Determinant of the Potts model transfer matrix 
and the critical point

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ABSTRACT

By using a decomposition of the transfer matrix of the $q$-state Potts Model on a three dimensional $m \times n \times n$ simple cubic lattice its determinant is calculated exactly. By using the calculated determinants a formula is conjectured which approximates the critical temperature for a d-dimensional hypercubic lattice.

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I. Introduction

The two dimensional $q$-state Potts models [1,2] for various $q$ have been of interest as examples of different universality classes for phase transitions and, for $q = 3, 4$ as models for the adsorption of gases on certain substrates [3,4,5]. For $q \geq 3$ the free energy has never been calculated in closed form for arbitrary temperature. Some exact results have been established for the model: from a duality relation, the critical point has been identified [1]. The free energy and latent heat [6,7,8], and magnetization [9] have been calculated exactly by Baxter at this critical point, establishing that the model has a continuous, second order transition for $q \leq 4$ and a first order transition for $q \geq 5$. Baxter has also shown that although the $q = 3$ model has no phase with antiferromagnetic long-range order at any finite temperature there is an antiferromagnetic critical point at $T = 0$ [9]. The values of the critical exponents (for the range of $q$ where the transition is continuous) have been determined [10-12]. Further insight into the critical behaviour was gained using the methods of conformal field theory [13]. Our knowledge about the three dimensional Potts model is much less than the two dimensional case. The three dimensional 3-state Potts ferromagnet serves as an important model in both condensed matter as well as high energy physics [2]. Experimental realizations are structural in some crystals, and theoretically this model has attracted much interest as a simple effective model of finite-temperature pure-gauge QCD. Consequently it has been studied in the past few years by many authors using quite a variety of different techniques, for an incomplete list see [14-20, and refs therein]. By using Monte Carlo simulations with the help of standard finite size scaling methods the characteristic parameters of the phase transition (transition temperature, latent heat, etc) have been estimated with varying accuracy [21]. As a result there is by now general consensus that this model undergoes on a simple cubic lattice a weak first order phase transition from a three fold degenerate ordered low temperature phase to a disordered phase at high temperature. However, our knowledge about exact value of the partition function and spectrum of the three dimensional $q$-state Potts model is almost nothing. It is thus of continuing value to obtain further information about the three dimensional Potts model. In this paper by using edge transfer matrices the product of the eigenvalues for the transfer matrices of the $q$-state Potts model on the three dimensional lattices is calculated. The paper is organized as follows: In section II, by using the standard representation of the transfer matrices for the $q$-state Potts model on $2 \times n \times n$ lattices and using a method which is suggested by R.J.Baxter [29], the determinants of the transfer matrices are calculated exactly and then the calculation is generalized to the three dimensional $m \times n \times n$ simple cubic lattices. Finally from the general relation for the determinant a formula for the $d$-dimensional $q$-state Potts model is conjectured which approximates the critical temperature with a few percent error.

II. Determinant of the Potts model transfer matrix

The $q$-state Potts model has served as a valuable model in the study of phase transition and critical phenomena. On a lattice, or more generally on a graph $G$, at temperature $T$
this model is defined by the partition function:

\[ Z(G, q, k) = \sum_{\{\sigma_n\}} e^{-\beta H} \]  

(1)

with the Hamiltonian

\[ H = -J \sum_{<i,j>} \delta(s_i, s_j) \]  

(2)

where \( \delta(s_i, s_j) \) is the kronecker delta and \( s_i = 1, \ldots, q \) are the spin variables on each vertex \( i \in G \), \( \beta = (k_B T)^{-1} \), \( k = \beta J \); and \( <i,j> \) denotes pairs of adjacent vertices. Consider an \( n \times n \) square lattice with periodic boundary conditions. For the two dimensional Ising model, partition function can be written as trace of the product of transfer matrices and the eigenvalues can be calculated exactly [22-27]. There are several representations for the transfer matrix of the two dimensional \( q \)-state Potts model [22,28] which can be used to represent the transfer matrices for m-layer models. Determinant of the transfer matrix for the two dimensional Potts model can be calculated by different methods [29,30,31]. It is quite hard if not impossible to generalize our method [30] to higher dimensions \( (d > 2) \). We will use a method which is suggested by R.J.Baxter and generalize it to calculate the determinant of the transfer matrix for the \( q \)-state Potts model on three dimensional \( m \times n \times n \) simple cubic lattices. At first we calculate the determinant for the two-layer lattice, generalization to m-layers is simple and straightforward. For a two layer lattice the transfer matrix element connecting the stripes \( s_1, \ldots, s_n, t_1, \ldots, t_n \) and \( s_1', \ldots, s_n', t_1', \ldots, t_n' \) can be written as

\[ < s_1, \ldots, s_n, t_1, \ldots, t_n | P | s_1', \ldots, s_n', t_1', \ldots, t_n' > = \prod_{k=1}^n e^{k[\delta(s_k,s_{k+1})+\delta(t_k,t_{k+1})+\delta(s_k,t_k)]} e^{k[\delta(s_k,s'_k)+\delta(t_k,t'_k)]} \]  

(3)

We consider the stripe \( s_1, \ldots, s_n, t_1, \ldots, t_n \) in a plane with a periodic boundary condition along one direction \( (x) \) and free boundary conditions in the other direction \( (y) \), i.e. \( s_{n+1} = s_1, t_{n+1} = t_1 \). The transfer matrix operates along the z direction which is perpendicular to the \( x-y \) plane and connects the two stripes. Let us define two \( q^{2n} \times q^{2n} \) matrices \( V_2 \) and \( V_1' \) whose matrix elements are given by

\[ < s_1, \ldots, t_n | V_2 | s_1', \ldots, t_n' > = \delta_{s,s'} \delta_{t,t'} \prod_{k=1}^n e^{k[\delta(s_k,s_{k+1})+\delta(t_k,t_{k+1})+\delta(s_k,t_k)]} \]  

(4)

\[ < s_1, \ldots, t_n | V_1' | s_1', \ldots, t_n' > = \prod_{k=1}^n e^{k[\delta(s_k,s'_k)+\delta(t_k,t'_k)]} \]  

(5)

where
\[ \delta_{s,s'} = \prod_{i=1}^{n} \delta(s_i, s'_i), \quad \delta_{t,t'} = \prod_{i=1}^{n} \delta(t_i, t'_i) \] (6)

Both \( V_2 \) and \( V'_1 \) are products of \( n \) matrices [29]:

\[ V_2 = W_{12}W_{23} \ldots W_{n,1} \] (7)

\[ V'_1 = U_1U_2 \ldots U_n \] (8)

where \( W_{\nu,\nu+1} \) is a diagonal matrix with entries

\[ [W_{i,i+1}]_{st,s't'} = e^{k[\delta(s_i, s_{i+1}) + \delta(t_i, t_{i+1}) + \delta(s_i, t_i)]}\delta_{s,s'}\delta_{t,t'} \] (9)

and \( U_i \) (\( i = 1, \ldots, n \)) is the matrix with entries

\[ [U_i]_{st,s't'} = e^{k[\delta(s_i, s'_i) + \delta(t_i, t'_i)]} \prod_{j=1, j \neq i}^{n} \delta(s_j, s'_j)\delta(t_j, t'_j) \] (10)

Simultaneously permuting \( s_1, \ldots, t_n \) and \( s'_1, \ldots, t'_n \) is equivalent to a rearrangement of the rows and columns of these matrices, so

\[ \det W_{12} = \det W_{23} = \cdots = \det W_{n1} \] (11)

\[ \det U_1 = \det U_2 = \cdots = \det U_n \] (12)

Hence

\[ \det P = (\det W_{12} \det U_1)^n \] (13)

\( W_{12} \) is a diagonal matrix and its determinant is the product of its diagonal entries

\[ \det W_{12} = \prod_{s_1, \ldots, s_n} \prod_{t_1, \ldots, t_n} e^{k\delta(s_1, s_2)}e^{k\delta(t_1, t_2)}e^{k\delta(s_1, t_1)} \] (14)

\[ = \left[ \prod_{s_1, s_2} \prod_{t_1, t_2} e^{k\delta(s_1, s_2)}e^{k\delta(t_1, t_2)}e^{k\delta(s_1, t_1)} \right] q^{2n-4} \] (15)

\[ = e^{3kq^3} q^{2n-4} \] (16)

\[ = e^{3kq^{n-1}} \] (17)

\( U_1 \) is a block-diagonal matrix, consisting of \( q^{2n-2} \) diagonal blocks, each of the form

\[ A = (e^kI_{q \times q} + \sigma_{q \times q}) \otimes (e^kI_{q \times q} + \sigma_{q \times q}) \] (18)
where $\sigma$ is a $q \times q$ matrix with zero diagonal elements and unit elements on all other entries and $I$ is a $q \times q$ unit matrix. The determinant of the $q^2 \times q^2$ matrix $A$ is given by,

$$\det A = (e^k - 1)^{2q} (e^k - 1)^{2q(q-1)}$$

(19)

by using the following definitions

$$x = \frac{e^k + q - 1}{e^k - 1}, \quad y = e^k$$

(20)

we arrive at

$$\det U_1 = (\det A)^{q^{2n-2}} = \left[x^{2q}(y - 1)^{2q^2}\right]^{q^{2n-2}}$$

(21)

so the determinant of the transfer matrix is given by

$$\det P = \left[x(y - 1)^q\right]^{2q^{2n-1}} y^{3q^{2n-1}}$$

(22)

For $m$-layer lattices after a straightforward calculation we get to the following results. The matrix $A$ is a direct product of $m$ factors

$$A = (e^k I_{q \times q} + \sigma_{q \times q}) \otimes (e^k I_{q \times q} + \sigma_{q \times q}) \otimes \cdots \otimes (e^k I_{q \times q} + \sigma_{q \times q})$$

(23)

and so we arrive at

$$\det A = x^{mq^{m-1}}(y - 1)^{mq^n}$$

(24)

$$(\det U_1)^n = (\det A)^{mq^{m(n-1)}}$$

(25)

$W_{12}$ is again a diagonal matrix and its determinant is the product of its diagonal entries

$$\det W_{12} = \prod_{s_1^{(1)}, \ldots, s_n^{(1)}} \cdots \prod_{s_1^{(m)}, \ldots, s_n^{(m)}} e^{k \sum_{i=1}^{m} \delta(s_1^{(i)}, s_2^{(i)})} e^{k \sum_{i=1}^{m-1} \delta(s_1^{(i)}, s_1^{(i+1)})}$$

(26)

$$= \left[\prod_{s_1^{(1)}, s_2^{(1)}} \cdots \prod_{s_1^{(m)}, s_2^{(m)}} e^{k \sum_{i=1}^{m} \delta(s_1^{(i)}, s_2^{(i)})} e^{k \sum_{i=1}^{m-1} \delta(s_1^{(i)}, s_1^{(i+1)})}\right] q^{m(n-2)}$$

(27)

$$= [e^{(2m-1)kq^{2m-1}}]^{q^{m(n-2)}}$$

(28)

$$= e^{(2m-1)kq^{mn-1}}$$

(29)

Finally we arrive at the following formula for the determinant of the transfer matrix for the $q$-state Potts model on a three dimensional $m \times n \times n$ simple cubic lattice

$$\det P = [x(y - 1)^q]^{mnq^{[m-n-1]}} y^n(2m-1)q^{[mn-n-1]}$$

(30)
Considering a periodic boundary condition in both x and y directions (a plane which is perpendicular to the direction that transfer matrix operates), a straightforward calculation shows that the determinant is given by the following simple equation

\[ \det P = [xy^2(y-1)^q]^m q^{m^2-1} \]  (31)

There is a temperature where the product of the eigenvalues does not depend on the size of lattices. It should be noted that all of the eigenvalues are positive and \( \det P = 1 \) can be simplified to the following equation

\[ xy^2(y-1)^q = 1 \]  (32)

It is clear that (29) has a solution for \( k = \beta J \) which is a function of \( q \) and does not depend on \( m \) or the size of lattices. There is another interesting point about the periodic boundary conditions in all directions. Consider a one dimensional lattice with a periodic boundary condition, the transfer matrix is given by

\[ P^{(1)} = e^k I_{q \times q} + \sigma_{q \times q} \]  (33)

The determinant can be calculated easily

\[ \det P^{(1)} = x(y-1)^q \]  (34)

For a two dimensional \( m \times m \) lattice with a periodic boundary condition the determinant is given by [29,30,32]

\[ \det P^{(2)} = [xy(y-1)^q]^m q^{m^2-1} \]  (35)

and the determinant for a three dimensional \( m \times m \times m \) lattice with a periodic boundary condition for the two dimensional plane which is perpendicular to the direction that the transfer matrix operates is given by

\[ \det P^{(3)} = [xy^2(y-1)^q]^m q^{m^2-1} \]  (36)

This calculation can be extended to the \( d \) dimensional lattices. Considering a toroidal boundary condition for the \( d-1 \) dimensional hypersurface which is perpendicular to the direction that the transfer matrix operates we arrive at the following relations

\[ (\det W_{12})^m = y^{s(d-1)q^{s-1}} \]  (37)

\[ (\det U_1)^m = (\det A)^{mq(s/m)(m-1)} \]  (38)

\[ \det A = x^{(s/m)q^{(s/m)-1}}(y-1)^{(s/m)q^{(s/m)}} \]  (39)

where \( s = m^{d-1} \). Finally we arrive at the following general formula for the determinant at any dimension \( (d = 1, 2, 3, \ldots) \) for \( m^{(1)} \times \cdots \times m^{(d)} \) hypercubic lattices
\[ \det P^{(d)} = [xy^{d-1}(y-1)^q]^{q^{d-1}} \] (40)

For a two dimensional lattice the critical point corresponds to the maximum of the following factor of the determinant.

\[ \frac{xy(y-1)^q}{(y-1)^q} = xy \] (41)

We may expect that the maximum of the following factor of the d-dimensional determinant will give us an approximate formula for the critical temperature (we cannot prove this except for the two dimensional lattices).

\[ \frac{xy^{d-1}(y-1)^q}{(y-1)^q} = xy^{d-1} \] (42)

The maximum occurs at the following point

\[ k_{\text{max}}(q, d) = \ln \left[ \frac{2(q-1) - d(q-2) + \sqrt{4q(d-1) + q^2(d-2)^2}}{2(d-1)} \right] \] (43)

So we may conjecture that (43) is an approximation for the critical temperature. Interested reader may compare (43) with data which is given in [2] (see tables II and III in page 256) and see that it is indeed a good approximation for the critical temperatures.

\[ k_{\text{crit}}(q, d) \approx k_{\text{max}}(q, d) \] (44)

It may be interesting to extend these results to other lattices with different boundary conditions. This decomposition of the transfer matrix may be useful for obtaining other exact results for the \( m \)-layer or three dimensional lattices.

V. Conclusion

In this work determinant of the transfer matrix for the \( q \)-state Potts model on a three dimensional \( m \times n \times n \) simple cubic lattice is calculated exactly and the critical temperature is approximated by a conjectured formula.

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