The Potts Model and Tutte Polynomial, and Associated Connections Between Statistical Mechanics and Graph Theory

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Introduction

Some Results from Statistical Physics

Statistical physics deals with properties of many-body systems. Description of such systems uses a specified form for the interaction between the dynamical variables. An example is magnetic systems, where the dynamical variables are spins located at sites of a regular lattice Λ; these interact with each other by an energy function called a Hamiltonian $\mathcal{H}$.

Simple example: a model with integer-valued (effectively classical) spins $\sigma_i = \pm 1$ at sites i on a lattice Λ, with Hamiltonian

$$\mathcal{H} = -J_I \sum_{e_{ij}} \sigma_i \sigma_j - H \sum_i \sigma_i$$

where J_I is the spin-spin interaction constant, e_{ij} refers to a bond on Λ joining sites i and j, and H is a possible external magnetic field. This is the Ising model.

Let T denote the temperature and define $\beta = 1/(k_B T)$, where $k_B = 1.38 \times 10^{-23}$ J/K $= 0.862 \times 10^{-4}$ eV/K is the Boltzmann constant. Consider a many-body system at thermal equilibrium at a temperature T.

A useful function in the description of this system is the partition function, which involves a sum over all of the possible spin configurations of $e^{-\beta\mathcal{H}}$:

$$Z = \sum_{\sigma_i} e^{-\beta\mathcal{H}} = \sum_{\sigma_i} \exp[K_I \sum_{e_{ij}} \sigma_i\sigma_j + h_I \sum_i \sigma_i]$$

where $K_I = \beta J_I$ and $h_I = \beta H$. If $J_I > 0$ (i.e., ferromagnetic, FM), the spin-spin interaction favors parallel spin configurations, while if $J_I < 0$ (antiferromagnetic, AFM), this interaction favors configurations in which neighboring spins are antiparallel. An external H favors σ to be in the direction of H.

Consider a regular d-dimensional lattice Λ. Define the thermodynamic limit as the limit in which the number of lattice sites $n \to \infty$ and the volume of this lattice goes to infinity. In this limit, we define the reduced dimensionless free energy (per site) as

$$f = \lim_{n\to\infty} \frac{1}{n} \ln Z$$

The Gibbs free energy (per site) $G(T, H) = -k_B T f$. The function f (or equiv. G) encodes much information about the system; partial derivatives yield various thermodynamic functions. For example,

$$\frac{\partial f}{\partial \beta} = -U, \quad \frac{\partial f}{\partial h} = M,$$

etc., where $U =$ internal energy and $M =$ magnetization (per site).

Phase Transitions

If $H = 0$ (i.e. no external magnetic field), the Hamiltonian is invariant under a global $\mathbb{Z}_2$ symmetry group containing the identity and the spin reversal operation, $\sigma_i \to -\sigma_i \; \forall \; i$. The presence of $H \neq 0$ breaks this symmetry explicitly.

On the infinite (thermodynamic) limit of a regular lattice of dimension $d \geq 2$, at sufficiently low temp. T, the zero-field ($H = 0$) Ising FM has a phase transition as T decreases below a certain value, T_c, involving spontaneous symmetry breaking (SSB) of the $\mathbb{Z}_2$ symmetry associated with the onset of ferromagnetic long-range order, i.e., a nonzero net magnetization. The high-temp., $\mathbb{Z}_2$-symmetric phase is the paramagnetic (PM) phase with $M = 0$, while the low-temp. phase with SSB of $\mathbb{Z}_2$ is the FM phase with $M \neq 0$.

If $J < 0$, then, depending on lattice Λ, there may also be a phase transition from the high-temp. PM phase to a low-temp. phase with AFM long-range order.

Thermodynamic functions behave nonanalytically as T passes through T_c; for example, in the Ising FM, the magnetization M is identically zero if $T > T_c$ and is a nonzero function for $0 \leq T < T_c$.

$G(T, 0)$ was calculated in closed form for the $H = 0$ Ising model on the square lattice by Onsager in 1944 and later for other 2D lattices (triangular, honeycomb, etc.), but it has never been calculated for regular lattices with $d \geq 3$. For $H \neq 0$, $G(T, H)$ has never been calculated for regular lattices with $d \geq 2$.

Zeros of Partition Function

Up to a prefactor, the Ising model partition function is a polynomial in the variables $y = e^{2K_I}$ and $\mu = e^{2h_I}$. An interesting question concerns the locations of the zeros of Z in the complex y plane for a given μ and in the complex μ plane for a given y. (We will also use the equivalent variable $v = y - 1$.)

Consider the zeros in the y plane for $H = 0$, i.e., $\mu = 1$. As $n \to \infty$, there is usually a merging of zeros to form curves. For example, for the square lattice, these are two circles of radius $\sqrt{2}$ (M. Fisher, 1965):

$$|y \pm 1| = \sqrt{2}$$

This locus of curves is invariant under (i) complex conjugation, since the coefficients of each term in y are real; (ii) inversion, $y \to 1/y$, reflecting a $K \to -K$ symmetry on a bipartite lattice, and (iii) $y \to -y$, reflecting the even vertex degree (coordination number).

These curves cross the real axis at $y_{PM-FM} = \sqrt{2} + 1$ and $y_{PM-AFM} = 1/y_{PM-FM} = \sqrt{2} - 1$, defining three physical phases in this square-lattice Ising model:

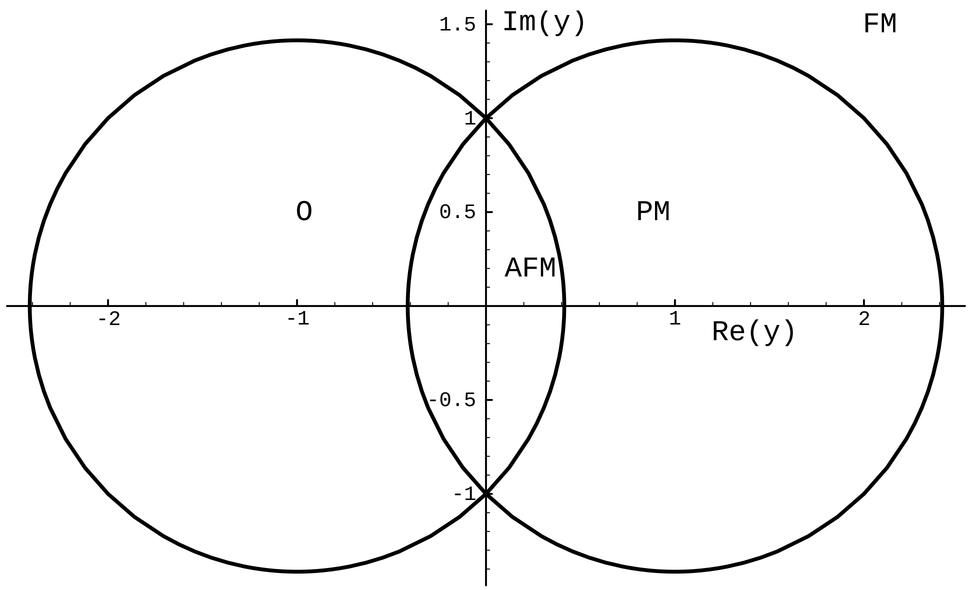


Figure 1: Locus $\mathcal{B}_y$ in the $y = e^{2K_I} = e^K$ plane for the $q = 2$ Potts model (= Ising model) on the square lattice.

1. PM: $y_{PM-AFM} \le y < y_{PM-FM}$, i.e., $0.414 < y < 2.414$
2. FM: $y > y_{PM-FM}$, i.e., $y > 2.414$
3. AFM: $0 \le y < y_{PM-AFM}$, i.e., $0 \le y < 0.414$

These physical phases have complex-y extensions as bounded by the curves $|y \pm 1| = \sqrt{2}$.

Special points:

1. The point $y = 1$ $(v = 0)$, i.e., $K = 0 \;\Leftrightarrow\;$ infinite temp., $\beta = 0$.
2. The point $y = \infty$ $(v = \infty)$, i.e., $K = \infty \;\Leftrightarrow T = 0$ with $J > 0$ (FM sign of coupling).
3. The point $y = 0$ $(v = 0)$, i.e., $K = -\infty \;\Leftrightarrow\; T = 0$ with $J < 0$ (AFM sign of coupling)

There are also two crossings at complex-temperature points, $-(\sqrt{2} \pm 1)$. The circles intersect each other at two complex-conjugate multiple points, $y = \pm i$.

The $y \to -y$ symmetry is incorporated via a conformal mapping to the variable $\eta = y^2$. In this variable, the image of the two circles is a limaçon-type curve that crosses the real η axis at $\eta_{PM-FM} = 3 + 2\sqrt{2}$, $\eta_{PM-AFM} = 1/\eta_{PM-FM} = 3 - 2\sqrt{2}$, and $\eta = -1$.

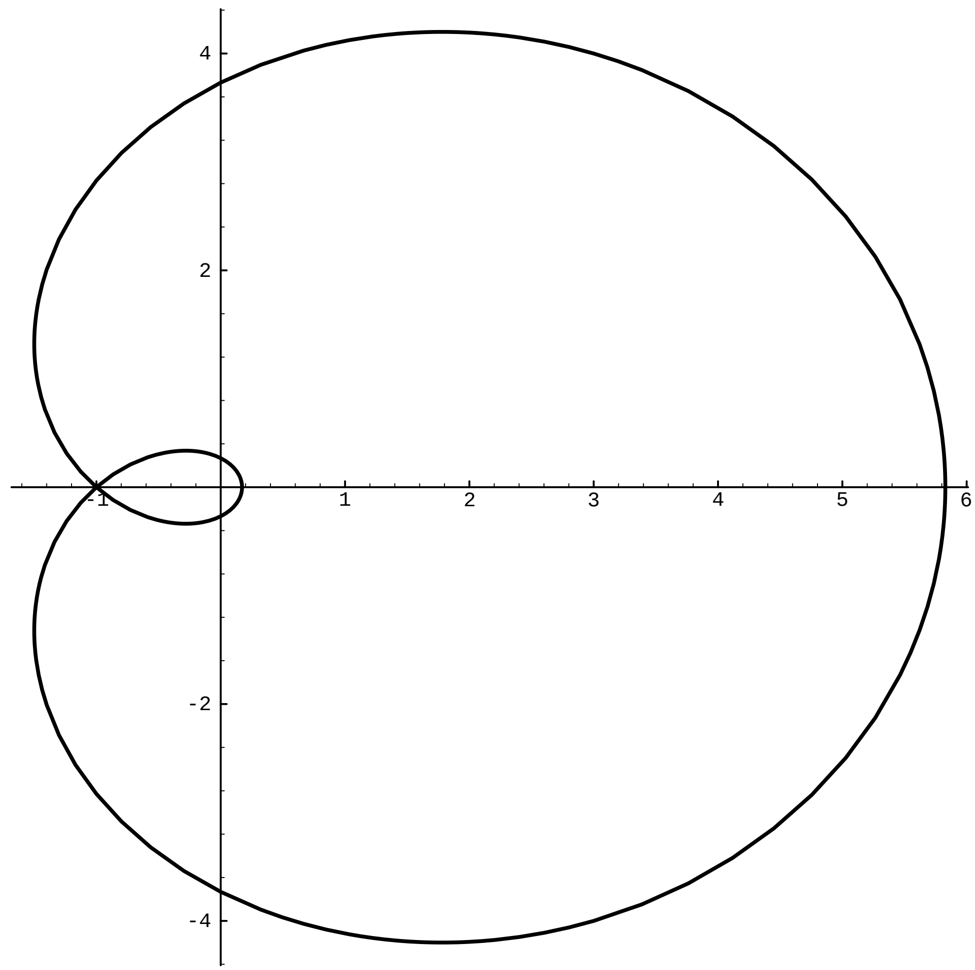


Figure 2: Locus $\mathcal{B}_\eta$ in the η plane for the $q = 2$ Potts model (= Ising model) on the square lattice.

(Matveev and Shrock, J. Phys. A28, 1557-1583 (1995)). One can also carry out this study of zeros and their accumulation sets $\mathcal{B}$ in the $n \to \infty$ limit for other lattices. We have done this for a number of different lattices (see refs. at end of Lecture 2).

Just as one learns more about functions of a real variable by considering their extension to functions of a complex variable, so also it is worthwhile to consider the complex-temperature extensions of physical phases. Although zeros usually merge to form algebraic curves, we showed that they do not always do this; for the 4-8-8 heteropolygonal lattice (vertex-transitive tiling of the plane with regular squares and octagons), they merge to form areas, which cross the real z axis at points (V. Matveev and R. Shrock, J. Phys. A 28, 5235-5256 (1995)).

For $H \neq 0$, it is also of interest to consider zeros of Z in the μ plane. T. D. Lee and C. N. Yang initiated this study in 1952 and showed that in the FM (but not AFM) case, the zeros of the Ising model partition function in the μ plane occur on arcs of the unit circle $|\mu| = 1$. On regular lattices, in the limit $n \to \infty$, these merge to form a continuous (self-conjugate) arc $\mathcal{B}_\mu$ on this circle.

For $T = \infty$, these are all at $\mu = -1$; on lattices where there is a PM-FM phase transition, as T decreases toward T_c, the arcs move out from $\mu = -1$ and pinch the positive real μ axis at $\mu = 1$ as T decreases below T_c. They remain on this closed unit circle $|\mu| = 1$ for $0 \le T < T_c$. For much of our discussion below, we will take $H = 0$.

One may generalize the analysis by considering the model on a graph G which is not necessarily a regular lattice. Here $G = G(V, E)$, where V is the set of vertices (= sites) and E is the set of edges (= bonds). The number of vertices is denoted $n = n(G) = |V|$ and the number of edges as $e(G) = |E|$. The number of disjoint components of G is $k(G)$.

We will also be interested in families of graphs that can be defined iteratively (recursively), such as (i) line graphs with n vertices; (ii) circuit graphs C_n with n vertices, (iii) ladder graphs, (iv) strips of regular lattices of length L_x vertices and width L_y vertices, etc. with various longitudinal and transverse boundary conditions (free, periodic, twisted periodic (Möbius), Klein-bottle).

Other families of graphs of interest are hierarchical graphs, e.g., Sierpinski, Diamond Hierarchical (DHL), such that the $(m+1)$'th member of a family is derived from the m'th by a specified operation. Work by P. Bleher, M. Lyubich, R. Roeder for DHL ...

Potts Model Partition Function, Tutte Polynomial, and Special Cases

An important further generalization in statistical mechanical spin models is as follows: in the Ising model, the variable σ_i can take on two values. In the above formulation, these are ± 1, and equivalently, they could be enumerated as 1,2. In the Potts model, the integer-valued variables located at each site on the lattice can take on q values rather than just two: $\sigma_i \in \{1, ..., q\}$, with the Hamiltonian

$$\mathcal{H} = -J \sum_{e_{ij}} \delta_{\sigma_i \sigma_j}$$

The Potts model partition function is then (with $K = \beta J$)

$$Z = \sum_{\{\sigma_i\}} e^{-\beta \mathcal{H}} = \sum_{\{\sigma_i\}} e^{K \sum_{e_{ij}} \delta_{\sigma_i \sigma_j}} = \sum_{\{\sigma_i\}} \prod_{e_{ij}} e^{K \delta_{\sigma_i \sigma_j}}$$

where $\delta_{\sigma_i \sigma_j}$ is the Kronecker delta. Here the spin-spin energy function takes on the two values 0 and J (in conventional Ising formulation, $\pm J_I$). The $q = 2$ Potts model is thus equivalent to the Ising model with $J = 2J_I$. The $J > 0$ and $J < 0$ cases define the Potts ferromagnet (FM) and antiferromagnet (AFM).

On the (thermodynamic limit of) 2D lattices, the Potts model has a continuous order-disorder phase transition for $q = 2,\ 3,\ 4$ with known critical exponents (universality classes). For general q, the Gibbs free energy $G(T, 0)$ of the Potts model has never been calculated exactly (in closed form) even for $H = 0$ on any regular lattice with $d \geq 2$.

One can reexpress the Potts model partition function on a graph G as a sum over contributions from spanning subgraphs of G without explicit reference to the sum over spin configurations. Define $v = y - 1$, so $0 \leq v < \infty$ for the FM case and $-1 \leq v \leq 0$ for the AFM case.

Def. A spanning subgraph G' of G is $G' = (V, E')$ with $E' \subseteq E$, i.e., it has the same vertices and a subset of the edges of G. (Recall $y = e^K$.) Observe that

$$e^{K\delta_{\sigma_i \sigma_j}} = 1 + (e^K - 1)\delta_{\sigma_i \sigma_j} = 1 + v\delta_{\sigma_i \sigma_j}$$

So $Z = \sum_{\{\sigma_i\}} \prod_{e_{ij}} (1 + v\delta_{\sigma_i \sigma_j})$. This can be reexpressed as

$$Z(G, q, v) = \sum_{G' \subseteq G} q^{k(G')} v^{e(G')}$$

where $k(G')$ = no. of connected components in G' and $e(G')$ = no. of edges in G'.

If G is the disjoint union $G = G_1 \cup G_2$, then $Z(G, q, v) = Z(G_1, q, v)Z(G_2, q, v)$ so, without loss of generality, we can take G to be connected.

The (Fortuin-Kastelyen) cluster representation shows that $Z(G, q, v)$ is a polynomial in q and v with positive integer coefficients for each term. Further, it allows one to generalize q from nonnegative integers to real (or complex) numbers.

The proof of this cluster formula is based on the 1-1 correspondence between the terms in $Z = \sum_{\{\sigma\}} \prod_{e_{ij}} (1 + v\delta_{\sigma_i\sigma_j})$ and spanning subgraphs $G' \subseteq G$.

Sketch of proof, using, as illustration, $G = C_3$, where C_n is the circuit graph with n vertices. Here

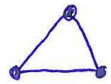
$$Z(C_3, q, v) = \sum_{\{\sigma_i\}} \prod_{e_{ij}} (1 + v\delta_{\sigma_i\sigma_j}) = \sum_{\{\sigma_i\}} (1 + v\delta_{\sigma_1\sigma_2})(1 + v\delta_{\sigma_2\sigma_3})(1 + v\delta_{\sigma_3\sigma_1})$$

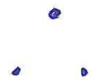
There are four types of terms that contribute:

- the term 1, corresponding to the G' with three disjoint vertices, no edges, (so $e(G') = 0$, $k(G') = 3$), for which the sum over the σ_i's yields q^3, i.e., one can choose the σ's independently in q^3 ways;

Example: $G = C_3$

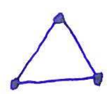
$G' = (V', E')$

$G =$  $\rightarrow$ $2^3 = 8$ resultant spanning subgraphs with $V' = V$ with $E' \subseteq E$ (don't confuse V and v)

 $k = 3$, $e = 0$ $\Rightarrow$ q^3

 $k = 2$, $e = 1$ $\Rightarrow$ $3q^2 v$

 $k = 1$, $e = 2$ $\Rightarrow$ $3qv^2$

 $k = 1$, $e = 3$ $\Rightarrow$ qv^3

$$\Rightarrow Z(C_3, q, v) = q^3 + 3q^2 v + 3qv^2 + qv^3$$
$$= (q+v)^3 + (q-1)v^3$$

This generalizes to

$$Z(C_n, q, v) = (q+v)^n + (q-1)v^n$$

- $v(\delta_{\sigma_1\sigma_2} + \delta_{\sigma_2\sigma_3} + \delta_{\sigma_3\sigma_1})$, corresponding to the three G's with one edge and one disjoint vertex, so $e(G') = 1$, $k(G') = 2$. The first of these terms contributes if $\sigma_1 = \sigma_2$; here one chooses $\sigma_1 = \sigma_2$ in any of q ways, and then σ_3 independently in any of q ways, for a total of q^2 ways; similarly for the other two terms, so these terms contribute $3q^2v$;
- $v^2(\delta_{\sigma_1\sigma_2}\delta_{\sigma_2\sigma_3} + \delta_{\sigma_2\sigma_3}\delta_{\sigma_3\sigma_1} + \delta_{\sigma_3\sigma_1}\delta_{\sigma_1\sigma_2})$, corresponding to G's with two edges, so $e(G') = 2$, $k(G') = 1$. For the first term to contribute, all of the σ's must be equal, and there are q ways of choosing them; similarly for the other two terms, so the total contribution is then $3qv^2$;
- $v^3(\delta_{\sigma_1\sigma_2}\delta_{\sigma_2\sigma_3}\delta_{\sigma_3\sigma_1})$, corresponding to $G' = G$, with all edges present, so $e(G') = 3$, $k(G') = 1$. For this term to contribute, all of the σ's must be equal, amounting to q possibilities, and yielding the term qv^3.

So combining all of these terms, one gets $Z(C_3, q, v) = q^3 + 3q^2v + 3qv^2 + qv^3$, which is precisely $\sum_{G' \subseteq C_3} q^{k(G')}v^{e(G')}$.

One can also express these terms in the form $Z(C_3, q, v) = (q + v)^3 + (q - 1)v^3$.

By the same methods, one obtains $Z(C_n, q, v) = (q + v)^n + (q - 1)v^n$ for general n.

Here we define two important graph-theoretic polynomials:

Def. The chromatic polynomial $P(G, q)$ is the number of ways of assigning q colors to the vertices of G such that no two adjacent vertices have the same color. This is called a proper q-coloring of (the vertices of) G. The minimum number of colors needed for a proper q-coloring of G is the chromatic number, $\chi(G)$.

In the antiferromagnetic Potts model, consider the limit $T \to 0$, so $K \to -\infty$ (since $K = \beta J$ and $J < 0$) and $v = e^K - 1 \to -1$. In this limit, the only spin configurations that contribute to $Z(G, q, v = -1)$ are those for which adjacent spins have different values. Hence, the $T = 0$ limit of the Potts antiferromagnet partition function is the chromatic polynomial:

$$Z(G, q, -1) = P(G, q)$$

Def. The Tutte (also called Tutte-Whitney) polynomial of a graph G is

$$T(G, x, y) = \sum_{G' \subseteq G} (x-1)^{k(G') - k(G)} (y-1)^{c(G')}$$

where $c(G')$ denotes the number of (linearly independent) cycles in G'. Note that $c(G) = e(G) + k(G) - n(G)$.

The Potts model partition function is equivalent to the Tutte polynomial. Let

$$x = 1 + \frac{q}{v}\,, \qquad y = v + 1 = e^K,$$

so $q = (x-1)(y-1)$ and $v = y-1$. Then, using the fact that $n(G') = n(G)$, so $c(G') = e(G') + k(G') - n(G)$, we have

$$\begin{aligned} T(G,x,y) &= (x-1)^{-k(G)} \sum_{G' \subseteq G} (x-1)^{k(G')}(y-1)^{c(G')} \\ &= (x-1)^{-k(G)} \sum_{G' \subseteq G} \left(\frac{q}{v}\right)^{k(G')} v^{e(G')+k(G')-n(G)} \\ &= (x-1)^{-k(G)}(y-1)^{-n(G)} \sum_{G' \subseteq G} q^{k(G')} v^{e(G')} \\ &= (x-1)^{-k(G)}(y-1)^{-n(G)} Z(G,q,v) \end{aligned}$$

i.e., with $x - 1 = q/v$ and $y - 1 = v$,

$$Z(G,q,v) = (q/v)^{k(G)} v^{n(G)} T(G,x,y)$$

This equivalence between $Z(G, q, v)$ and $T(G, x, y)$ is an important connection between statistical mechanics and mathematical graph theory. The Tutte polynomial encodes much information about a graph.

Special valuations of $T(G, x, y)$ count various types of subgraphs of G. Setting $x = 1$ in $T(G, x, y)$ restricts the G's that contribute to those that are connected, i.e., $k(G') = k(G) = 1$. Setting $y = 1$ restricts the G's that contribute to those having no cycles, so that $c(G') = 0$.

Def. A connected graph with no cycles is a tree. Setting $x = y = 1$ picks out G's that are connected spanning subgraphs with no cycles, i.e., spanning trees. So

$$T(G, 1, 1) = N_{ST}(G)$$

Def. A spanning subgraph G' with no cycles is a spanning forest of G. One can relax the restriction on connectedness by setting $x = 2$, so that $(x - 1)^{k(G')-k(G)} = 1$, independent of $k(G')$. Then

$$T(G, 2, 1) = N_{SF}(G)$$

where $N_{SF}(G)$ is the number of spanning forests of G.

One can keep the restriction on connectedness but include G's with cycles by setting $y = 2$; then $(y-1)^{c(G')} = 1$ independent of $c(G')$. Hence

$$T(G, 1, 2) = N_{CSSG}(G)$$

where N_{CSSG} is the number of connected spanning subgraphs of G.

If one sets $x = y = 2$, then the summand is just 1, so this counts all of the spanning subgraphs of G. This is enumerated by noting that all of the vertices are present, but each edge may be present or absent, a 2-fold choice. So

$$T(G, 2, 2) = N_{G' \subseteq G} = 2^{e(G)}$$

Special cases of the Tutte polynomial yield many graph-theoretic functions of interest.

We will focus on one of these special cases here, namely the chromatic polynomial $P(G,q)$. We have shown that for $v=-1$, $Z(G,q,v)$ is equal to this polynomial, i.e., $Z(G,q,-1)=P(G,q)$. Now $v=-1$ means $y=0$ and $x=1-q$, so, using the $Z-T$ relation,

$$P(G,q)=(-q)^{k(G)}(-1)^{n(G)}T(G,x=1-q,y=0)$$

Graph coloring has long been of interest in mathematical graph theory; early work by Birkhoff and Whitney, subsequent work by Tutte, Read, and many others.

The chromatic polynomial is of interest not just in graph theory but also in applied mathematics and engineering. One application is the following frequency allocation problem. Consider n radio broadcast transmitter stations; let each of these be represented by a vertex of a graph G and define two transmitters as being adjacent (joined by a edge) if they are closer than a certain distance to each other. Then assign frequencies from a set of q values to these transmitters, subject to the condition that adjacent stations should use different frequencies to avoid interference. The number of ways of doing this is $P(G,q)$.

Some Easy Cases

We mention some cases of graphs and/or values of q, v, where the calculation of $Z(G,q,v)$ or $P(G,q) = Z(G,q,-1)$ is easy.

At $q = 0$, since $k(G') \ge 1$, all terms vanish and hence $Z(G,0,v) = 0$. Since Z is a polynomial, this means that $Z(G,q,v)$ always has an overall factor of q.

At $v = 0$ (i.e., $\beta = 0$, infinite temperature), all terms in the cluster formula with $e(G') \ge 1$ vanish, and the only term that remains is for the G' consisting of n disjoint vertices, E_n (the "empty" graph), so $Z(G,q,0) = q^n$. The same result holds for any v if G itself is E_n.

At $q = 1$, in the Hamiltonian form, the Kronecker delta functions $\delta_{\sigma_i \sigma_j} = 1$ for all edges e_{ij}, since all $\sigma' s$ have the same value, and hence, with $y = e^K$,

$$Z(G,1,v) = y^{e(G)} = (v+1)^{e(G)}$$

As $v \to \infty$ (infinitely strong ferromagnetic coupling J or $T \to 0$ for finite $J > 0$, so $K \to \infty$), all spins prefer to be aligned, so $Z(G,q,v) \to q y^{e(G)} = q(v+1)^{e(G)}$.

Def. The complete graph K_n is the graph with n vertices such that each pair of vertices is connected by an edge (so $e(K_n) = \binom{n}{2}$).

Then by a simple combinatoric argument, $P(K_n, q) = \prod_{j=0}^{n-1}(q - j)$.

This follows since one uses one color for the first vertex, which can be chosen in any of q ways; then one must use a different color for the second vertex, which can be chosen in any of $q - 1$ ways, and so forth up to the n'th vertex. So, e.g., $P(K_3, q) = q(q - 1)(q - 2)$. In general, $\chi(K_n) = n$.

Def. A loop is an edge that connects a vertex to itself. Thus this vertex is adjacent to itself via such a loop. Since adjacent vertices must have different colors in a proper q-coloring of the vertices of G, this is not possible if G contains any loops, and hence $P(G, q)$ vanishes identically if G contains one or more loops.

If and only if G is bipartite, i.e., $G = G_1 \bigoplus G_2$, where each vertex in G_1 has only adjacent vertices in G_2 and vice versa, then $P(G, 2) = 2$, since there are two ways to perform a proper 2-coloring of G. Iff G is k-partite, then $P(G, k) = k!$; e.g., triangular lattice is tripartite: $P(tri, 3) = 3!$.

Corresponding results hold for $T(G, x, y)$.

Calculational Methods

Let $G - e$ denote the graph G with the edge e deleted and let G/e denote the graph G with the edge e deleted and the two vertices which it connected identified, i.e., G contracted on the edge e. $Z(G, q, v)$ satisfies a deletion-contraction relation (DCR),

$$Z(G, q, v) = Z(G - e, q, v) + vZ(G/e, q, v)$$

This can be seen from the Hamiltonian representation of $Z(G, q, v)$ and is equivalent to the identity (for $e = e_{ij}$) $\exp(K\delta_{\sigma_i \sigma_j}) = 1 + v\delta_{\sigma_i \sigma_j}$; there are two possibilities: the two σ's on the vertices joined by the edge e are (i) different, in which case Z is the same as if this edge were removed, corresponding to the 1; or (ii) the σ's are the same, which is accounted for by the $v\delta_{\sigma_i \sigma_j}$ term in the above identity.

For example, consider $G = C_4$, with $Z(C_4, q, v) = (q + v)^4 + (q - 1)v^4$. Now, for any edge e, $C_4 - e = T_4$, and $Z(T_4, q, v) = q(q + v)^3$. Contracting on e gives $C_4/e = C_3$, and $Z(C_3, q, v) = (q + v)^3 + (q - 1)v^3$. The RHS of the DCR is then

$$Z(T_4, q, v) + vZ(C_3, q, v) = q(q + v)^3 + v\Big[(q + v)^3 + (q - 1)v^3\Big]$$

which equals $(q + v)^4 + (q - 1)v^4 = Z(C_4, q, v)$, the LHS of the DCR.

From the DCR for $Z(G, q, v)$, there follows a DCR for $P(G, q) = Z(G, q, -1)$:

$$P(G, q) = P(G - e, q) - P(G/e, q)$$

i.e., $P(G - e, q) = P(G, q) + P(G/e, q)$. This has a combinatoric interpretation: labelling the two vertices connected by the edge e as v_i and v_j, this relation expresses the fact that in the proper q-coloring of $H = G - e$, if the colors assigned to v_i and v_j are denoted $\mathrm{color}(v_i)$ and $\mathrm{color}(v_j)$, then there are precisely two (disjunct) possibilities:

1. $\mathrm{color}(v_i) \neq \mathrm{color}(v_j)$, which is equivalent to the situation in which there is an edge connecting these vertices (since this requires that these colors be different), as enumerated by $P(G, q)$, and
2. $\mathrm{color}(v_i) = \mathrm{color}(v_j)$, which is equivalent to the situation in which these vertices are the same, as enumerated by $P(G/e, q)$.

There is a corresponding DCR for $T(G, x, y)$. For E_n, $T(E_n, x, y) = 1$. Def.: an edge in G is a bridge iff removing it increases the number of components, k. If $e = e_b$ is a bridge, $T(G - e_b, x, y) = xT(G/e_b, x, y)$; if $e = e_\ell$ is a loop, then $T(G - e_\ell, x, y) = yT(G/e_\ell, x, y)$. If e is not a bridge or a loop, then

$$T(G, x, y) = T(G - e, x, y) + T(G/e, x, y)$$

For example, again consider the circuit graph C_4, for which $T(C_4, x, y) = x + x^2 + x^3 + y$, $C_4 - e = T_4$, and $T(T_4, x, y) = x^3$; $C_4/e = C_3$, and $T(C_3, x, y) = x + x^2 + y$. The RHS of the DCR is then $x^3 + (x + x^2 + y)$, which is equal to the LHS.

By the use of the DCR, one can calculate $Z(G, q, v)$ in terms of the Z's of graphs with one less edge, namely $G - e$ and G/e, the latter of which also has one less vertex. One can use the DCR iteratively to calculate $Z(G, q, v)$ in terms of smaller graphs. Similar comment for $T(G, x, y)$.

Some Simple Examples

We next give some simple examples of calculation of $Z(G,q,v)$, $T(G,x,y)$, and $P(G,q)$:

Denote a tree graph with n vertices as T_n. Since $e(T_n) = n-1$, one has $T(T_n,x,y) = x^{n-1}$. Then, since $k(T_n) = 1$ and $n(T_n) = n$, one can use the $Z-T$ relation to calculate $Z(T_n,q,v)$ as follows (with $x = 1 + (q/v)$)

$$Z(T_n,q,v) = (q/v)v^n T(T_n,x,y) = qv^{n-1}\Big(1+\frac{q}{v}\Big)^{n-1} = q(q+v)^{n-1}$$

Illustration of use of DCR to obtain this: $T_2 - e = E_2 = \bullet \ \ \bullet$ and $T_2/e = T_1 = E_1 = \bullet$, so with $Z(E_n) = q^n$,

$$Z(T_2) = Z(E_2) + vZ(E_1) = q^2 + vq = q(q+v)$$

Iterating, we get (with $T_n - e = T_{n-1} \bullet$ and $Z(T_{n-1} \bullet) = Z(T_{n-1})Z(\bullet)$)

$$Z(T_n) = Z(T_{n-1})Z(E_1) + vZ(T_{n-1}) = (q+v)T(T_{n-1}) = q(q+v)^{n-1}$$

Note that for $n \geq 4$, there is more than one different tree graph; for example, for $n = 4$, there are two such graphs: the path graph L_4 and the star graph, S_4 (a central vertex with three outer vertices connected to it). As this shows, although $T(G, x, y)$ and $Z(G, q, v)$ encode information about a graph, two different graphs can have the same $T(G, x, y)$ and $Z(G, q, v)$.

For a circuit graph C_n, we have shown that $Z(C_n, q, v) = (q + v)^n + (q - 1)v^n$. Using $x - 1 = q/v$ and $q = (x - 1)(y - 1)$, we can write this as

$$Z(C_n, q, v) = v^n \Big[\Big(1 + \frac{q}{v} \Big)^n + (q - 1) \Big] = v^n \Big[x^n + (q - 1) \Big]$$

$$= (q/v) v^n \Big[\frac{x^n + (q - 1)}{x - 1} \Big]$$

and hence we have

$$T(C_n, x, y) = \Big[\frac{x^n + (xy - y - x)}{x - 1} \Big]$$

where C_1 is a single vertex with loop, so $T(C_1, x, y) = y$.

N.B.: The factor $1/(x - 1)$ is always cancelled so that $T(G_m, x, y)$ is a polynomial in x and y.

For $n \geq 2$, using $(x^n - x)/(x-1) = \sum_{j=1}^{n-1} x^j$, one can write $T(C_n, x, y)$ as

$$T(C_n, x, y) = \Big(\sum_{j=1}^{n-1} x^j\Big) + y$$

Setting $v = -1$ in the results for $Z(G, q, v)$ yields $P(G, q)$. For example,

$$P(T_n, q) = q(q-1)^{n-1}$$

$$P(C_n, q) = (q-1)^n + (q-1)(-1)^n = q(q-1)D_n(q)$$

where

$$D_n(q) = \sum_{j=0}^{n-2} (-1)^j \binom{n-1}{j} q^{n-2-j}$$

so $D_2 = 1$, $D_3 = q - 2$, $D_4 = q^2 - 3q + 3$, etc.

Using the deletion-contraction relation, one progressively reduces the number of edges in the graphs that enter into the calculation. However, for an arbitrary graph, using the DCR does not reduce the complexity of the calculation since, in general, at each step one is doubling the number of terms, leading to an exponential increase in the time of the calculation with $e(G)$.

In Lecture 2, we will consider some families of graphs for which the DCR can be used to calculate $Z(G, q, v)$ obtaining new exact results.

Partition Function Zeros and their Accumulation Sets as $n \to \infty$

Just as the zeros of $Z(G, q, v)$ in the plane of the temperature-dependent variable v, or equivalently, $y = v + 1$, for fixed q, and their accumulation set in the $n \to \infty$ limit, denoted $\mathcal{B}_v$, are of interest, so also the zeros of $Z(G, q, v)$ in the complex q plane for fixed v, and their continuous accumulation set $\mathcal{B}_q$, are of interest. Specific important case: zeros of the chromatic polynomial, $P(G, q)$, called chromatic zeros.

We have calculated (i) $Z(G, q, v)$ for general q and v (equivalently, $T(G, x, y)$) and (ii) $P(G, q)$ for a variety of families of graphs for arbitrarily large n and have studied the limit $n \to \infty$. We denote this limit on a particular family of graphs, e.g., lattice strip graphs with fixed width L_y, arbitrary length L_x, and a given set of boundary conditions, as $\{G\}$ and the resultant functions (i) f and (ii) W as $f(\{G\}, q, v)$ and $W(\{G\}, q)$.

In particular, for $T = 0$ Potts AFM, $W(\{G\}, q)$ can exhibit nonanalytic behavior for one or more values of q where the singular locus $\mathcal{B}_q$ in the complex q plane crosses the real q axis. We denote the largest such value as $q_c(\{G\})$.

Viewing the singular locus as a subvariety in the $\mathbb{C}^2$ space of variables (q, v), when $q_c(\{G\})$ is a positive integer, this is equivalent to the singular locus $\mathcal{B}_v$ in the complex v plane of the q-state Potts antiferromagnet crossing the real v axis at $v = -1$, i.e., at $T = 0$, so that this q_c-state Potts AFM has a zero-temperature critical point. Examples:

1. $q_c = 2$ for $n \to \infty$ limit of cyclic graph $\iff$ Ising ($q = 2$ Potts) AFM has $T_c = 0$ (and, since sq. lattice is bipartite, also equiv. to Ising FM having $T_c = 0$ here).
2. $q_c = 3$ for infinite square lattice $\iff$ $q = 3$ Potts AFM has $T_c = 0$ on square lattice; We also find this to be true for self-dual families of square-lattice graphs.
3. $q_c = 4$ for infinite triangular lattice $\iff$ $q = 4$ Potts AFM has $T_c = 0$ on triangular lattice;

Illustrative calculation of $\mathcal{B}_v$ and $\mathcal{B}_q$ for a given limit $\{G\}$. Let us consider the family of circuit graphs C_n. We have

$$Z(C_n, q, v) = (q+v)^n + (q-1)v^n = \lambda_0^n + (q-1)\lambda_1^n$$

where $\lambda_0 = q + v$ and $\lambda_1 = v$.

In the $n \to \infty$ limit, denoted $\{C\}$, one or the other of these λ's will generically have a larger magnitude than the other and hence will dominate the limit, so that the reduced free energy

$$f = f(\{C\}, q, v) = \lim_{n\to\infty} \frac{1}{n} \ln Z(C_n, q, v)$$

is $f = \ln(q+v)$ in the region $|q+v| > |v|$ and $f = \ln v$ in the region $|v| > |q+v|$. On the boundary curve separating these two regions, f changes form nonanalytically. The limits $n \to \infty$ and $q \to 1$ do not commute; we discuss this more generally later.

This boundary curve is given by the condition of equality in magnitude of the two λ's, namely $|q+v| = |v|$. Since zeros of $Z(C_n, q, v)$ occur where the two (dominant) λ's are equal in magnitude, enabling cancellation, this is also the continuous accumulation set of zeros of $Z(C_n, q, v)$ as $n \to \infty$.

In the complex v plane, the locus of solutions to the condition $|q+v| = |v|$, $\mathcal{B}_v$, is the infinite vertical line $v = -(q/2) + ir$, $-\infty < r < \infty$, which crosses the real-v axis at $v = -q/2$. Equivalently, in the y plane, this is the infinite vertical line $\mathcal{B}_y$: $y = 1 - (q/2) + ir$.

Although this locus is noncompact in the y plane, it is compact in the $z = y^{-1}$ plane, where, for $q \neq 2$, it is the circle

$$\left| z + \frac{1}{q-2} \right| = \frac{1}{|q-2|}$$

Evidently, this circle is centered at $z = -1/(q-2)$ with radius $1/|q-2|$, which crosses the real z axis at $z = 0$ and $z = -2/(q-2)$. If $q = 2$, this locus is the imaginary z axis.

The solution to $|q+v| = |v|$ in the complex q plane, $\mathcal{B}_q$, is the circle centered at $q = -v$ with radius $|v|$. This crosses the real q axis at $q = -2v$ and $q = 0$. In particular, for the chromatic polynomial, for which $v = -1$, this is the circle $|q-1| = 1$ centered at $q = 1$, passing through $q = 0$ and $q = 2$. Thus, $q_c = 2$ in this chromatic-polynomial case.

In Lecture 2 we will discuss more complicated examples.

Chromatic polynomials and Ground State Entropy of Potts AFM

A quantity of particular interest is the ground state degeneracy, per site, of the Potts antiferromagnet,

$$W(\{G\}, q) = \lim_{n\to\infty} P(G, q)^{1/n}$$

The associated ground state entropy per site is $S_0 = k_B \ln W$.

The q-state Potts antiferromagnet at $T = 0$ is noteworthy as a system that, for a given type of graph G and sufficiently large q, exhibits nonzero ground state entropy (per site) S_0, or equivalently, $W > 1$.

There are physical systems that exhibit this type of residual low-temperature entropy, such as water ice, for which $W = 1.51$, i.e., the entropy per molecule is $S_0/k_B = 0.41$. This is due to the fact that ice is a hydrogen-bonded molecular crystal and there is a twofold possibility for the H atom in each hydrogen bond, to be closer to one oxygen or the other. Even with the constraint of local electric neutrality, this produces exponentially many ground state configurations of equal (minimal) energy, and hence a finite ground state entropy of ice.

Note that both of these cases, this entropy does not involve frustration; i.e., each spin-spin contribution to the energy is minimal.

Simple proof of $S_0 > 0$ for the Potts antiferromagnet on a bipartite graph $G_{bp.}$ for $q > 2$. An elementary lower bound on $P(G, q)$ is obtained by assigning one color to all of the vertices on the even sublattice, which can be done in any of q ways. Then independently for each vertex on the odd sublattice, one can choose the color in any of $q - 1$ ways. Therefore,

$$P(G_{bp,}, q) \geq q(q-1)^{n/2}$$

Hence, for $n \to \infty$, one has $W(\{G\}, q) \geq \sqrt{q-1}$ and

$$S_0 \geq (k_B/2) \ln(q-1)$$

So for $q > 2$, there is nonzero ground state entropy per site.

Historical Note on Graph Coloring

The early interest by Birkhoff and Whitney in chromatic polynomials was motivated by their connection with the map coloring problem, i.e. face-colorings of planar graphs.

Def. a proper q-coloring of the faces of a graph is an assignment of colors, from a set of q colors, to the faces of a graph such that no two adjacent faces (faces that share an edge) have the same color.

For a planar graph G, there is a 1-1 correspondence between the vertices of G and the faces of the planar dual graph G^*. Therefore, $P(G, q)$ equivalently counts the proper q-colorings of the vertices of G and the proper q-colorings of the faces of G^*.

Def. An edge of G which, if cut, would increase the number of components of G by 1 is called a bridge. A bridge in G leads to a face being adjacent to itself across the bridge. Since adjacent faces must have different colors in a proper q-coloring of the faces of a planar graph G^*, this is not possible if G^* contains any bridges.

The Four-Color Theorem is the statement that if G is a planar graph with no loops, so G^* is a planar graph with no bridges, then $P(G, 4) > 0$, i.e., there exists a proper q-coloring of the vertices of G with $q = 4$ colors, or equivalently, there exists a proper q-coloring of the faces of G^* with $q = 4$ colors.

Conclusions

- Important connection between the Potts model in statistical mechanics and the Tutte polynomial in mathematical graph theory.
- $T = 0$. Potts antiferromagnet partition function is identical to the chromatic polynomial relevant for graph coloring.
- We have given some calculational methods and simple examples.
- Worthwhile to study pattern of zeros of $Z(G, q, v)$ in v plane for fixed q and in q plane for fixed v. Merging of these zeros produces curves in the $n \to \infty$ limit; locations where these cross the real v or real q axis are physically significant.
- Including external magnetic field, one can carry out a similar study for the zeros in the complex μ plane.
- Connection of $P(G, q)$ with ground-state entropy per site of Potts AFM.
- Thus, study of the properties of the Potts model partition function and Tutte polynomial on various families of graphs, together with the asymptotic behavior as $n \to \infty$, involves interesting confluence of statistical physics, graph theory, combinatorics, complex analysis, and algebraic geometry. Many opportunities for further work.