FIRST ORDER PHASE TRANSITION OF THE Q-STATE POTTS MODEL IN TWO DIMENSIONS

H. ARISUE, K. TABATA
Osaka Prefectural College of Technology, Saiwai-cho, Neyagawa
Osaka 572, Japan
E-mail: arisue@las.osaka-pct.ac.jp

We have calculated the large-q series of the energy cumulants, the magnetization cumulants and the correlation length at the first order phase transition point both in the ordered and disordered phases for the $q$-state Potts model in two dimensions. The series enables us to estimate the numerical values of the quantities more precisely by a factor of $10^2 - 10^4$ than the Monte Carlo simulations. From the large-q series of the eigenvalues of the transfer matrix, we also find that the excited states form a continuum spectrum and there is no particle state at the first order phase transition point.

1 Introduction

In many of the physical systems that exhibit the first order phase transition, the order of the transition changes to the second order by changing the parameter of the system. It is important to know how the quantities at the first order phase transition point diverge when the parameter approaches the point at which the order of the transition changes. The $q$-state Potts model\(^1,2\) in two dimensions gives a good place to investigate this subject. It exhibits the first order phase transition for $q > 4$ and the second order one for $q \leq 4$. Many quantities of this model are known exactly at the phase transition point $\beta = \beta_t$ for $q > 4$, including the latent heat\(^3\) and the correlation length in the disordered phase\(^4,5,6\) which vanishes and diverges, respectively, in the limit $q \to 4_+$. One the other hand other physically important quantities such as the specific heat, the magnetic susceptibility, and the correlation length (in the ordered phase) at the transition point, which also diverge as $q \to 4_+$, are not solved exactly.

Here we calculate the large-$q$ expansion series of the energy cumulants including the specific heat and the magnetization cumulants including the magnetic susceptibility in both the phases and the correlation length in the ordered phase at the transition point using the finite lattice method\(^7,8,9\). Obtained long series for the energy and magnetization cumulants give the estimates of the quantities that are more precise by a factor of $10^2 - 10^4$ than the Monte Carlo simulations. Especially its estimates are within an accuracy of 0.1% at $q = 5$, where the correlation length is as large as a few thousands of the lattice spacing. Bhattacharya et al\(^10\) made a stimulating conjecture on the asymptotic behavior of the energy cumulants at the first order transition point; the relation
between the energy cumulants and the correlation length in their asymptotic behavior at the first order transition point for $q \rightarrow 4^+$ will be the same as their relation in the second order phase transition for $q = 4$ and $\beta \rightarrow \beta_t$, which is well known from their critical exponents. The obtained series enables us to confirm the correctness of the conjecture.

As for the correlation length at the first order phase transition point, the results of the Monte Carlo simulation\(^1\)\(^1\)\(^1\)\(^1\) and the density matrix renormalization group\(^1\)\(^2\) indicate that the correlation lengths are very close to each other in the ordered and disordered phases for $q \geq 10$. On the other hand, at the second order phase transition point($q \leq 4$) their ratio is known to be $1/2$. It is interesting whether the ratio is exactly equal to unity, remains close to unity, or approaches $1/2$ when $q \rightarrow 4^+$. To investigate it we calculate the first few terms of the large-$q$ expansion for the eigenvalues of the transfer matrix and find that from the second largest to the $N$-th largest eigenvalues with $N$ the one-dimensional size of the lattice make a continuum spectrum in the thermodynamic limit both in the ordered and disordered phases. We also calculate the long series of the second moment correlation length in both the phases, which serve to investigate the behavior of the spectrum of the eigenvalues of the transfer matrix in the region of $q$ close to 4.

2 Finite lattice method

Here we use the finite lattice method\(^7\)\(^,\)\(^8\)\(^,\)\(^9\) to generate the large-$q$ series for the Potts model, instead of the standard diagrammatic method used by Bhattacharya et al.\(^1\)\(^3\) The finite lattice method can in general give longer series than those generated by the diagrammatic method especially in lower spatial dimensions. In the diagrammatic method, one has to list up all the relevant diagrams and count the number they 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\(^1\)\(^4\)\(^,\)\(^15\) without the diagrammatic 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. We note that this method is applicable to the series expansion with respect to any parameter other than the temperature or the coupling constant. Using this method we calculated\(^17\)\(^,\)\(^21\) the series for the $n$-th energy cumulants ($n = 0 - 6$) to $z^{23}$, $n$-th magnetization cumulants ($n = 1 - 3$) to $z^{21}$, and second moment correlation length to $z^{19}$ with $z \equiv 1/\sqrt{q}$.
Figure 1: Padé approximants of $F^{(2)}_d \mathcal{L}^p$ at $q = 4$ plotted versus $p$.

3 Energy cumulants

The latent heat $\mathcal{L}$ at the transition point are known to vanish at $q \to 4_+$ as

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

with $x = \exp(\pi^2/2\theta)$ and $2\cosh\theta = \sqrt{q}$. Bhattacharya et al.’s conjecture says that the $n$-th energy cumulants $F^{(n)}_{d,o}$ at the first order transition point $\beta = \beta_t$ will diverge for $q \to 4_+$ as

$$F^{(n)}_{d} , (-1)^n F^{(n)}_{o} \sim \alpha B^{n-2} \frac{\Gamma \left( n - \frac{4}{3} \right) }{\Gamma \left( \frac{4}{3} \right) } x^{3n/2-2} . \quad (1)$$

The constants $\alpha$ and $B$ in Eq.(1) should be common to the ordered and disordered phases from the duality relation for each $n$-th cumulants.

If this conjecture is true, the product $F^{(n)} \mathcal{L}^{3n-4}$ is a smooth function of $\theta$, so we can expect that the Padé approximation of $F^{(n)} \mathcal{L}^p$ will give convergent result at $p = 3n - 4$. It has been examined for the large-$q$ series obtained by the finite lattice methods for $n = 2, \cdots, 6$ both in the ordered and disordered phases, which in fact give quite convergent Padé approximants for $p = 3n - 4$ and as $p$ leaves from this value the convergence of the approximants becomes bad rapidly. An example can be seen in Fig. 1 for $n=2$ in the disordered phase. We give in Table 1 the values of the specific heat $C = \beta^2 F^{(2)}$ evaluated from these Padé approximants for some values of $q$. These estimates are three or four orders of magnitude more precise than (and consistent with) the previous result for $q \geq 7$ from the large-$q$ expansion to order $z^{10}$ by Bhattacharya et al. and the result of the Monte Carlo simulations for $q = 10, 15, 20$ carefully done by Janke and Kappler as in Table 2. What should be emphasized is that we obtained the values of the specific heat in the accuracy of about 0.1 percent at
Table 1: The specific heat for some values of $q$. The exact correlation length is also listed.

<table>
<thead>
<tr>
<th>$q$</th>
<th>$C_d$</th>
<th>$C_o$</th>
<th>$\xi_d$ (exact)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>2889(2)</td>
<td>2886(3)</td>
<td>2512.2</td>
</tr>
<tr>
<td>6</td>
<td>205.93(3)</td>
<td>205.78(3)</td>
<td>158.9</td>
</tr>
<tr>
<td>7</td>
<td>68.78(2)</td>
<td>68.513(2)</td>
<td>48.1</td>
</tr>
<tr>
<td>8</td>
<td>36.938(2)</td>
<td>36.5235(3)</td>
<td>23.9</td>
</tr>
<tr>
<td>9</td>
<td>24.58761(8)</td>
<td>24.20344(7)</td>
<td>14.9</td>
</tr>
<tr>
<td>10</td>
<td>18.38543(2)</td>
<td>17.93780(2)</td>
<td>10.6</td>
</tr>
<tr>
<td>15</td>
<td>8.6540358(4)</td>
<td>7.9964587(2)</td>
<td>4.2</td>
</tr>
<tr>
<td>20</td>
<td>6.13215967(2)</td>
<td>5.36076877(1)</td>
<td>2.7</td>
</tr>
</tbody>
</table>

Table 2: Comparison with the Monte Carlo simulations by Janke and Kappler (1997).

<table>
<thead>
<tr>
<th></th>
<th>$q = 10$</th>
<th>$q = 15$</th>
<th>$q = 20$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_d$</td>
<td>18.38543(2)</td>
<td>8.6540358(4)</td>
<td>6.13215967(2)</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>18.44(4)</td>
<td>8.651(6)</td>
<td>6.133(4)</td>
</tr>
<tr>
<td>$C_o$</td>
<td>17.93780(2)</td>
<td>7.9964587(2)</td>
<td>5.36076877(1)</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>18.0(1)</td>
<td>7.99(2)</td>
<td>5.361(9)</td>
</tr>
</tbody>
</table>

$q = 5$ where the correlation length is as large as 2500. As for the asymptotic behavior of $F^{(n)}$ at $q \to 4_+$, the Padé data of $F_d^{(2)}/x$ and $F_o^{(2)}/x$ have the errors of a few percent around $q = 4$ and their behaviors are enough to convince us that the conjecture (1) is true for $n = 2$ with $\alpha = 0.073 \pm 0.002$. Furthermore, from the conjecture (1) the combination $\{ \Gamma(n - \frac{1}{4}) |F^{(n)}|/\Gamma\left(\frac{3}{4}\right) F^{(2)} \}^{\frac{1}{n-2}} x^{-\frac{3}{2}}$ is expected to approach the constant $B$ for each $n(\geq 3)$, and in fact the Padé data for every $n(= 3, \cdots, 6)$ gives $B = 0.38 \pm 0.05$, which also gives strong support to the conjecture for $n \geq 3$.

4 Magnetization cumulants

The behavior of the $n$-th magnetization cumulants $M^{(n)}$ for $\beta \to \beta_l$ at $q = 4$ is well known as $M^{(n)}_{d,o} \simeq A^{(n)}_{d,o}(\xi)^{\frac{15}{8} n - 2}$ and parallel to the conjecture for the energy cumulants by Bhattacharya et al. we can make a conjecture that

$$M^{(n)}_{d,o} \sim \mu^{(n)}_{d,o} x^{-\frac{15}{8} n - 2},$$

in the limit $q \to 4_+$ with $\beta = \beta_l$. We have examined the Padé approximation of $M^{(n)} L^p$ for the large-$q$ series generated by the finite lattice method for $n = 2$ and 3 both in the ordered and disordered phases, which in fact gives
Table 3: The magnetic susceptibility for some values of $q$.

<table>
<thead>
<tr>
<th>$q$</th>
<th>$\chi_d$</th>
<th>$\chi_o$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>$9.13(3) \times 10^2$</td>
<td>$9.01(3) \times 10^2$</td>
</tr>
<tr>
<td>6</td>
<td>$6.585(4) \times 10^2$</td>
<td>$6.665(4) \times 10^2$</td>
</tr>
<tr>
<td>7</td>
<td>70.54(1)</td>
<td>77.31(1)</td>
</tr>
<tr>
<td>8</td>
<td>19.359(1)</td>
<td>21.525(1)</td>
</tr>
<tr>
<td>9</td>
<td>8.0579(1)</td>
<td>9.0106(2)</td>
</tr>
<tr>
<td>10</td>
<td>4.23276(2)</td>
<td>4.73823(4)</td>
</tr>
<tr>
<td>15</td>
<td>0.7304214(1)</td>
<td>0.8056969(2)</td>
</tr>
<tr>
<td>20</td>
<td>0.309365682(1)</td>
<td>0.33556421(1)</td>
</tr>
</tbody>
</table>

Table 4: Comparison with the Monte Carlo simulations by Janke and Kappler(1997).

<table>
<thead>
<tr>
<th>$q$</th>
<th>$M_d^{(2)}$</th>
<th>$M_o^{(2)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$q = 10$</td>
<td>$q = 15$</td>
</tr>
<tr>
<td>large-$q$</td>
<td>4.23276(2)</td>
<td>0.7304214(1)</td>
</tr>
<tr>
<td>M.C.</td>
<td>4.233(2)</td>
<td>0.73039(8)</td>
</tr>
<tr>
<td>large-$q$</td>
<td>4.73823(4)</td>
<td>0.8056969(2)</td>
</tr>
<tr>
<td>M.C.</td>
<td>4.74(4)</td>
<td>0.805(3)</td>
</tr>
</tbody>
</table>

quite convergent Padé approximants for $p = 15n/4 - 4$ and as $p$ leaves from this value the convergence of the approximants becomes bad rapidly again. In Table 3 we present the resulting estimates of the magnetic susceptibility $\chi_{d,o} = M_{d,o}^{(2)}$. Our result is much more precise than the Monte Carlo simulation at least by a factor of 100 as in Table 4. From the behavior of $M_{d,o}^{(n)}/x^{(15n/8-2)}$ we obtain the coefficients in Eq.(2) as $\mu_d^{(2)} = 0.0020(2)$, $\mu_o^{(2)} = 0.0016(1)$ and $\mu_d^{(3)} = 7.4(5) \times 10^{-5}$, $\mu_o^{(3)} = 7.9(2) \times 10^{-5}$. These convince us that the conjecture made for the magnetization cumulants is also true.

5 Exponential correlation length

Next we investigate the exponential correlation length $\xi_{1,o}$ in the ordered phase. Here the exponential correlation length is defined by $\xi_1 = \log (\Lambda_1/\Lambda_0)$ with $\Lambda_0$ and $\Lambda_1$ the largest and the second largest eigenvalues of the transfer matrix, respectively. (We have omitted the subscript '1' in the previous sections) There is an obstacle to extract the correction to the leading term of the large-$q$ expansion for the correlation length at the phase transition point from the correlation function $<O(t)O(0)>_c$, since we know from the graphical expansion that it
behaves like
\[
\langle \mathcal{O}(t)\mathcal{O}(0) \rangle \propto z^t (1 + 2zt^2 + \cdots) \neq \exp(-mt).
\]
for a large distance \(t\). Thus we will diagonalize the transfer matrix \(T\) directly for large-\(q\). The eigenfunction for the largest eigenvalue \(\Lambda_0\) in the leading order of \(z\) is
\[
|0\rangle \equiv |0 \ 0 \ \ldots \ 0 \ 0 \rangle_N
\]
where all of the \(N\) spin variables (each of which can take the value of \(s = 0, 1, \cdots, q - 1\)) are fixed to be zero, with the element of the transfer matrix \(\langle 0|T|0\rangle = 1 + O(z^2)\) and the corresponding eigenvalue is \(\Lambda_0 = 1 + O(z)\). The eigenfunctions for the second largest eigenvalue are
\[
|I\rangle \equiv \frac{1}{\sqrt{N - I + 1}} \sum_{I} |0 \ \ldots \ 0 \ e \ e \ \ldots \ e \ 0 \ \ldots \ 0 \rangle,
\]
\[
(I = 1, \cdots, N),
\]
\[
|e\rangle \equiv \frac{1}{\sqrt{q - 1}} \sum_{s=1}^{q-1} |s\rangle
\]
with the diagonal matrix elements
\[
\langle I|T|I\rangle = z + O(z^2),
\]
and the off-diagonal matrix elements starting from higher orders in \(z\). The second largest eigenvalues of \(T\) degenerate in the leading order with \(\Lambda_i = z + O(z^{3/2})\). The degeneracy of the eigenvalues of the first \(N\) 'excited states' is the reason why the expansion series (3) of the correlation function cannot be exponentiated into a single exponential term. The off-diagonal matrix elements resolve the degeneracy with
\[
\Lambda_i/\Lambda_0 = z + 4z^{3/2} + 6z^2 + O(z^3),
\]
\[
\cdots
\]
\[
\Lambda_N/\Lambda_0 = z - 4z^{3/2} + 6z^2 + O(z^3).
\]
for \(N \to \infty\). These eigenvalues constitute a continuum spectrum. It appears to be kept in any higher order of \(z\). From Eq.(4) we obtain
\[
1/\xi_{1,o} = - \log z - 4z^{1/2} + 2z + 8/3z^{3/2} + O(z^2).
\]
This is the same as the large-$q$ expansion of $1/\xi_{1,d}$ given by Buffenoir and Wallon$^5$ to this order.

In the disordered phase the situation is quite similar. The eigenvalues of the transfer matrix for the first $N$ excited states constitute a continuum spectrum with their values exactly the same as in the ordered phase at least to the order of $z^{3/2}$.

The eigenvalues form the continuum spectrum just on the first order phase transition point. Off the transition point, we can see that the spectrum is discrete with $\Lambda_i - \Lambda_{i+1} \sim O(\epsilon)$ for $\sqrt{z} \ll \epsilon \ll 1$ and $\Lambda_i - \Lambda_{i+1} \sim O(\epsilon^{2/3})$ for $\epsilon \ll \sqrt{z} \ll 1$ where $\epsilon \equiv \beta/\beta_t - 1$.

6 Second moment correlation length

Here we give the results of the large-$q$ expansion of the second moment correlation lengths $\xi_{2nd,o}$ in the ordered phase and $\xi_{2nd,d}$ in the disordered phase defined by

$$\xi_{2nd}^2 = \frac{\mu_2}{2d\mu_0},$$

where $\mu_2$ and $\mu_0$ are the second moment of the correlation function and the magnetic susceptibility, respectively. The obtained expansion coefficients$^8$ for the ordered and disordered phases coincide with each other to order $z^3$ and differ from each other in higher orders. The ratio of the second moment correlation length in the ordered phase to that in the disordered phase is estimated by the Padé analysis to be not far from unity even in the limit of $q \to 4$ ($\xi_{2nd,o}/\xi_{2nd,d} = 0.930(3)$). Another point is that the ratio $\xi_{2nd,d}/\xi_{1,d}$ of the second moment correlation length to the exponential correlation length is much less than unity in the region of $q$ where the correlation length is large enough. It approaches 0.51(2) for $q \to 4$. It is known that in the limit of the large correlation length,

$$\frac{\xi_{2nd}^2}{\xi_1^2} \to \frac{\sum_{i=1}^{\infty} c_i^2 (\xi_i/\xi_1)^3}{\sum_{i=1}^{\infty} c_i^2 (\xi_i/\xi_1)} < 1,$$

with $\xi_i \equiv -\log (\Lambda_i/\Lambda_0)$. If the 'higher excited states' ($i = 2, 3, \cdots$) did not contribute so much, this ratio would be close to unity, as in the case of the Ising model on the simple cubic lattice, where $\xi_{2nd}/\xi_1 = 0.970(5)$ at the critical point.$^8,19$ Our result implies that the contribution of the 'higher excited states' is large in the disordered phase of the Potts model in two dimensions even when $q$ is close to 4. This strongly suggests that the eigenvalues of the transfer matrix for the first $N$ excited states in the disordered phase form the continuum spectrum not only in the large-$q$ region but also when $q$ approaches 4.
As for the exponential correlation length $\xi_{1,o}$ in the ordered phase for $q \to 4$, it is difficult to calculate the eigenvalues of the transfer matrix in much higher orders. It is quite natural, however, to expect that the ratio $\xi_{1,o}/\xi_{1,d}$ would be close to unity even in the limit of $q \to 4$. The reason is the following. If the ratio $\xi_{1,o}/\xi_{1,d}$ would be $1/2$ in the limit of $q \to 4$, which is the known ratio in the second order phase transition point ($q \leq 4$), then the ratio $\xi_{2nd,o}/\xi_{1,o}$ should be close to unity, which would imply that the higher excited states would not contribute so much to $\xi_{2nd,o}$ and the eigenvalue of the transfer matrix for the first excited state would be separated from the higher excited states. This scenario is not plausible, since as already mentioned in section 5 the continuum spectrum of the eigenvalues of the transfer matrix appears to be maintained in any high order in $z$. In this case, we can expect that the ratio $\xi_{2nd,o}/\xi_{1,o}$ would be around $1/2$ as is the case in the disordered phase, resulting that $\xi_{1,o}/\xi_{1,d}$ is close to unity.

7 Summary

We generated the large-$q$ series for the energy and magnetization cumulants at the first order phase transition point of the two-dimensional $q$-state Potts model in high orders using the finite lattice method. They gave very precise estimates of the cumulants for $q > 4$ and confirmed the correctness of the Bhattacharya et al.'s conjecture that the relation between the cumulants and the correlation length for $q = 4$ and $\beta \to \beta_t$ (the second order phase transition) is kept in their asymptotic behavior for $q \to 4$, at $\beta = \beta_t$ (the first order transition point). If this kind of relation is satisfied as the asymptotic behavior for the quantities at the first order phase transition point in more general systems when the parameter of the system is varied to make the system close to the second order phase transition point, it would serve as a good guide in investigating the system.

Further the large-$q$ expansion of the eigenvalues of the transfer matrix was calculated in the first 4 terms. We found that they have the same spectra of the eigenvalues of the transfer matrix in the ordered and disordered phases giving the same exponential correlation length ($\xi_{1,o} = \xi_{1,d}$) to the order of $z^{3/2}$ and that the spectra are continuous in the thermodynamic limit. We also calculated the large-$q$ expansion of the second moment correlation length in the ordered and disordered phases in high orders and found that they differ from each other in higher orders than $z^3$, but that the ratio $\xi_{2nd,d}/\xi_{1,d}$ is not far from unity for all region of $q > 4$. We also found that $\xi_{2nd,d}/\xi_{d,1}$ is far from unity even in the limit of $q \to 4$. It receives significant contributions not only from the 'first excited state' but also 'higher excited states' and this suggest
strongly that the continuum spectrum would be maintained (i.e. there would be no particle state) in the disordered phase. From these results it is quite natural to expect that the exponential correlation length $\xi_{1,o}$ in the ordered phase is not far from that in the disordered phase even in the limit of $q \to 4$ and it is not plausible that their ratio approaches $1/2$ that is their ratio in the second order phase transition point ($q \leq 4$).

References