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An Analytical Study of Three-State Potts Model on Lattice

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Abstract *We investigate the phase structure of the three-state Potts model by the variational cumulant expansion approach. It is shown that there is a weak first-order phase transition in three and four dimensions. The critical coupling given by this method is in good agreement with MC data.*

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1 Introduction

It has been argued[1] that an effective theory for the order parameter of a (3+1)-dimensional SU(N) gauge theory has the same global symmetry as the three-dimensional $Z(N)$ spin model. $Z(N)$ spin model plays an important role in understanding the critical behavior of SU(N) gauge theories.

Considerable research has been invested in the study of the behavior of the three-dimensional three-state Potts model.[2] The important and controversial question concerning the three-state Potts model in three dimensions is whether its transition is of the first or the second order and where the transition point β_c is.

Mean-field theory predicted a first-order transition independent of the dimension of the lattice.[2] Approximate renormalization group calculations by Golner[3] and ϵ-expansion calculation by Amit and Shcherbakov, Rudnick[4] for $d = 3$ predicted a first-order transition. Levy and Sudako[5] also predicted a first-order transition for $d = 3$ using the cluster variation method. Using high-temperature series expansions, Ditzian and Oitmaa,[6] Kim and Joseph[7] calculated the three-state Potts model and got a first-order transition for $d = 3$.

In contrast, modified mean-field approximation predicted a continuous transition for all dimensions.[8] Burkhard *et al.*[9] found a second-order transition via the Kadanoff variational method. Straley and Fisher,[10] relying mainly on low-temperature series expansion, favored a second-order transition and reported estimates of the critical exponents. With high-field expansion, Miyashita *et al.*[11] claimed that this transition also should be of the second order.

Since 1979, numerical simulation has been the main approach to attack this problem. A small but clear jump of the internal energy was found.[12−19] A general consensus has been reached that it possesses a weak first-order transition. Thus, it leads us to expecting that the transition of pure SU_3 gauge theory is also a first-order one.

But there is also some circumstantial evidence[20−23] of three-states Potts model by Monte Carlo studies indicating that the correlation length increases towards the critical point with a power-law divergence which is usually taken as a characteristic of a second-order phase transition.

Recently, the properties of Potts model have been the subject of renewed interest because of a claim made by the APE collaboration[24] that the finite-temperature phase transition of SU_3 gauge theory may be of the second order. The correlation length of SU_3 system appears to be divergent. On the other hand, Columbia University Group[25] still found a small but finite discontinuity in the internal energy at the transition point. This status looks similar to that for the three-dimensional three-state Potts model ($q = 3$).

The variational cumulant expansion is developed for the investigation of lattice gauge theories. It has given many encouraging results.[26] In this paper, we try to apply this analytical method to three-dimensional three-state Potts model with aim to investigate the question of the order of the transition. We shall calculate the internal energy, specific heat, and order parameter. The results in $4 \sim 6$ dimensions are also given. The comparison with the results from other procedure is presented.

2 Calculation

The three-state Potts model is given by the Hamiltonian

$$H = -\frac{3}{2}\sum_{\langle ij\rangle}(\delta_{\sigma_i\sigma_j} - 1)\,, \tag{1}$$

where $\langle ij\rangle$ is the sum over the nearest neighbor spin pairs and the spin variable σ_i takes $q = 3$ states. We can recast Hamiltonian (1) into

$$\begin{aligned} H &= -\sum_{\langle ij\rangle}[\,\mathrm{Re}(s_i s_j^*) - 1] \\ &= -\frac{1}{2}\sum_{\langle ij\rangle}(s_i s_j^* + s_i^* s_j - 2) \end{aligned} \tag{2}$$

with a Z_3 valued spin variables s_i and s_j defined at the sites i and j,

$$s_j = \exp\Big(\frac{2\pi i n_j}{3}\Big), \quad n_j = 0, 1, 2\,. \tag{3}$$

The partition function of this statistical system is defined by

$$Z = \sum_{\{S_i\}} \mathrm{e}^{-\beta H} = \mathrm{e}^{-\beta N_i d} \sum_{\{S_i\}} \mathrm{e}^{S} \tag{4}$$

with action S,

$$S = \frac{\beta}{2} \sum_{\langle ij \rangle} (s_i s_j^* + s_i^* s_j)\,, \tag{5}$$

where N_i is the number of site, d is the dimensionality, and $\beta = 1/T$ is the inverse temperature.

The free energy F is obtained by

$$F = -\frac{1}{N_l} \ln Z\,, \tag{6}$$

where $N_l = N_i d$ is the total number of links.

We calculate the internal energy per link as

$$E = \frac{1}{N_l} \langle H \rangle = \frac{\partial F(\beta)}{\partial \beta}\,, \tag{7}$$

the specific heat

$$C = \frac{\partial E}{\partial T}\,, \tag{8}$$

and the order parameter

$$P \equiv \max(P_0, P_1, P_2) \tag{9}$$

with P_α defined by

$$P_\alpha = \mathrm{Re}(\,\mathrm{e}^{-\mathrm{i}(2\pi/3)\alpha} \langle s_i \rangle)\,, \quad \alpha = 0, 1, 2\,. \tag{10}$$

Here, $\langle X \rangle$ denotes the thermal expectation value of the observable X with respect to Z.

Now let us apply the variational cumulant expansion to this model. In order to solve this statistical system in variational cumulant expansion approach, one can introduce an "effective" action $S_0(s, J)$, which is as "close" to the action S as possible. S_0 system should be easy to be solved. J is a variational parameter, which is determined by minimizing the free energy in cumulant expansion (see below). In this way, actually, S_0 system becomes an approximate effective one of S system. We solve the problem in S_0 system. The effect due to the difference between S and S_0 can be calculated by cumulant expansion.

As usual, one can choose S_0 as

$$S_0 = \sum_i (J s_i^* + J^* s_i)\,, \tag{11}$$

where J is a complex variational parameter $J = x + \mathrm{i}y$. According to the cumulant expansion, the partition function can be expanded as

$$\begin{aligned} Z &= \mathrm{e}^{-\beta N_i d} \sum_{\{s_i\}} \mathrm{e}^{S} = \mathrm{e}^{-\beta N_i d} Z_0 \langle\, \mathrm{e}^{S - S_0} \rangle_0 \\ &= \mathrm{e}^{-\beta N_i d} Z_0 \exp\Big(\sum_{n=1}^{\infty} \frac{1}{n!} K_n\Big)\,, \end{aligned} \tag{12}$$

where

$$\begin{aligned} Z_0 &\equiv \sum_{\{s_i\}} \mathrm{e}^{S_0} = (FI)^{N_i}\,, \\ FI &= \sum_{\{s_i\}} \mathrm{e}^{J s_i^* + J^* s_i} \\ &= \mathrm{e}^{2x} + \mathrm{e}^{-x+\sqrt{3}y} + \mathrm{e}^{-x-\sqrt{3}y}\,, \\ \langle X \rangle_0 &\equiv \frac{1}{Z_0} \sum_{\{s_i\}} X\, \mathrm{e}^{S_0}\,, \end{aligned} \tag{13}$$

$$\begin{aligned} K_1 &= \langle S - S_0 \rangle_0\,, \\ K_2 &= \langle (S - S_0)^2 \rangle_0 - \langle S - S_0 \rangle_0^2\,, \\ K_3 &= \langle (S - S_0)^3 \rangle_0 - 3 \langle S - S_0 \rangle_0 \langle (S - S_0)^2 \rangle_0 \\ &\quad + 2 \langle S - S_0 \rangle_0^3\,, \\ K_4 &= \langle (S_0 - S)^4 \rangle_0 - 4 \langle S_0 - S \rangle_0 \langle (S_0 - S)^3 \rangle_0 \\ &\quad + 12 \langle (S_0 - S)^2 \rangle_0 \langle S_0 - S \rangle_0^2\,, \\ &\quad - 3 \langle (S_0 - S)^2 \rangle_0^2 - 6 \langle S_0 - S \rangle_0^4\,. \end{aligned} \tag{14}$$

Thus the free energy F can be expressed as a function of β and J,

$$F(\beta, J) = -\frac{1}{N_l} \ln Z(\beta, J)\,. \tag{15}$$

Using the expression of $S_0(s, J)$, each term in expansions (12) $\sim$ (14) can be calculated analytically as a function of β and J. Here, we give an example, the calculation of K_1 and K_2,

$$\begin{aligned} K_1 &= \langle S - S_0 \rangle_0 \\ &= \Big\langle \frac{\beta}{2} \sum_{\langle ij \rangle} (s_i s_j^* + s_i^* s_j) - \sum_i (J s_i^* + J^* s_i) \Big\rangle_0 \\ &= \frac{\beta}{2} N_i d \cdot 2 \langle s_i \rangle_0 \langle s_j^* \rangle_0 - N_i (J \langle s_i^* \rangle_0 + J^* \langle s_i \rangle_0)\,. \end{aligned} \tag{16}$$

One can see that in S_0 system, the expectation value of $\langle s_i s_j^* \rangle_0$ can be factorized into $\langle s_i \rangle_0 \langle s_j^* \rangle_0$,

$$\Big\langle \sum_{\langle ij \rangle} s_i s_j^* \Big\rangle_0 = N_i d \langle s_i \rangle_0 \langle s_j^* \rangle_0\,, \tag{17}$$

where $N_i d$ is the total number of the spin pairs, and $\langle s_i \rangle_0 \langle s_i^* \rangle_0$ can be calculated analytically,

$$\begin{aligned} \langle s_i \rangle_0 &\equiv \frac{1}{Z_0} \sum_{\{s_i\}} s_i \exp\Big[\sum_j (J s_j^* + J^* s_j)\Big]\,, \\ \langle s_i^* \rangle_0 &\equiv \frac{1}{Z_0} \sum_{\{s_i\}} s_i^* \exp\Big[\sum_j (J s_j^* + J^* s_j)\Big]\,. \end{aligned} \tag{18}$$

In the following, for simplicity, we use two graphs to stand for these combinations,

$$\langle | \rangle_0 \to \langle s_i s_j^* + s_i^* s_j \rangle_0\,, \quad \langle \cdot \rangle_0 \to \langle J s_i^* + J^* s_i \rangle_0\,. \tag{19}$$

Therefore

$$K_1 = \frac{\beta}{2} N_i d \langle | \rangle_0 - N_i \langle \cdot \rangle_0\,. \tag{20}$$

Similarly, we have

$$K_2 = \langle (S - S_0)^2 \rangle_0 - \langle S - S_0 \rangle_0^2$$

$$
\begin{aligned}
&= \Big(\frac{\beta}{2}\Big)^2 N_i d\,[\langle\|\rangle_0 - \langle|\rangle_0^2] \\
&\quad + \Big(\frac{\beta}{2}\Big)^2 N_i 2d\,(2d-1)[\langle|_-\rangle_0 - \langle|\rangle_0^2] \\
&\quad - 2\Big(\frac{\beta}{2}\Big) 2N_i d\,[\langle|.\rangle_0 - \langle|\rangle_0\langle\cdot\rangle_0] \\
&\quad + N_i[\langle\cdot\cdot\rangle_0 - \langle\cdot\rangle_0^2]\,. \qquad (21)
\end{aligned}
$$

The contribution of these graphs is

$$
\begin{aligned}
\langle\|\rangle_0 &= 2(1 + \langle s_i^2\rangle_0\langle s_i^{*2}\rangle_0)\,, \\
\langle|_-\rangle_0 &= 2\langle s\rangle_0\langle s_i^*\rangle_0 + \langle s_i^2\rangle_0\langle s^*\rangle_0^2 + \langle s\rangle_0^2\langle s_i^{*2}\rangle_0\,, \\
\langle|.\rangle_0 &= J(\langle s\rangle_0\langle s^{*2}\rangle_0 + \langle s^*\rangle_0) + J^*(\langle s^*\rangle_0\langle s^2\rangle_0 \\
&\quad + \langle s\rangle_0)\,, \\
\langle\cdot\cdot\rangle_0 &= J^2\langle s^{*2}\rangle_0 + 2J\ J^* + J^{*2}\langle s^2\rangle_0\,. \qquad (22)
\end{aligned}
$$

With the Z_3 valued spin variable, it is useful to show

$$
\langle s^{*2}\rangle_0 = \langle s\rangle_0\,, \quad \langle s^2\rangle_0 = \langle s^*\rangle_0\,. \qquad (23)
$$

One can prove from Eq. (14) that only connected graphs give non-zero contribution to K_n. Therefore, to calculate the n-th order contribution K_n, one has to list all the n-th order connected graphs and the number of topological graphs of each order in d dimensions. Then, using Eqs. (14), (18), and (23), one obtains K_n.

In this paper, we calculate the free energy to the fourth-order cumulant expansion. The topological graphs and the numbers of graphs in K_3 and K_4 are listed in Appendix. Therefore, the free energy F, internal energy E, and specific heat C can be expressed as functions of β, J and J^* analytically. It is found easily that this approach is invariant under Z_3 transformation of the variational parameter J,

$$
J \to J' = \mathrm{e}^{\mathrm{i}(2\pi/3)\alpha} J\,, \quad (\alpha = 0, 1, 2)\,, \qquad (24)
$$

because of Z_3 symmetry of spin variable.

Physical state is in the minimum of the free energy. Under this physical requirement, the variational parameter J is determined as a function of β (Meanwhile the free energy of this physical system is also determined). For simplicity, in this work, we find the minimum of the free energy by directly comparing the values of free energy calculated by computer instead of solving the extreme differential equation.

We calculate the free energy to the n-th order expansion ($n = 1, 2, 3, 4$). In each order, when $\beta < \beta_{\mathrm{cn}}$, we find one minimum in $J = 0$. When $\beta > \beta_{\mathrm{cn}}$, for each value of β, there are 3 equivalent minimums (with the same value of the free energy). Three variational parameters J's determined from these 3 equivalent minimums are indeed Z_3 symmetry as mentioned before. So three variational parameters J are equivalent. Substituting one of the three variational parameters determined above into the expression of E and C, we obtain the internal energy and specific heat. One can see that β_{cn} is the transition point in the n-th order approximation.

On the other hand, the expectation value of the spin variable s_i can be expressed in the cumulant expansion as

$$
\langle s_i\rangle = \frac{1}{Z}\sum_{\{s_i\}} s_i\,\mathrm{e}^{-\beta H} = \frac{\langle\,\mathrm{e}^{S_0 - S} s_i\rangle_0}{\langle\,\mathrm{e}^{S_0 - S}\rangle_0} = \sum_{m=1}^{\infty}\frac{1}{m!}L_m\,, \qquad (25)
$$

where

$$
\begin{aligned}
L_1 &= \langle s_i\rangle_0\,, \\
L_2 &= 2\langle s_i(S_0 - S)\rangle_0 - 2\langle s_i\rangle_0\langle S_0 - S\rangle_0\,, \\
L_3 &= 3\langle s_i(S_0 - S)^2\rangle_0 - 6\langle s_i(S_0 - S)\rangle_0\langle S_0 - S\rangle_0 \\
&\quad + 6\langle s_i\rangle_0\langle S_0 - S\rangle_0^2 - 3\langle s_i\rangle_0\langle(S_0 - S)^2\rangle_0\,, \\
L_4 &= 4\langle s_i(S_0 - S)^3\rangle_0 - 12\langle s_i(S_0 - S)^2\rangle_0\langle S_0 - S\rangle_0 \\
&\quad - 24\langle s_i\rangle_0\langle S_0 - S\rangle_0^3 + 24\langle s_i(S_0 - S)\rangle_0\langle S_0 - S\rangle_0^2 \\
&\quad + 24\langle s_i\rangle_0\langle S_0 - S\rangle_0\langle(S_0 - S)^2\rangle_0 \\
&\quad - 12\langle s_i(S_0 - S)\rangle_0\langle(S_0 - S)^2\rangle_0 \\
&\quad - 4\langle s_i\rangle_0\langle(S_0 - S)^3\rangle_0\,. \qquad (26)
\end{aligned}
$$

The calculation of L_m is similar to that of K_n. It is also a function of β and J. Substituting into Eqs. (25) and (26) the variational parameter $J(\beta)$, and using Eqs. (9) and (10), we obtain the order parameter $\langle\phi\rangle$.

3 Results and Discussions

Our result shows the internal energy of three-dimensional three-state Potts model in the 1st-, 2nd-, 3rd-, and 4th-order approximation.

Obviously, the phase transition is a weak first-order one. In the transition point, the gap of internet energy ΔE is

$$
\Delta E = \begin{cases} 0.1439 & \text{(Our result, to the 4th order)}, \\ 0.080 \pm 0.004 & \text{(MC result in Ref. [17])}. \end{cases} \qquad (27)
$$

Our analytical result conforms with that from MC numerical simulation. For comparison, we also present MC data for internal energy which only covers a very narrow region of β. Table 1 lists the transition point β_c in the first-, second-, third-, and fourth-order approximation.

Table 1 The transition point β_c of $Z(3)$ Potts model in d dimensions and in the n-th order approximation.

order	first	second	third	fourth
$d = 3$	0.3084	0.3479	0.3545	0.3577
$d = 4$	0.2313	0.2528	0.2553	0.2567
$d = 5$	0.1850	0.1986	0.1997	0.2004
$d = 6$	0.1542	0.1634	0.1641	0.1645

In the $d = 4$ case, the phase transition is also a weak first-order one.

Table 2 gives the values of β_c determined by other methods.

Table 2 The values of β_c determined by other methods.

d	e^{-K_c}	β_c	Method
3	0.5784	0.364 99	Low-temperature series[11]
	0.571	0.373 57	High-temperature series[7]
	0.577	0.366 60	MCRG[12]
	0.5769	0.366 72	MC[14]
		$0.3678 \pm 0.000\ 02$	MC[17]
		0.367 03	MC[16]
		$0.367\ 015\ 4 \pm 0.000\ 064$	MC[18]
		0.367 08	MC[19]
4	0.6788	0.2582	MC[12]

Our result shows that it has a good convergence to MC data. The deviation from MC data is only about 3%. We believe that the expansion will give more precise values of β_c in higher-order approximation.

Our result gives the specific heat. There is not a sharp peak but only an enhancement there.

Our result gives the order parameter P in three dimensions for the third order. The MC data are also presented for comparison. The gap of order parameter P is

$$\Delta P = \begin{cases} 0.5105 & \text{(Our result, to the third order)}, \\ 0.395 \pm 0.005 & \text{(MC result in Ref. [17])}. \end{cases} \tag{28}$$

Our study also shows that the variational cumulant expansion looks well for the three-state Potts model. We expect to apply this technique to many other statistical and gauge models.

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Appendix: Connected Graphs and Their Numbers

K_3 Order

Graph	$\langle\vert\vert\vert\rangle$	$\langle\vert_{=}\rangle$	$\langle\vert\overline{\ }\rangle$	$\langle\overline{\vert}\overline{\ }\rangle$	$\langle\vert\vert_{\cdot}\rangle$	$\langle\vert_{-}\rangle$	$\langle\vert_{-\cdot}\rangle$	$\langle\vert_{\cdot\cdot}\rangle$	$\langle\vert_{\cdot}\rangle$	$\langle\cdots\rangle$
Number	$N_i d$	$6N_i d(2d-1)$	$6N_i d(2d-1)^2$	$4N_i d(d-1)^2$	$2N_i d$	$2N_i d(2d-1)$	$4N_i d(2d-1)$	$2N_i d$	$2N_i d$	$N_i d$

K_4 Order

Graph	$\langle\vert\vert\vert\vert\rangle$	$\langle\vert\vert\vert^{-}\rangle$	$\langle\vert\vert^{=}\rangle$	$\langle\vert\vert^{--}\rangle$
Number	$N_i d$	$8N_i d(2d-1)$	$6N_i d(2d-1)$	$24N_i d(2d-1)^2$
Graph	$\langle\vert\vert^{<}\rangle$	$\langle\vert\vert\overline{\ }\rangle$	$\langle\vert\overline{\ }^{-}\rangle$	$\langle\vert\overline{\vert}\rangle$
Number	$12N_i d(2d-1)(2d-2)$	$12N_i d(2d-1)^2$	$24N_i d((2d-1)^3-(2d-2))$	$6N_i d(2d-2)$
Graph	$\langle\vert^{-<}\rangle$	$\langle-\overline{\vert}\rangle$	$\langle\vert\vert\vert_{\cdot}\rangle$	$\langle\vert\vert^{-}_{\cdot}\rangle$
Number	$24N_i d(2d-1)^2(2d-2)$	$2N_i d(2d-1)(2d-2)(2d-3)$	$2N_i d$	$6N_i d(2d-1)$
Graph	$\langle\vert\vert^{-}_{\cdot}\rangle$	$\langle\vert\vert^{-}_{\cdot}\rangle$	$\langle\vert^{--}_{\cdot}\rangle$	$\langle\vert^{-}_{\cdot}{}^{-}\rangle$
Number	$6N_i d(2d-1)$	$6N_i d(2d-1)$	$12N_i d(2d-1)^2$	$12N_i d(2d-1)^2$
Graph	$\langle\vert^{<}_{\cdot}\rangle$	$\langle\vert^{<}_{\cdot}\rangle$	$\langle\vert\vert^{\cdot\cdot}\rangle$	$\langle\vert\vert_{\cdot}^{\cdot}\rangle$
Number	$2N_i d(2d-1)(2d-2)$	$6N_i d(2d-1)(2d-2)$	$2N_i d$	$2N_i d$
Graph	$\langle\vert^{\cdot\cdot-}\rangle$	$\langle\vert^{-\cdot\cdot}\rangle$	$\langle\vert^{\cdot-}_{\cdot}\rangle$	$\langle\vert^{-}_{\cdot\cdot}\rangle$
Number	$2N_i d$	$4N_i d$	$8N_i d$	$4N_i d$
Graph	$\langle\vert^{\cdots}\rangle$	$\langle\vert_{\cdot}^{\cdot}\rangle$	$\langle\cdots\cdot\rangle$	
Number	$2N_i d$	$6N_i d$	$N_i d$	

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