Variational analyses of series expansions of the Potts model

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A linked-cluster type of series expansion of the free energy with a variational parameter is developed to the eighth order for the q-state Potts model. The order parameter and the internal energy are then derived. By analyzing these series expansions, critical temperatures T_c, latent heats, and discontinuities of the order parameters at T_c are determined for the cubic lattices.

The analysis of series expansions for thermodynamic functions has been a powerful method to study phase transitions and critical phenomena for spin systems.[1,2] There are three types of series expansions: high-temperature series expansions, low-temperature series expansions, and linked-cluster series expansions. In the linked-cluster series expansion,[2,3] a parameter which is the mean-field order parameter is introduced, such that the series expansions give approximations to thermodynamic functions at low temperatures as well as at high temperatures. The linked-cluster series expansions, therefore, can be used to study critical properties for systems which undergo either first-order or second-order phase transitions.

In this article we study critical properties of the q-state Potts model[4,5] by the series-expansion method. It is known that the Potts model on three-dimensional lattices undergoes first-order phase transitions for $q \geq 3$.[6-14] Determinations of critical parameters for first-order phase transitions are more difficult and less successful than those for continuous transitions. Previous studies on three-dimensional Potts model have determined the critical temperature T_c quite accurately. But estimates of the discontinuities of the order parameters, to be denoted as ΔM, and the latent heats, denoted as ΔU, are sparse.[10-14] Although there are numerous series-expansion studies of the Potts model,[2,5,6,15] to the best of our knowledge, linked-cluster series expansions of general q-state Potts model have not been reported before. Here we derive series expansions similar to the linked-cluster series expansions, but the parameter involved is considered as a variational parameter. We have obtained the series expansions to the eighth order. Critical parameters are then determined for the Potts model on cubic lattices for general values of q.

For convenience we let $q=2S+1$. The q-state Potts model can be considered as a spin-S Ising-like model with spin-multipole interactions.[15] The Hamiltonian of the spin-S Potts model is

$$-\beta H=(J/kT)\sum_{\langle ij\rangle}\delta(S_{iz},S_{jz}) =K\sum_{\langle ij\rangle}\sum_{l=0}^{2S}A(S,l)Q_0^{(l)}(S_{iz})Q_0^{(l)}(S_{jz}) , \quad (1)$$

where $\beta=1/kT$, J is the coupling constant, $\delta(n,m)$ is the Kronecker delta function, $K=J/kT$, and the summation $\sum_{\langle ij\rangle}$ is over nearest-neighbor pairs of spins. The coefficients $A(S,l)$ are

$$A(S,l)=2^{2l}(2l+1)(2S-l)!/(2S+l+1)! , \quad (2)$$

and $Q_0^{(l)}$ are spin multipole moments:

$$\begin{aligned} Q_0^{(0)}&=1 ,\\ Q_0^{(1)}&=S_z ,\\ Q_0^{(2)}&=(3/2)S_z^2-S(S+1)/2 ,\\ Q_0^{(3)}&=(5/2)S_z^3-[3S(S+1)-1]S_z/2, \text{ etc.} \end{aligned} \quad (3)$$

It has been shown that under the mean-field approximation the Potts model has exactly the same thermodynamic properties as the exchange-interaction model.[16] For the ferromagnetic case, these two models have only one order parameter. At $T=0$, all spins are in the same state, say, $|\alpha\rangle$. The thermal averages $\langle Q_0^{(l)}\rangle$ normalized by the matrix elements $\langle\alpha|Q_0^{(l)}|\alpha\rangle$ are independent of l for $l\geq 1$. We can define the order parameter as $M=\langle Q_0^{(l)}\rangle/\langle\alpha|Q_0^{(l)}|\alpha\rangle$. The mean-field Hamiltonian of these models is then given by[17]

$$-\beta H_{\mathrm{MFA}}=KzM\sum_i\rho_\alpha(S_{iz}) , \quad (4)$$

where z is the coordination number of the lattice, and $\rho_\alpha(S_{iz})$ is the density matrix that the spin S_{iz} is in the pure state $|\alpha\rangle$, which is any eigenstate of S_z.

In this article we define a single-spin Hamiltonian H_0 with a variational parameter μ:

$$-\beta H_0=Kz\mu\sum_i\rho_\alpha(S_{iz})\equiv L\sum_i\rho_\alpha(S_{iz}) , \quad (5)$$

where the summation is taken over all spins. The partition function of the Potts model is then expressed as

$$Z=\mathrm{Tr}\,\exp(-\beta H)=Z_0\langle\exp[-\beta(H-H_0)]\rangle_0 , \quad (6)$$

where

$$Z_0=\mathrm{Tr}\exp(-\beta H_0)=\exp(L)+2S , \quad (7)$$

and the average $\langle A\rangle_0$ for any operator A is defined as

$$\langle A\rangle_0=\mathrm{Tr}\,A\exp(-\beta H_0)/Z_0 . \quad (8)$$

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Following the standard series-expansion method,[1,2] the exponential function in the bracket of Eq. (6) is expanded in power series

$$Z(K,L)=Z_0\left[1+\sum_{n=1}^{\infty}\left\langle\left[K\sum_{\langle ij\rangle}\delta(S_{iz},S_{jz})-L\sum_i\rho_\alpha(S_{iz})\right]^n\right\rangle_0\Big/n!\right] . \quad (9)$$

The free energy $F=-kT\ln Z$ is then expressed as

$$-\beta F(K,L)=\ln Z_0+\sum_{n=1}^{\infty}[a_{n,0}K^n+a_{n,1}K^{n-1}L+\cdots+a_{n,n}L^n]/n! . \quad (10)$$

The coefficients $a_{n,m}$ can be calculated by the diagrammatic method, or by the cluster expansion method.[1,2]

If the summation is taken up to the nth order, we obtain the nth-order free energy, denoted as $F^{(n)}$. The first-order and the second-order free energies depend only on the coordination number z. They are

$$-\beta F^{(1)}=\ln Z_0+[(zD_2/2)K-xL] , \quad (11)$$

$$-\beta F^{(2)}=-\beta F^{(1)}+[z^2(D_3-D_2^2)+z(D_2^2+D_2-2D_3)/2]K^2/2+zx(D_2-x)KL+(x-x^2)L^2/2 , \quad (12)$$

where

$$x\equiv\exp(L)/[\exp(L)+2S] , \quad (13)$$

and

$$D_n\equiv[\exp(nL)+2S]/[\exp(L)+2S]^n . \quad (14)$$

$F^{(3)}$ and higher-order free energies depend on the details of the lattice structure. We have calculated the coefficient $a_{n,m}$ to the eighth order ($m\le n\le 8$) numerically for the general lattices. It is too lengthy to present these coefficients in this article. If $L=0$, Eq. (10) reduces to the high-temperature series expansion; and if $L=Kz[\exp(KzM)-1]/[\exp(KzM)+2S]$, Eq. (10) is the same as the linked-cluster expansion. In the present method, L (or $\mu=L/Kz$) is a variational parameter.

As defined in Eq. (5), $z\mu$ is the effective field (or the symmetry breaking field) acting on each spin. The effective field is related to the thermal average $\langle Q_0^{(l)}\rangle$, and is nonzero if and only if the system is ordered. Therefore, the stable value of μ (or L) may be considered as the order parameter of the system. But it is important to note that μ (or L) is not the conventional order parameter M defined as the thermal averages of the spin multiple moments.

We consider L as the Landau order parameter, and $F^{(n)}(K,L)$ as the Landau free energy of the systems. At a given temperature K^{-1}, one can plot $F^{(n)}$ versus L. The values of L which has the lowest free energy $F^{(n)}$ is the stable value of L (or μ) at the given temperature. For the nth-order free energy, the stable value of L at the temperature K^{-1} will be denoted as $L_s^{(n)}(K)$. We calculate $L_s^{(n)}$ as functions of the temperature numerically. At low temperatures, $L_s^{(n)}$ are positive, and above a critical temperature, $kT_c^{(n)}/J(=1/K_c^{(n)}), L_s^{(n)}$ vanishes. For $q=2, L_s^{(n)}$ are continuous as expected for second-order phase transitions. For $q\ge 3$, $L_s^{(n)}$ are discontinuous at $T_c^{(n)}$. For example, $kT_c^{(n)}/J$ for the three-state Potts model on the face-centered-cubic (f.c.c.) lattice are 4.328 09, 4.078 58, 4.000 94, 3.963 73, 3.942 53, 3.929 00, 3.919 72, and 3.912 45, for $n=1$ through 8, respectively. The values of $L_s^{(n)}$ at $T_c^{(n)}$ (or the discontinuities of $L_s^{(n)}$) are 1.386 29, 1.276 81, 1.183 62, 1.116 55, 1.066 55, 1.028 88, 0.999 192, and 0.963 757, respectively.

As mentioned above $L_s^{(n)}/Kz$ are not the conventional order parameters (defined as $\langle Q_0^{(l)}\rangle/\langle\alpha|Q_0^{(l)}|\alpha\rangle$) of the system. It can be shown that the nth-order parameter $M^{(n)}$ is given by

$$(2SM^{(n)}+1)/(2S+1)=(\partial/\partial L)[\beta F^{(n)}(K,L,a_{i,j})] . \quad (15)$$

The coefficients $a_{i,j}$ are functions of L as illustrated in Eqs. (11)–(14). But, in the above equation Z_0 and $a_{i,j}$ are regarded as constants when we take the derivative of $F^{(n)}$ with respect to L. Similarly, the nth-order internal energy of the system is given by

$$U^{(n)}/J=(\partial/\partial K)[\beta F^{(n)}(K,L,a_{i,j})] . \quad (16)$$

TABLE I. Critical temperatures kT_c/J, discontinuities of the order parameters ΔM, and latent heats (per spin) $\Delta U/J$ of the q-state Potts model on the cubic lattices. Values with superscript indices are results of previous studies.

Lattice	q	KT_c/J	ΔM	ΔU
f.c.c.	3	3.861	0.421	0.482
	3	3.90[a]	0.448[a]	0.585[a]
	4	3.345	0.620	1.338
	5	3.032	0.721	2.056
	6	2.816	0.783	2.602
	7	2.655	0.824	3.028
b.c.c.	3	2.515	0.426	0.293
	4	2.187	0.628	0.840
	5	1.990	0.718	1.306
	6	1.850	0.778	1.668
	7	1.745	0.819	1.985
s.c.	3	1.807	0.427	0.199
	3	1.826[b]	0.4[b]	0.24[b]
	3	1.816[c]	0.460[c]	0.222[c]
	3	1.816[d]	0.434[d]	0.197[d]
	3	1.816[e]	0.395[e]	0.240[e]
	3	1.817[f]		0.17[f]
	4	1.583	0.611	0.573
	5	1.444	0.715	0.899
	6	1.347	0.777	1.178
	7	1.274	0.830	1.367

[a]Kikuchi variational method using a four-site cluster (Ref. 7).
[b]Monte Carlo simulation via a coarse-grained averages on a $N=30^3$ lattice (Ref. 11).
[c]Multilattice microcannonical simulation for $N=16^3$ (Ref. 12).
[d]Multilattice microcannonical simulation for $N=32^3$ (Ref. 12).
[e]Metropolis Monte Carlo simulation for $N=48^3$ (Ref. 13).
[f]Histogram Monte Carlo method for $N=15^3$ (Ref. 14).

In Eqs. (15) and (16), $M^{(n)}$ and $U^{(n)}$ are evaluated at $L=L_s^{(n)}$ for the given temperature. In this article, we are interested in the critical parameters, i.e., the discontinuities of $M^{(n)}$ and $U^{(n)}$ at $T_c^{(n)}$, denoted as $\Delta M^{(n)}$ and $\Delta U^{(n)}$, respectively. For illustration consider the three-state Potts model on the f.c.c. lattice again. We obtain $\Delta M^{(n)}=0.5, 0.492\,181, 0.478\,300, 0.467\,349, 0.458\,758, 0.452\,344, 0.447\,329,$ and $0.439\,354$; and $\Delta U^{(n)}/J$ (per spin) $=1, 0.860\,667, 0.767\,994, 0.707\,238, 0.664\,359, 0.633\,534, 0.610\,112,$ and $0.581\,002$ for $n=1$ to 8, respectively.

When $n=1$, the present results are the same as those of the mean-field theory, and $M^{(1)}=L_s^{(1)}/Kz$. As n approaches infinity, $F^{(n)}$ gives exact free energy. Similarly, $T_c^{(n)}$, $\Delta M^{(n)}$, and $\Delta U^{(n)}$ approach the correct critical values as $n\rightarrow\infty$. It is not known theoretically how these nth-order critical parameters converge to their limiting values. Our numerical results show that $X^{(n)}$ ($X=T_c, \Delta M$ or ΔU) can be fitted quite well in the form

$$X^{(n)}=X+cn^{-1}+Q(n^{-2}) . \tag{17}$$

Extrapolation of the nth-order critical parameters to $n\rightarrow\infty$ yields critical properties of the Potts model. Our results based on the series expansion up to the eighth order are shown in Table I. Results of previous studies which have determined ΔM or ΔU (available only for $q=3$) are also included for comparison.

The uncertainties in our estimates of T_c are within one percent; and those for ΔM and ΔU are within a few percent. In general, the successive orders of critical parameters converge more rapidly for the f.c.c. lattice than for other cubic lattices. Our results are in reasonable agreement with (although a little lower than) various Monte Carlo studies for the three-state Potts model on the simple cubic lattice. We are presently deriving higher-order coefficients $a_{n,m}$ for the Potts model. It is expected that more accurate estimates of the critical parameters can be obtained from longer series expansions.

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