, and most likely the prediction is closer to the exact value than the third-order correction when the linearity is especially good; for example, for $d=2$ and $s=\frac{1}{2}$, the "most reliable" value list in Ref. 8 is 0, and that is just our prediction.

## V. FURTHER DISCUSSION

There are some results which can be inferred about the critical temperatures of the Heisenberg model on two- and three-dimensional lattices. For $s=\frac{1}{2}$ on the square lattice, Ref. 9 gives $T_c$ several methods, such as Weiss molecular field (MF), 1.000; Oguchi two-spin cluster (OTSC), 0.845; three-spin cluster (TSC), 0.572; Kramers-Opechowski (KO), 0.55. Reference 8 with an effective-field theory (EFT) gives it as 0.704, while Ref. 10 with the same method modifies it as 0.659, but they think the most reliable result should be 0. The first order of the $1/z$ expansion derives $T_c$ as 0.500. In this paper, the third order of the VCE gives $T_c$ as 0.333, and the prediction of the fitting result is 0 (see Table II). For $s=\frac{1}{2}$ on the cubic lattice, Ref. 9 lists $T_c$ as MF, 1.500; OTSC, 1.400; TSC, 1.041; KO, 0.915. Reference 8 with the EFT gives it as 1.223, while Ref. 10 modifies it as 1.078, but they all think the reliable result should be 0.84. The $1/z$ expansion derives $T_c$ as 1.000. In this paper, the third order of the VCE gives $T_c$ as 0.917, and the prediction of the fitting result is 0.603 (see Table II).

It should be emphasized that the linear fitting method is just a trial for the Heisenberg model. The method is not perfect, and the datum size is small; therefore, the prediction cannot be very reliable. But the result of the third order of VCE is strict, and it is more accurate than the second-order correction and can be relied on.

From calculations of the Ising and Heisenberg models, one can see that the VCE is an effective method to study model systems. We find that the first order of the VCE is equivalent to the zero order of the $1/z$ expansion, and the second order of the VCE corresponds to the first order of $1/z$ expansion; therefore, the VCE may have some qualities common with the $1/z$ expansion. If the hypothesis is right, the third-order VCE should correspond to the second order of the $1/z$ expansion. It seems that each method has its singular advantages over the other. The relation of the two methods needs further investigation.

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