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許許與 模型的解析計算

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The transfer matrix method in the Fortuin-Kasteleyn representation has been used to calculate the partition function of the $q$-state Potts model for arbitrary (not necessarily integer) $q$ on lattice strips of fixed width and arbitrarily great length. We had extended the method for planar strips of the square, triangular and honeycomb lattices with free and cylindrical boundary conditions to cyclic and Möbius boundary conditions. Now we have succeeded in generalizing the method to non-planar strips with toroidal and Klein bottle strips by taking into account the rotational symmetry of these strips. Especially, the expression for the sum of coefficients is obtained, and the size of the transfer matrix is determined. In addition to the full-temperature $q$-state Potts model, the structure of the transfer matrix for the zero-temperature Potts antiferromagnet, i.e. the chromatic polynomial, is also obtained. In another direction, we introduced a novel method to derive the boundary-boundary correlation function for the rectangular Ising lattice strip with infinite length and finite width $L$. In the thermodynamic limit such that $L$ approaches to infinity, the boundary-boundary correlation function yields the square of the boundary spontaneous magnetization. We have also studied the asymptotic behavior of the boundary-boundary correlation function when the temperature is above, at, and below the critical temperature. As the nearest-neighbor correlation function could be derived in the same formalism, this provides a unified way to consider both long-range boundary correlation function and the short-range correlation function at once.

keywords:
Potts model, chromatic polynomial, Ising model, critical phenomena, boundary effect, exact solution
My research work has been in statistical mechanics. A major part of my research has been concerned with a very fundamental topic, namely, the phenomenon of nonzero ground state entropy. Physical examples of this include ice and certain other hydrogen-bonded molecular crystals. A particularly simple model exhibiting ground state entropy without the complication of frustration is the $q$-state Potts antiferromagnet for sufficiently large values of $q$. The Potts model [1] is a generalization of the Ising model, and has been a subject of central interest. The famous review paper [2] on this model given by Professor F. Y. Wu has been cited for more than a thousand times. This subject also has a deep connection with mathematical graph theory, since the $q$-state Potts model partition function $Z(G,q,v)$ on a lattice, or more generally, a graph $G$, is, up to a prefactor, the same as the Tutte-Whitney polynomial in modern mathematical graph theory [3-5], where $v$ is the temperature variable. Specifically, the zero-temperature partition function of the $q$-state Potts antiferromagnet is identical to the chromatic polynomial $P(G,q)$ [6-9]. This polynomial yields the number of ways of coloring the vertices of the lattice $G$ with $q$ colors such that no two adjacent vertices have the same color.

Together with my thesis advisor, Professor Robert Shrock, when I was a Ph.D. student in the C. N. Yang Institute for Theoretical Physics and Department of Physics and Astronomy at the State University of New York at Stony Brook, we obtained exact results for the zero-temperature partition functions of the $q$-state Potts antiferromagnet for several lattice strips of finite width and arbitrarily great length, with a variety of different boundary conditions, including free, cylindrical, cyclic, Möbius, toroidal, and Klein bottle [10-17]. Once the polynomial $P(G,q)$ is calculated, $q$ can be generalized from a positive integer to a complex variable. We calculated the zeros of $P(G,q)$, called chromatic zeros, for the strips of the square, triangular and honeycomb lattices. Since our exact results apply for arbitrary length, we were able to study the infinite-length limit in which a subset of these zeros accumulate to form curves, denoted $\mathcal{B}$, across which the degeneracy per site is nonanalytic. This is analogous to the generalization that Yang and Lee carried out of the magnetic field from real to complex values [18] and their study of the zeros of the Ising model partition function. Another analogy is to the corresponding generalization carried by M. E. Fisher of the temperature from physical to complex values and his study of the continuous accumulation set of Fisher zeros [19]. We found that although the thermodynamics of these infinite strips is quasi-one-dimensional, a disorder quantity such as the ground state degeneracy per site can, for even moderately large widths, be very close to its value for the infinite 2D lattice.

In a series of papers, we performed exact calculations of the full temperature-dependent partition function of the $q$-state Potts model, $Z(G,q,v)$ for arbitrary (not necessarily integer) $q$ on lattice strips of fixed width and arbitrarily great length, again with a variety of boundary conditions [20-27]. Our results apply for both the ferromagnetic and antiferromagnetic cases of the Potts model. With these exact results in hand, we went on to determine the singular locus $\mathcal{B}$ where the free energy is singular. This is now a complex hypersurface in the full $\mathbb{C}^2$ space spanned by the
variables \((q,v)\). We showed how the zeros of the partition function in the \(q\) plane for fixed \(v\) and in the \(v\) plane for fixed \(q\) accumulate to form this locus.

The transfer matrix method for lattice strips of the square and triangular lattices with free longitudinal boundary conditions and free or cylindrical transverse boundary conditions in the Fortuin-Kasteleyn representation was explained in detail by Salas and Sokal [28]. By using the bases for the chromatic polynomials in terms of the compatibility matrix [29-31], we succeeded in extending the method to cyclic and Möbius strips for various planar lattices, i.e., square, triangular and honeycomb lattices [32, 33]. We also proved a number of theorems concerning the general structure of the Potts model partition function for these strips with not just arbitrary length, but also arbitrary width \(L\) [13, 22, 25, 26]. The partition functions for cyclic strips can be written as

\[
Z(G,q,v) = \sum_{d=0}^{L} c^{(d)} \sum_{j=1}^{n_{Z,cyc}(L,d)} (\lambda_{Z,L,d,j})^{m},
\]

where \(m\) is the number of repeated subgraph in the longitudinal direction. We found the coefficient of degree \(d\) in \(q\) is \(c^{(d)} = U_{2d}(\sqrt{q} / 2)\), where \(U_{2d}(x)\) is the Chebyshev polynomial of the second kind. The transfer matrix has a block structure, and each block has the size \(n_{Z,cyc}(L,d)\) with \(\lambda_{Z,L,d,j}\) as its eigenvalues. Although the structure of the Potts model partition function for cyclic strips has been discussed by Saleur [34, 35] by a different approach, our results extend his to consider the structure of the chromatic polynomial for both cyclic and Möbius strips. In addition, our determination of the structure of the partition function for self-dual cyclic strips of the square lattice filled out the relevant Bratteli diagrams.

One purpose of the proposed project is to continue the research results given above. As we have already extended the transfer matrix method to cyclic and Möbius strips [32, 33], it is desirable to apply the method to toroidal and Klein bottle strips that are not planar and more difficult. I am happy to report here that we have succeeded in this extension, and the results are in press to be published in Physica A. For toroidal and Klein bottle strips, we knew the coefficient of degree \(d\) is not unique [14, 23, 36], in contrast to the coefficient for cyclic and Möbius strips. As the slice of the toroidal strips is a circle, the rotational symmetry should be taken into account. We found that the partition functions for toroidal strips can be written as

\[
Z(G,q,v) = \sum_{d=0}^{L} \sum_{j} b_{j}^{(d)} (\lambda_{Z,L,d,j})^{m},
\]

where there is only one coefficient \(b_{j}^{(d)}\) for both \(d=0\) and \(d=1\), but there are two coefficients for \(d=2\) and \(d=3\). The reason is due to the possible permutation of the color assignments for the bases. A set of \(d!\) eigenvalues should have their coefficients summed to be equal to \(b_{j}^{(d)}\) which can be determined by the sieve formula [29-31]. For \(d=0, 1, 2\), \(b_{j}^{(d)}\) are the same as \(c^{(d)}\), and
\[ b^{(d)} = c^{(d)} - c^{(d-1)} + (-1)^d c^{(1)} \] for \( d \) larger or equal to two. We have also determined the reduced size of the transfer matrix \( n_{Z_{\text{tor}}}(L,d) \) without the permutation of color assignments. For \( d \) equal to zero and one, \( n_{Z_{\text{tor}}}(L,0) = \frac{1}{L+1} \binom{2L}{L} \) and \( n_{Z_{\text{tor}}}(L,1) = \binom{2L-1}{L-1} \) that are obtained by the Narayana number, \( N(n,k) \), the number of partitions of size \( n \) with \( k \) components. For \( d \) equal to zero and one, \( n_{Z_{\text{tor}}}(L,0) = \binom{2L}{L} \) and \( n_{Z_{\text{tor}}}(L,1) = \sum_{d=0}^L n_{Z_{\text{cyc}}}(L,d') \) that is obtained through the comparison with the corresponding size of the transfer matrix for cyclic strips. When the longitudinal boundary condition is changed from toroidal to Klein bottle, the eigenvalues remain the same and we observed the changes of coefficients. Certain coefficients become zero for the Klein bottle strips so that the number of eigenvalues for Klein bottle strips always appears to be less than the number for the corresponding toroidal strips. We also worked out the corresponding results for the zero-temperature Potts antiferromagnet as follows. It is necessary that adjacent vertices are not assigned the same color for the chromatic polynomials. Denote the reduced size of the transfer matrix for the square and triangular lattices as \( n_{P_{\text{tor}}}(L,d) \). For \( d=0 \), \( n_{P_{\text{tor}}}(L,0) \) is the number of non-crossing non-nearest-neighbor partitions of \( L \) vertices on a circle, namely, the Riordan number. We found \( n_{P_{\text{tor}}}(L,1) = \sum_{k=1}^{\left\lfloor \frac{L}{2} \right\rfloor} \binom{L}{k} \binom{L-1-k}{k-1} \) that is obtained by the number of diagonal dissections of a convex \( n \)-gon into \( k \) regions. For \( d \) between two and \( L \), \( n_{P_{\text{tor}}}(L,d) \) is again obtained through the comparison with the corresponding size of the transfer matrix for cyclic strips. For a strip of the honeycomb lattice with toroidal boundary conditions, the width \( L \) must be even. In each transverse slice of the strip, the \( L \) vertices are connected in a pairwise manner. That is, compared with the square and triangular lattices, only half edges are kept. Denote the reduced size of the transfer matrix as \( n_{P_{\text{tor, hc}}}(L,d) \) without the permutation of the color assignments. \( n_{P_{\text{tor, hc}}}(L,0) \) is the same as the corresponding number \( n_{P_{\text{cyc, hc}}}(L,0) \) for cyclic strips. We found \( n_{P_{\text{tor, hc}}}(L,1) = \sum_{d=0}^{L-1} n_{P_{\text{cyc, hc}}}(L,d') \) and \( n_{P_{\text{tor, hc}}}(L,d) = \sum_{d'=0}^d n_{P_{\text{cyc, hc}}}(L,d') \) for \( d \) larger or equal to two. In addition to the above general structure results which apply to arbitrary width and length for the strips with toroidal boundary conditions, we also performed explicit calculations for the square and honeycomb lattices with \( L=4 \) and for the triangular lattice with \( L=3 \). These reduce to the zero-temperature partition function of the \( q \)-state Potts antiferromagnet that we had in Ref. [12].

I have been also working with Professor Masuo Suzuki, a world authority in statistical mechanics, with a new research direction, namely, the mesoscopic phenomena in infinite systems. It is intriguing to study the mesoscopic phenomena in infinite systems. That is, impose a perturbative
interaction on only a part of an infinite system, but keep the size of the affected part infinite. The result is then compared with both macroscopic and microscopic phenomena. It is well known that the Ising model is one of the simplest models in the study of critical phenomena since Onsager’s celebrated work on the free energy of the rectangular lattice without magnetic field [37], followed by Yang’s derivation of the spontaneous magnetization [38]. One interesting direction is to study boundary effects in an infinite system, and the approach of the boundary result to the bulk result. In Ref. [39], we calculated the long-range correlation functions of the rectangular Ising model between two spins on the same row along the direction with free boundary conditions. Expressing the final result as a low-temperature series expansion with the same spin-spin couplings in both directions and applying D Log Padé approximant to the series [40], we showed that if one spin is on the $m$-th row from one boundary, and the other spin is on the $n$-th row from the other boundary, their long-range correlation function is the product of the corresponding $m$-th and $n$-th row spontaneous magnetizations. In terms of low-temperature series expansions, the approach of the correlation function between two $m$-th row spins to the bulk correlation function could be understood as follows: the dominant terms of their series expansions are the same and the number of these terms increases monotonically as $m$ increases.

One purpose of the proposed project is to investigate a special mesoscopic phenomenon, the boundary effect of an infinite system where the size of boundaries is infinite. In collaboration with Professor Masuo Suzuki and his student (now postdoc) Hidenori Suzuki, we proposed a novel method to derive the boundary-boundary correlation function. The results have been published in Journal of Mathematical Physics, 46, 1 (2005). Consider the rectangular Ising lattice strip with infinite length and finite width $L$ and ferromagnetic interactions. Take periodic boundary condition in the horizontal direction and free boundary conditions in the transverse direction, then impose a topological spin-spin interaction $J'$ between the spins on the free boundaries. The boundary-boundary correlation function $C_L$ is essentially the derivative of the free energy with respect to $J'$, followed by taking the limit $J'=0$. When the width $L$ approaches to infinity, the boundary-boundary correlation function is equal to square of the boundary spontaneous magnetization $m_b$ given by McCoy and Wu [41] as expected. Furthermore, we determined the asymptotic behavior of the boundary-boundary correlation functions as follows.

When the temperature is above the critical temperature $T_c$, $C_L$ is proportional to $e^{-L/\xi}/\sqrt{L}$, where $\xi$ is the same as the ordinary correlation length with exponent $\nu=1$. At the critical temperature, we found $C_L$ is proportional to $1/L$. It becomes more complicated when the temperature is below $T_c$ and we found that $C_L - m_b^2$ is proportional to $e^{-L/\xi}$. As temperature is low, it is interesting to note that $C_L$ is nonmonotonic with respect to the width $L$. On the other hand, $L$ approaching to infinity limit can be taken first before the limit $J'=0$. We found these two limits are interchangeable for the two-dimensional rectangular lattice. That is, if $L$ approaching to infinity is taken first for the two-dimensional lattice, then the limit $J'=0$ gives the same long-range boundary-boundary correlation function. Furthermore, after the infinite $L$ limit if $J'$ is taken to be
the regular spin-spin interaction, we rederived the ordinary nearest-neighbor correlation function [42, 43]. That is, $J'$ changes the topology of the system according to its value. If $J'$ is not equal to zero, we have the short-range correlations; while for $J'=0$, we have the long-range boundary-boundary correlations for the two-dimension lattice. This procedure was checked first on the Ising chain by imposing a topological spin-spin interaction $J'$ between the edge spins. It is straightforward to calculate the partition function of this Ising chain for non-zero magnetic field and we compared the boundary magnetization where a magnetic field only applies on an edge spin with the uniform magnetization per site where the magnetic field applies to all the spins.

References:
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In retrospect, the main projects proposed were completed in the due period. We have succeeded in generalizing the transfer matrix method in the Fortuin-Kasteleyn representation to the strips of the square, triangular and honeycomb lattices with toroidal and Klein bottle boundary conditions. The structure of the transfer matrix was obtained for both the full-temperature $q$-state Potts model and the zero-temperature Potts antiferromagnet, i.e. the chromatic polynomial. Now the method is very general to be applied to both planar and non-planar two-dimensional lattice strips with all the boundary conditions. We also proposed to investigate the special interval $0 \leq q \leq 4$ when the phase transition for two-dimension lattices is known to be second-order from a high-temperature paramagnetic phase to a low-temperature phase with ferromagnetic long-range order. The result is out of our expectation, and this work is still in progress. In another direction, we introduced a novel method to derive both the nearest-neighbor and boundary-boundary correlation functions for the rectangular Ising lattice strip with infinite length and finite width $L$. The thermodynamic limit, infinite $L$, is interchangeable with the topological spin-spin interaction $J'=0$ to give the long-range boundary-boundary correlation function. We also showed the asymptotic behavior of the boundary-boundary correlation function for large $L$ when the temperature is above, at, and below the critical temperature.