Microcanonical Transfer Matrix and Yang-Lee Zeros of the $Q$-State Potts Model

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1 Introduction

The $Q$-state Potts model in two dimensions is very fertile ground for the investigation of phase transitions and critical phenomena. For $Q = 2$ and 3 there is a second order phase transition between $Q$ ferromagnetic ordered states and a disordered state. For $Q = 4$ the transition is also second order, but the usual critical behavior is modified by strong logarithmic corrections. For $Q > 4$ the transition is first order, with $Q = 5$ exhibiting weak first order behavior and a very large correlation length at the critical point.

The Hamiltonian for the Potts model is

$$\mathcal{H} = J \sum_{<i,j>} (1 - \delta(q_i, q_j)),$$

where $J$ is the coupling constant and $0 \leq q_i \leq Q - 1$ are the Potts spin variables. The energies (in units of $J$) are evenly spaced and take on integer values in the range $0 \leq E \leq N_b$ where $N_b$ is the number of bonds on the lattice. Here we will consider simple square lattices with periodic, cylindrical, and self-dual boundary conditions.

In addition to the energy there are $Q$ order parameters

$$M_q = \sum_k \delta(q_k, q),$$

which for the Ising model is simply related to the magnetization. The possible values of the order parameter are also integers, $0 \leq M \leq N_s$, where $N_s$ is the number of sites on the lattice.

If we denote the number of states with energy $E$ by $\Omega(E)$, then the canonical partition function for the $Q$-state Potts model is

$$Z_Q(y) = \sum_E \Omega_Q(E)y^E,$$

where $y = e^{-\beta J}$. From (3) it is clear that $Z$ is simply a polynomial in $y$, and the analytic structure of $Z$ is completely determined by the zeros of this polynomial, as first discussed by Lee and Yang[1, 2].
If we wish to study the partition function in an external field which couples to the order parameter, \( (2) \), then one needs to enumerate the number of states with fixed energy \( E \) and fixed order parameter \( M, \Omega(E, M) \). The partition function is again a polynomial given by

\[
Z_Q(y, x) = \sum_E \sum_M \Omega_Q(E, M) x^M y^E, \tag{4}
\]

where \( x = e^{-\beta h} \), and \( h \) is the external field. As discussed in the second \( 2 \) of Lee and Yang’s two famous papers, the zeros of the partition function for the Ising model in the complex-\( x \) plane all lie on the unit circle.

For finite systems the analyticity of \( Z \) in both \( x \) and \( y \) ensures that no zeros lie on the real axis. However, according to Lee and Yang, in the thermodynamic limit the zeros of the partition function in either the complex-\( x \) or -\( y \) planes approach arbitrarily close to the real axis at the critical point, leading to nonanalytic behavior in the partition function.

If the zeros lie on a one-dimensional locus in the thermodynamic limit one can define the density of zeros (per site) \( g(\theta) \) in terms of which the free energy per site is

\[
f(y) = -\int g(\theta) \log[y - y_0(\theta)] d\theta. \tag{5}\]

In the critical region the singular part of the free energy is a homogeneous function of the reduced temperature, \( y - y_c \), from which it follows\( ^2 \) that \( g(\theta) \) must also be a homogeneous function for small \( \theta \) of the form

\[
g(\theta) = b^{(-d+y_T)} g(\theta b^{y_T}). \tag{6}\]

This in turn implies that \( g(\theta) \) vanishes as \( \theta^\kappa \) as \( \theta \) goes to zero where \( \kappa = (d - y_T)/y_T \). On the other hand, if the system has a first order transition, \( \kappa = 0 \) and the discontinuity in the first derivative of \( f \), the latent heat, is given by \( L = 2\pi g(0) \). Exactly parallel arguments hold in the complex-\( x \) plane if one replaces the temperature exponent \( y_T \) by the magnetic exponent \( y_h \).

In a recent paper Creswick\( ^6 \) has shown how the numerical transfer matrix of Binder\( ^7 \) can be generalized to allow the evaluation of the density of states \( \Omega(E) \) and the restricted density of states, \( \Omega(E, M) \) for the \( Q \)-state Potts model. Similar calculations of \( \Omega(E) \) have been carried out by Bhanot\( ^8 \) in both two and three dimensions for the \( Q = 2 \) and \( Q = 3 \) Potts models, and Pearson\( ^9 \) for the 4\(^3 \) Ising model. Beale\( ^10 \) has used the exact solution for the partition function of the Ising model on finite square lattices to calculate \( \Omega(E) \). Bhanot’s method is far more complex than the \( \mu TM \) and requires essentially the same computer resources. Pearson’s method is only applicable to lattices with very few spins (e.g. 64) and Beale’s approach makes essential use of the exact solution for the Ising model and so can not be used for other values of \( Q \) or in three dimensions. The \( \mu TM \) is quite general and the algorithm itself requires less than 100 lines of code. In addition, it is straightforward to generalize the \( \mu TM \) to count
states with fixed energy and magnetization, or any other function of the Potts variables.

2 Results

The partition function for the Potts model maps into itself under the dual transformation

\[ u \rightarrow \frac{1}{u}, \]

(7)

where

\[ u = \frac{y^{-1} - 1}{\sqrt{Q}}. \]

(8)

In the complex \( u \)-plane a subset of the zeros of the partition function tend to lie on a unit circle (which maps into itself under (7)); however, cylindrical and periodic boundary conditions are not self-dual, and this causes the zeros to move slightly off the unit circle. For this reason we have modified the \( \mu TM \) for the self-dual lattice introduced by Wu et al. [11], so that the zeros do indeed lie on the unit circle and therefore are simply parameterized by the phase \( \theta \).

In the complex \( x \)-plane the zeros of the partition function for the Ising model are guaranteed to lie on the unit circle by the circle theorem of Lee and Yang [2], irrespective of the boundary conditions.

Given that the zeros are well parameterized by a single variable, we can define the density of zeros for finite lattices as

\[ g\left(\frac{1}{2}(\theta_{k+1} - \theta_k)\right) = \frac{1}{N} \frac{1}{\theta_{k+1} - \theta_k}. \]

(9)

In Fig.1 we show the density of zeros in the complex-\( x \) plane for the Ising model at \( y = y_c \) and \( y = 0.5y_c \). Note that at the critical temperature \( g \) tends to zero as one approaches the real axis, but below the critical temperature it approaches a constant

\[ 2\pi g(0, y) = m_0(y), \]

(10)

where \( m_0(y) \) is the spontaneous magnetization. We have applied finite-size scaling to the density of zeros calculated in this way and find excellent agreement with the exact solution for the magnetization except close to the critical point where crossover complicates the FSS analysis. There is reason to hope that a more sophisticated FSS analysis will improve these results substantially.

Finally, in Fig.2 we show the density of zeros in the complex \( y \)-plane for the 3-state Potts model, which is known to have a second-order transition at the critical point.
3 Conclusions

The \( \mu T M \) and its extensions offer a new way of obtaining exact information about finite two dimensional lattices. While the method is easily extended to three dimensions, memory requirements limit its use to the 2-state model on \( 4^2 \times L \) lattices. However, Monte Carlo techniques have been developed\([12]\) which have no such limitations and show great promise in extending many of these results to larger lattices. Preliminary studies indicate that while most of the Yang-Lee zeros are very sensitive to the exact value of \( \Omega(E) \), the edge singularity and the next two nearest the critical point are not.

In addition, it is possible to generalize the \( \mu TM \) to calculate the microcanonical distribution of any function of the Potts variables, and in particular the order parameter and correlation function.

References

[1] C. N. Yang and T. D. Lee, Phys. Rev. 87, 404 (1952).
[2] T. D. Lee and C. N. Yang, Phys. Rev. 87, 410 (1952).
[3] R. Abe, Prog. Theor. Phys. 38, 72 (1967).
[4] M. Suzuki, Prog. Theor. Phys. 38, 1225 (1967).
[5] R. J. Creswick and S.-Y. Kim, Phys. Rev. E 56, 2418 (1997).
[6] R. J. Creswick, Phys. Rev. E 52, R5735 (1995).
[7] K. Binder, Physica 62, 508 (1972).
[8] G. Bhanot, J. Stat. Phys. 60, 55 (1990).
[9] R. B. Pearson, Phys. Rev. B 26, 6285 (1982).
[10] P. D. Beale, Phys. Rev. Lett. 76, 78 (1996).
[11] C.-N. Chen, C.-K. Hu, and F. Y. Wu, Phys. Rev. Lett. 76, 169 (1996).
[12] G. Bhanot, R. Salvador, S. Black, P. Carter, and R. Toral, Phys. Rev. Lett. 59, 803 (1987); K.-C. Lee, J. Phys. A 28, 4835 (1995); C. M. Care, \textit{ibid.} 29 L505 (1996); A. Pavel’yev, Ph.D. thesis, University of South Carolina, 1997 (unpublished).
Figure 1: Density of zeros in the complex $x$-plane for the Ising model for $L = 14$, cylindrical boundary conditions, for $y = y_c$ (filled circles) and $y = 0.5y_c$ (open triangles).
Figure 2: Density of zeros in the complex $y$-plane for the 3-state Potts model for $L = 10$, self-dual boundary conditions.