Large-q expansion of the specific heat for the two-dimensional q-state Potts model

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We have calculated the large-q expansion for the specific heat at the phase transition point in the two-dimensional q-state Potts model to the 23rd order in $1/\sqrt{q}$ using the finite lattice method. The series obtained allows us to give highly convergent estimates of the specific heat for $q>4$ on the first-order transition point. The result confirms the correctness of the conjecture by Bhattacharya *et al.* [Nucl. Phys. B **435**, 526 (1995); J. Phys. I **7**, 1155 (1997)] on the asymptotic behavior of the specific heat for $q\to 4$. [S1063-651X(99)05101-6]

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The q-state Potts model [1,2] in two dimensions has been investigated intensively as the test ground for analyzing the phase transition in many physical systems. In particular it is interesting because the order of the phase transion changes from first order to the second order when the parameter q is varied, that is, first order for $q>4$ and second order for $q\leqslant 4$. The amplitudes of many quantities at the first-order transition point are known exactly, including the free energy, the internal energy [3], and the correlation length [4–6]. The correlation length at the transition point increases to infinity as $q\to 4$ and at $q=4$ the transition becomes second order. Physically important quantities such as the specific heat and the susceptibility at the transition point, which also increase to infinity as $q\to 4$, are not solved exactly. Bhattacharya *et al.* [7] made a stimulating conjecture on the asymptotic behavior of the energy cumulants (including the specific heat) at the first-order transition point: The asymptotic relation of the energy cumulants and the correlation length at the first-order transition point for $q\to 4$ will be equal to the one at the second-order phase transition point with $q=4$ fixed. If this conjecture is true not only in the q-state Potts model but also in general physical systems that have a phase transition whose order changes from first order to second order when some parameter of the system is varied, it would give a good guide in investigating such systems, for instance, the order of the phase transition. Bhattacharya *et al.* [8] also made the large-q expansion of the energy cumulants to order 10 in $z\equiv 1/\sqrt{q}$, with which they could use the conjecture to give the estimates of the cumulants at the transition point for $q\geqslant 7$ that are better than those given by other methods including the Monte Carlo simulations [9] and the low- (and high-) temperature expansions [10–12]. The series obtained by Bhattacharya *et al.* are, however, not long enough to investigate the behavior of the energy cumulants for q close to 4.

In this paper we will enlarge the large-q series for the specific heat at the transition point to order 23 in z using the finite lattice method [13–15] instead of the standard graphical method used by Bhattacharya *et al.* The finite lattice method can in general give longer series than those generated by the graphical method especially in lower space (and time) dimensions. In the graphical method, one has to list all the relevant diagrams and count how many appear. In the finite lattice method we can skip this job and reduce the main work to the calculation of the expansion of the partition function for a series of finite size lattices, which can be done using the straightforward site-by-site integration [16,17] without the graphical technique. This method has been used mainly to generate the low- and high-temperature series in statistical systems and the strong coupling series in lattice gauge theory. One of the purposes of this paper is to demonstrate that this method is also applicable to the series expansion with respect to the inverse of the number of degrees of freedom for each local dynamical variable in a physical system. The long series obtained here by the finite lattice method enables us to examine the conjecture by Bhattacharya *et al.* on the asymptotic behavior of the specific heat for q very close to 4. We can also give the estimates of the specific heat for each $q=5,6,7,\ldots$ that are much more precise than those given in previous works and they would serve as a target in investigating this model in various contexts, for example, in testing the efficiency of a new algorithm of the numerical simulation.

The model is defined by the partition function

$$Z=\sum_{\{s_i\}}\exp(-\beta H),\quad H=-\sum_{\langle i,j\rangle}\delta_{s_i,s_j}, \tag{1}$$

where $\langle i,j\rangle$ represents the pair of nearest neighbor sites and $s_i=1,2,\ldots,q$. The phase transition point β_t is given by $\exp(\beta_t)-1=\sqrt{q}$. We will consider the free energy density in the disordered phase, which is given by

$$F_d(\beta)=\lim_{L_x,L_y\to\infty}(L_xL_y)^{-1}\ln Z_d(L_x,L_y), \tag{2}$$

where the partition function for the $L_x\times L_y$ lattice should be calculated with the free boundary condition corresponding to the disordered phase. The large-q expansion of the partition function can be given through the Fortuin-Kasteleyn representation [18] as

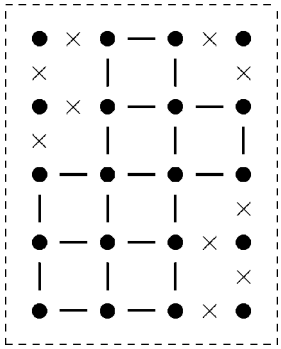

FIG. 1. Example of the cluster consisting of a single polymer that contributes to the lowest-order term of $W(l_x,l_y)$ with $l_x=4$ and $l_y=5$. The closed circles are the sites and the solid lines and the crosses are the bonds connecting and disconnecting the nearest neighbor sites, respectively, in the Fortuin-Kasteleyn representation.

$$Z_d(L_x,L_y)=q^{L_xL_y}\sum_{l,j} N_{l,j}(e^{\beta}-1)^l q^{-j}$$

$$=q^{L_xL_y}\sum_{l,j} N_{l,j}Y^l z^{2j-l}, \tag{3}$$

where $N_{l,j}$ is the number of configurations of l bonds connecting the nearest neighbor sites on the $L_x\times L_y$ lattice with L_xL_y-j independent clusters of sites and $Y\equiv(e^{\beta}-1)/\sqrt{q}$. (Two sites connected to each other belong to the same cluster.)

We define $H(l_x,l_y)$ for each $l_x\times l_y$ lattice $(l_x,l_y=1,2,3,\ldots)$ as [15]

$$H(l_x,l_y)=\ln[Z_d(l_x,l_y)/q^{l_xl_y}], \tag{4}$$

where $Z_d(l_x,l_y)$ is the partition function with the free boundary condition, and define $W(l_x,l_y)$ recursively as

$$W(l_x,l_y)=H(l_x,l_y)$$

$$-\sum_{l_x'\le l_x,l_y'\le l_y}{}' (l_x-l_x'+1)(l_y-l_y'+1)W(l_x',l_y'). \tag{5}$$

Here the $'$ indicates that a term with $l_x'=l_x$ and $l_y'=l_y$ should be excluded in the summation. Then the free energy density defined by Eq. (2) is given by

$$F_d(\beta)=\ln(q)+\sum_{l_x,l_y} W(l_x,l_y). \tag{6}$$

We can prove [15] that the Taylor expansion of $W(l_x,l_y)$ with respect to z and Y includes the contribution from all the clusters of polymers in the standard cluster expansion that can be embedded in the $l_x\times l_y$ lattice but cannot be embedded in any of its rectangular sublattices. Each cluster that contributes to the lowest-order term of $W(l_x,l_y)$ consists of a single polymer and is of order $z^{l_x+l_y-2}$. An example of such a single polymer is shown in Fig. 1. Therefore, to obtain the series to order z^N we only have to take into account all the rectangular lattices that satisfy $l_x+l_y-2\le N$. If we set $Y=1+y$ [19], then we only have to keep the expansion with respect to y to order y^n to obtain the nth energy cumulant at the phase transition point as

$$F_d^{(n)}=\frac{d^n}{d\beta^n}F_d(\beta)\big|_{\beta=\beta_t}=\sum_m a_m^{(n)}z^m. \tag{7}$$

[We note that $(d/d\beta)=(1+y+z)(d/dy)$ and $y=0$ at $\beta=\beta_t$.] We can also calculate the series for the energy cumulant $F_o^{(n)}$ at β_t in the ordered phase by using the duality relation

$$F_d^{(2)}-F_o^{(2)}=-z[F_d^{(1)}-F_o^{(1)}]. \tag{8}$$

We have calculated the series to order $N=23$ in z for $n=0,1$, and 2. The series obtained for the zeroth and first cumulants (i.e., the free energy and the internal energy) agree with the expansion of the exactly known expressions. The series for the second cumulants are listed in Table I. The coefficients for $F_o^{(2)}$ agree with those by Bhattacharya *et al.* to order 10.

TABLE I. Large-q expansion coefficients $a_m^{(2)}$ for the second energy cumulant.

m	$a_m^{(2)}$ (disordered)	$a_m^{(2)}$ (ordered)
0	0	0
1	2	0
2	14	16
3	26	34
4	118	114
5	250	254
6	894	882
7	1936	1944
8	6160	6128
9	13538	13550
10	39774	39698
11	88360	88360
12	245188	245036
13	547468	547356
14	1457976	1457784
15	3264012	3263316
16	8410284	8410596
17	18868858	18865590
18	47391870	47395762
19	106180532	106166828
20	261607968	261629456
21	586199668	586145660
22	1415497756	1415594740
23	3174285456	3174081000

The latent heat $\mathcal{L}$ [3] and the correlation length ξ [4–6] at the transition point are known, respectively, to vanish and to diverge at $q\to 4$ as

$$\mathcal{L}\sim 3\pi x^{-1/2}, \tag{9}$$

$$\xi\sim\frac{1}{8\sqrt{2}}x, \tag{10}$$

TABLE II. Specific heat for some values of q.

q	C_d	C_o
5	2889(2)	2886(3)
6	205.93(3)	205.78(3)
7	68.738(2)	68.513(2)
8	36.9335(3)	36.6235(3)
9	24.58761(8)	24.20344(7)
10	18.38543(2)	17.93780(2)
12	12.401336(3)	11.852175(2)
15	8.6540358(4)	7.9964587(2)
20	6.13215967(2)	5.36076877(1)
30	4.2989934145(6)	3.4128952554(3)

with $x=\exp(\pi^2/2\theta)$ and $2\cosh\theta=\sqrt{q}$. Bhattacharya *et al.* [7] made the conjecture that $F^{(2)}_{d,o}$ will diverge at $q\to 4$ as

$$F^{(2)}_{d,o}\sim \alpha x. \tag{11}$$

This is from the fact that for $\beta\to\beta_t$ with $q=4$ fixed the correlation length and the second cumulant diverge, respectively, as $\xi\sim\lambda|\beta-\beta_t|^{-2/3}$ and $F^{(2)}\sim\mu|\beta-\beta_t|^{-2/3}$, so that $\xi/F^{(2)}\sim$ const, and the assumption that this relation between the correlation length and the second cumulant is also kept for $q\to 4$ with $\beta=\beta_t$. The constant α in Eq. (11) should be common for the ordered and disordered phases from Eqs. (8) and (9). Here we follow this conjecture. Then the product $F^{(2)}\mathcal{L}^2$ is expected to be a smooth function of θ, so we apply the Padé approximation to this quantity as

$$F^{(2)}_d\mathcal{L}^2=zP_M(z)/Q_L(z)+O(z^{M+L+2}),$$

$$F^{(2)}_o\mathcal{L}^2=z^2R_M(z)/S_L(z)+O(z^{M+L+3}), \tag{12}$$

where $P_M(z)$ and $Q_L(z)[R_M(z)$ and $S_L(z)]$ are the Mth- and Lth-order polynomials with $M+L+1\leqslant N[M+L+2\leqslant N]$. We give in Table II the values of the specific heat $C_{d,o}$ evaluated from these Padé approximants for some values of q and present in Fig. 2 the behavior of the ratio of $F^{(2)}$ to x plotted versus θ. The averages and errors are taken from all the

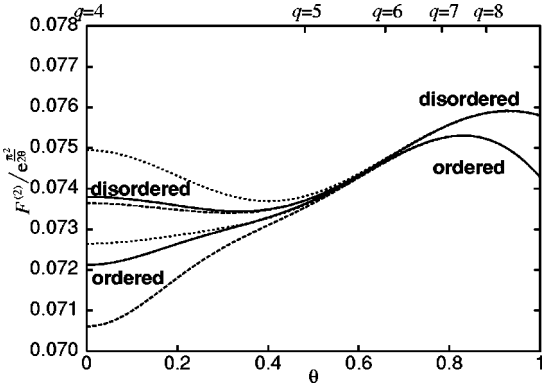

FIG. 2. Ratio of $F^{(2)}$ to x plotted versus θ. The dashed and dotted lines represent the errors for the ordered and disordered phases, respectively.

$[M,L]$ Padé approximants with $M\geqslant 8$ and $L\geqslant 8$, excluding that whose denominator has zero at some point in $4<q<\infty$. We have checked that the duality relation (8), which is not respected exactly by the Padé approximants, is really satisfied within the accuracy for the whole range of $q>4$. These estimates are more precise by three or four orders of magnitude than (and of course consistent with) the previous result for $q\geqslant 7$ from the large-q expansion to order z^{10} by Bhattacharya *et al.* [8] and the result for $q=10,15,20$ from the Monte Carlo simulations carefully done by Janke and Kappler [9]. What should be emphasized is that we obtained the values of the specific heat to an accuracy of about 0.1% at $q=5$, where the correlation length is as large as 2500 [4]. As for the asymptotic behavior of $F^{(2)}$ at $q\to 4$, the Padé data of $F^{(2)}_d/x$ and $F^{(2)}_o/x$ have relatively large errors of a few percent around $q=4$, but their behaviors shown in Fig. 2 are enough to convince us that the conjecture (11) is true with

$$\alpha=0.073\pm 0.002. \tag{13}$$

The extension of the large-q expansion to the higher-energy cumulants and the magnetization cumulants is rather straightforward and now in progress, which would also enable us to investigate the asymptotic behavior of these quantities for $q\to 4$.

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