The Potts model and Graphs Theory

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Outline

Some questions that I will attempt to answer, at least partially, are:

- Where does the Potts model come from?
- Why the Potts model?
- How is the Potts model related to graph/knot theory?

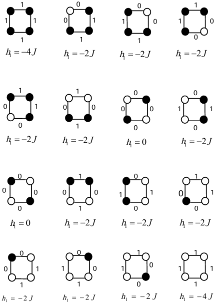
A little Statistical Mechanics

- Time evolution is encoded in a quantity called the Hamiltonian $\mathcal{H}$ (which in most cases can be thought of as energy).
- The kinetic energy term of Hamiltonians usually is not of interest, so it is ignored leaving only the potential energy term.
- The Potts model Hamiltonian can be defined on a graph as a sum over its edges E, with a function along each vertex $\sigma(v_i) \in \{1, \ldots, q\}$ along with an exchange constant $J \in \mathbb{R}$.

$$\mathcal{H} = -J \sum_{v_i, v_j \in E} \delta(\sigma(v_i), \sigma(v_j))$$

A little Statistical Mechanics

We may as well label each vertex with q colors instead of q natural numbers. The Potts Hamiltonian then becomes $-J \cdot (\#$edges not properly colored by $\sigma)$, where an edge E is properly colored when $\sigma(v_1) \neq \sigma(v_2)$ for $v_1, v_2 \in E$.



(figure from Beaudin 2007)

A little Statistical Mechanics

Statistical physics studies the properties of very large systems ($\sim 10^{23}$ vertices) using the partition function defined as the following sum over all possible states S of the system:

$$\mathcal{Z} = \sum_{S} e^{-\beta \mathcal{H}(S)}$$

Where β is the inverse of temperature: $\frac{1}{k_b T}$.

- In the case of the potts model, a state is a choice of coloring for all vertices.
- Since the relative probability of a system being in state S' is $e^{-\beta \mathcal{H}(S')}$ the probability of a state is

$$P(S') = \frac{e^{-\beta \mathcal{H}(S')}}{\sum_S e^{-\beta \mathcal{H}(S)}} = \frac{e^{-\beta \mathcal{H}(S')}}{\mathcal{Z}}$$

A little Statistical Mechanics

The partition function is important because it allows the computation of the expected values for useful quantities. Suppose a quantity A is given by the derivative of the hamiltonian w.r.t some parameter α, $A(S) = \frac{\partial \mathcal{H}(S)}{\partial \alpha}$:

$$\langle A \rangle = \sum_S P(S)A(S) = \frac{1}{\mathcal{Z}} \sum_S \frac{\partial \mathcal{H}(S)}{\partial \alpha} e^{-\beta \mathcal{H}(S)}$$

$$= \frac{-1}{\beta} \frac{1}{\mathcal{Z}} \frac{\partial}{\partial \alpha} (\sum_S e^{-\beta \mathcal{H}(S)}) = \frac{-1}{\beta} \frac{1}{\mathcal{Z}} \frac{\partial}{\partial \alpha} (\mathcal{Z}) = \frac{\partial}{\partial \alpha} (-\frac{\ln(\mathcal{Z})}{\beta})$$

$F := -\frac{\ln(\mathcal{Z})}{\beta} = -k_b T \ln(\mathcal{Z})$ is called the free energy and derivatives with respect to parameters gives the expected values for quantities of interest (e.g. magnetization, energy, moments of distribution, etc.)

A little Statistical Mechanics

It is worth noting the asymptotic behavior of the probabilities of each state as $T \to 0^+$ (low T) and $T \to \infty$ (high T):

- At low T ($\beta \to \infty$), for a state of minimum energy S_{min} and a state that is not a minimum S, $\frac{e^{-\beta\mathcal{H}(S)}}{e^{-\beta\mathcal{H}(S_{\text{min}})}} \to 0$
- Each minimum energy state will be equiprobable and the probability of any other state is 0, meaning the system settles in it's lowest energy state.
- At high T ($\beta \to 0$), $e^{-\beta\mathcal{H}(S)} \to 1$ for all states. Meaning every state is equiprobable.
- This aligns with the intuitive notion that temperature "scrambles" a system and causes disorder.

A little Statistical Mechanics

One reason why it is useful to distinguish between $J > 0$ (ferromagnetic ordering) and $J < 0$ (antiferromagnetic ordering) in the Potts model is that they have different qualitative behavior as demonstrated by the $T \to 0$ limit:

- When $J > 0$ the energy decreases with the number of non-properly colored edges, the minimum energy states will have the same color at every vertex and $\mathcal{Z}(q) = q$
- When $J < 0$ the energy decreases with the number of properly colored edges, so assuming the number of proper colorings is non-zero $\mathcal{Z}(q) = \chi(q)$ where $\chi(q)$ is the chromatic polynomial.
- Lattices with $\chi(q) = 0$ are called "frustrated" and have been heavily studied from both physical and mathematical standpoints.

A little Statistical Mechanics

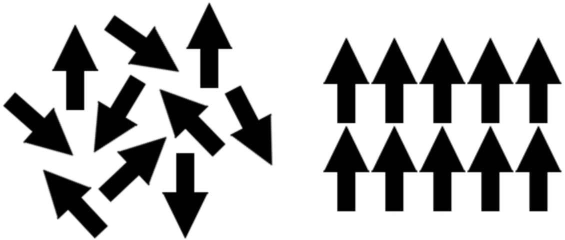
A typical question in statistical mechanics describing sudden changes in the behavior of matter called phase transitions (Boiling, Freezing, etc.).

- Phase transitions correspond to some kind of non-analyticity.
- Assuming $\mathcal{H}$ is analytic and G is finite, $\mathcal{Z}$ is analytic because it is the finite sum of analytic functions.
- Phase transitions are only well defined in infinite systems and are regions of non-analyticity in the vertex averaged free energy f in the "thermodynamic limit". ($-k_b T$ in this context will be ignored because it is analytic)

$$f := \lim_{k \to \infty} \frac{\ln(\mathcal{Z}_{G_k})}{\nu(G_k)}$$

A little Statistical mechanics

The phase transition we will be interested in is the ferromagnetic "order-disorder" transition, discovered by Pierre Curie in 1895. He discovered that below a certain temperature (Curie Temperature) some materials retain a magnetization in the absence of a magnetic field (spontaneous magnetization):



Ising Model

- The Ising model is a model for spontaneous magnetic ordering investigated by Ernest Ising in 1924, created and given to him by his advisor Wilhelm Lenz.
- The Ising Hamiltonian on a graph is a sum over it's edges E, described by spins at each vertex $\sigma(v_i) \in \{-1, 1\}$, along with a exchange constant $J \in \mathbb{R}$:

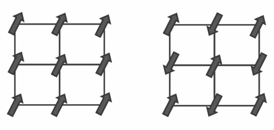
$$\mathcal{H} = -J \sum_{v_i, v_j \in E} \sigma(v_i)\sigma(v_j)$$

  or with magnetic field h included:

$$\mathcal{H} = -J \sum_{v_i, v_j \in E} \sigma(v_i)\sigma(v_j) - h \sum_{v_i} \sigma(v_i)$$

- Since $\delta(\sigma(v_i), \sigma(v_j)) = \frac{1}{2}(1 + \sigma(v_i)\sigma(v_j))$ the $h = 0$ Ising model is equivalent to the $q = 2$ Potts model.

Ising Model



The Ising model the interaction of electron "spins" and a number of assumptions are made and effects ignored:

- The electron's "spin" is restricted to a single axis.
- The atoms reside on a regular lattice/material is crystalline.
- Only short range "nearest-neighbor" interactions are taken into account. (no domain or hysterisis)
- Electrons are assumed to be "tightly bound" to their atoms.
- Magnetic contributions from the nucleus, electron's orbit and confounding effects from interaction are ignored.

Ising Model

It is important to keep in mind the Ising model was only meant to investigate the relationship between ferromagnetism (magnetic ordering) and local magnetic interactions:

- The model should be as simple as possible math can actually be done.
- Treating each atom individually would not lead to any non-analyticity (trivial thermodynamic limit).
- Heuristically, the nucleus is much heavier than the electron so it "spins" slower.
- By the Bohr-van Leeuwen theorem classical physics (Newton's laws and Electromagnetism) can't describe magnetism, thus some quantum effect such as spin is necessary.
- "Exchange interaction" is dominant, being proportional to $-\vec{s}_i \cdot \vec{s}_j$

Ising Model

The crudeness of the model does not limit it’s usefulness and actually part of the reason why it’s useful:

- From "universality", behavior of many systems near certain types (continuous) phase transition depend on broad characteristics, like symmetry.
- Due to possible asymmetry in crystalline lattices, it is possible that one direction of spin is heavily favored.
- Simple, yet retains the many important features of statistical mechanical systems.

Ising Model

- Ising solved his model in the 1 dimensional lattice case and found no phase transition. He incorrectly extrapolated this result to higher dimension.
- In 1933 Peierls gave a argument for the existence of an order-disorder phase transition when $D \geq 2$.
- In 1941 Kramers and Wannier use a duality argument to give the exact critical temperature for a 2D square lattice.
- This culminated with Onsager's celebrated closed form solution to the 2D Ising model on a 2D square lattice with $h = 0$ published in 1944.
- No closed form solution to the Ising model in 2D for $h \neq 0$ or for cubic lattice with $D \geq 3$ has been found since then.

Ising Model

Work on the Ising model and it's generalizations have been very influential:

- The 2024 Nobel Prize in physics was awarded to Hopfield and Hinton for their work involving the application of the Sherrington-Kirkpatrick model for "spin glasses" (The Ising model but on a symmetric graph and J is a random variable that changes by edge) to machine learning.
- The 2024 Abel Prize was awarded to Michel Talagrand partly for his work on a rigorous solution to the Sherrington-Kirkpatrick model.

Ising Model

Work done on the Ising model has also had it's impact on Knot theory.

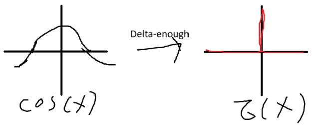
- "Transfer matrices" introduced by Kramers and Wannier, and used by Onsager inspired "Temperley-Lieb algebras".
- Vaughan Jones found the Jones polynomial in his study of this algebra.
- Kauffman introduced Dirac's bracket notation to knot theory in analogy with this algebra.
- The partition function is a knot invariant, and in particular Type III Reidemeister moves correspond to the "star-triangle" relation that Onsager suggested in his 1944 paper. (See Adam's Knot book ch. 7)

Potts Model

Renfrey Pott's advisor Cyril Domb suggested a model that is now known as the "clock" or "vector Potts" model with the Hamiltonian:

$$\mathcal{H} = -J \sum_{v_i, v_j \in E} \cos\left(\frac{2\pi(\sigma(v_i) - \sigma(v_j))}{q}\right)$$

Potts had trouble finding the critical points of this model for $q > 4$ so he simplified the model to what's known today.



(Wu 1982) discusses historical details and gives a interpretation of the Potts model using a $q - 1$ dimension hypertetrahedron.

Potts Model

Experimental realizations of the Potts model in physics relies on "universality". Applications of the model have spread outside of physics:

- Flocking of birds.
- Tumor growth.
- Image processing.
- Foam behavior.
- Social clustering.

Dichromatic Polynomial

- The relationship between the Potts Model partition function and the Tutte polynomial was first noticed by Fortuin and Kastelyn (1972) investigating contraction-deletion relations on variety of systems along side the potts model (electric resistor networks, percolation)
- Fortuin and Kastelyn generalize the ferromagnetic Potts model along with the aformentioned systems to "Random-Cluster models"

Dichromatic Polynomial

Recall that the dichromatic polynomial of graph G, Z_G can be defined as a sum over the q-colorings S. If we define $u(S) := \{\#$ edges that are not properly colored$\}$ then:

$$Z_G(q, v) = \sum_S (1+v)^{u(S)}$$

since $\mathcal{H}(S) = -Ju(S)$, the partition function $\mathcal{Z}_G$ is related to the dichromatic polynomial by the substitution $v = e^{\beta J} - 1$

$$Z_G(q, e^{\beta J} - 1) = \sum_S (e^{\beta J})^{u(S)} = \sum_S e^{\beta J u(S)} = \sum_S e^{-\beta \mathcal{H}(S)} = \mathcal{Z}_G(q)$$

A contraction-deletion proof can be found in (Beaudin 2007, Adam's Knot book ch.8).

Dichromatic Polynomial

Recall that the Dichromatic polynomial is related to the Tutte polynomial $T_G(x, y)$ through a change of variables (with $\kappa(G)$ and $r(G)$ being the number of connected components and rank of G):

$$Z_G(q, v) = q^{\kappa(G)} v^{r(G)} T_G(1 + qv^{-1}, 1 + v)$$

This leads to the following relation between the Tutte polynomial and the q-Potts partition function:

$$\mathcal{Z}_G(q) = q^{\kappa(G)}(e^{\beta J} - 1)^{r(G)} T_G(1 + \frac{q}{e^{\beta J} - 1}, e^{\beta J})$$

Dichromatic Polynomial

Since $x = 1 + \frac{q}{e^{\beta J}-1}$ and $y = e^{\beta J}$, $(x-1)(y-1) = q$ so the Potts partition function is the specialization of the Tutte polynomial on such hyperbola. This leads to the following table from (Welsh and Marino 2000):

Q-state Potts	Tutte polynomial
Ferromagnetism	Positive branch H_Q^+ of H_Q
Antiferromagnetism	Negative branch H_Q^- of H_Q restricted to $y>0$
High temperature both ferromagnetic and antiferromagnetic	Portion of H_Q asymptotic to $y=1$
Low temperature ferromagnetic	H_Q^+ asymptotic to $x=1$
Absolute zero antiferromagnetic	$x=1-Q,\ y=0$

Duality

The Tutte polynomial can be defined with the relations:

$$T_{\bullet} = 1$$
$$T_{G_1 \sqcup G_2} = T_{G_1} \cdot T_{G_2}$$
$$T_G = xT_{G/e}, e \text{ is a bridge}$$
$$T_G = yT_{G\backslash e}, e \text{ is a loop}$$
$$T_G = T_{G/e} + T_{G\backslash e}, e \text{ is not a loop or bridge}$$

To see how this changes under planar duality, recall deletion and contraction are adjoint in the sense that duality interchanges them:

$$(G/e)^* = (G^* \backslash e^*)$$
$$(G\backslash e)^* = (G^* / e^*)$$

Duality

So the Tutte-Polynomial relations become under duality:

$$T_{\bullet} = 1$$

$$T_{G_1^* \sqcup G_2^*} = T_{G_1^*} \cdot T_{G_2^*}$$

$$T_{G^*} = xT_{G^* \setminus e^*}, \; e^* \text{ is a loop}$$

$$T_{G^*} = yT_{G^* / e^*}, \; e^* \text{ is a bridge}$$

$$T_{G^*} = T_{G^* \setminus e^*} + T_{G^* / e^*}, \; e^* \text{ is not a loop or bridge}$$

therefore:

$$T_G(x, y) = T_{G*}(y, x)$$

Duality

(Kazhakov 2024) makes a connection between Tutte duality and the Kramers-Wannier duality equation, defining the dual of β, β^* satisfying the following equation:

$$T_G(1 + \frac{q}{e^{\beta J} - 1}, e^{\beta J}) = T_{G^*}(1 + \frac{q}{e^{\beta^* J} - 1}, e^{\beta^* J})$$
$$\Rightarrow (e^{\beta J} - 1)(e^{\beta^* J} - 1) = q$$

This leads to the following questions:

- How is the Tutte duality connected to the duality of Kramers and Wannier between high and low temperature expansions?
- How can generalized dualities be used with the Potts model on non-planar graphs?

Duality

This relation can also be applied to find the critical temperature of a square lattice. Defining G_k as a square lattice with $k \times k$ vertices, the free energy per vertex in the thermodynamic limit f is:

$$f(\beta, q) = \lim_{k\to\infty} \frac{\ln(\mathcal{Z}_{G_k}(\beta, q))}{\nu(G_k)} = \lim_{k\to\infty} (\kappa(G_k)\ln(q) + r(G_k)\ln(e^{\beta J} - 1) + \ln(T_{G_k}(1 + \frac{q}{e^{\beta J} - 1}, e^{\beta J})))$$

Because the first 2 terms are analytic, the regions of non-analyticity of $f(\beta, q)$ are the regions of non-analyticity of:

$$\tilde{f}(\beta, q) := \lim_{k\to\infty} \frac{\ln(T_{G_k}(1 + \frac{q}{e^{\beta J}-1}, e^{\beta J}))}{\nu(G_k)}$$

Duality

And on G_k^* (notice that $\lim_{k\to\infty} G_k = \lim_{k\to\infty} G_k^*$) the reduced free energy can be defined similiary:

$$\tilde{f}^*(\beta, q) := \lim_{k\to\infty} \frac{\ln(T_{G_k^*}(1 + \frac{q}{e^{\beta J}-1}, e^{\beta J}))}{\nu(G_k^*)}$$

because of time constraints the following lemma will not be proved:

Lemma (Kazakhov 2024)

$$\tilde{f}^*(\beta, q) - \ln(q) = \tilde{f}(\beta, q)$$

Duality

By the definition of β^*:

$$\lim_{k\to\infty} \frac{\ln(T_{G_k}(1+\frac{q}{e^{\beta J}-1}, e^{\beta J}))}{\nu(G_k)} = \lim_{k\to\infty} \frac{\nu(G_k^*)}{\nu(G_k)} \frac{\ln(T_{G_k^*}(1+\frac{q}{e^{\beta^* J}-1}, e^{\beta^* J}))}{\nu(G_k^*)}$$
$$= \lim_{k\to\infty} \frac{\ln(T_{G_k^*}(1+\frac{q}{e^{\beta^* J}-1}, e^{\beta^* J}))}{\nu(G_k^*)}$$

so by the definitions of $\tilde{f}, \tilde{f}^*$ and the previous lemma:

$$\tilde{f}(\beta, q) = \tilde{f}^*(\beta^*, q) = \tilde{f}(\beta^*, q) + \ln(q)$$

so if there is a phase transition at β_c, there is also one at β_c^*.

Duality

Assuming there is only one phase transition (uniqueness hypothesis) then $\beta_c = \beta_c^*$ meaning the critical temperature can be calculated from:

$$(e^{\beta_c J} - 1)^2 = q$$

(Beffara and Duminil-Copin 2011) prove a similiar result using random cluster models.

- Can a similar result for non-planar graphs be obtained using generalized dualities?

Misc

A number of relationships (that I find interesting) exist between the graph theory and the Potts model that haven't been mentioned. Some of them are:

- Through the Lee-Yang theorem zeroes of the Dichromatic polynomial are related to phase transitions in the Potts model.
- A specialization of the Tutte polynomial called the flow polynomial which is related to the "random current expansion" of the Ising model.
- The colored Tutte polynomial is associated with the Random cluster model.

Misc

- Many applications of the potts model include an external magnetic field, the Potts-Tutte connection in this case has been extended using the V-polynomial. What insights come from this connection?
- Penrose-Kauffman polynomial corresponds to Potts model partition function at imaginary β. Finding implications of this is an open question.
- The presentation uses a minimally quantum approach (because most quantum effects will not matter for continuous phase transitions). Can the Potts model in the full quantum mechanical formalism be used to define a corresponding "Quantum" Tutte polynomial?

Acknowledgement

I would like to thank Dr. Ilya Gruzberg for many useful discussions regarding phase transitions and teaching me condensed matter physics.

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