From Potts to Tutte and back again...
A graph theoretical view of statistical mechanics

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The Ising Model

1925—(Lenz)

Consider a sheet of metal:

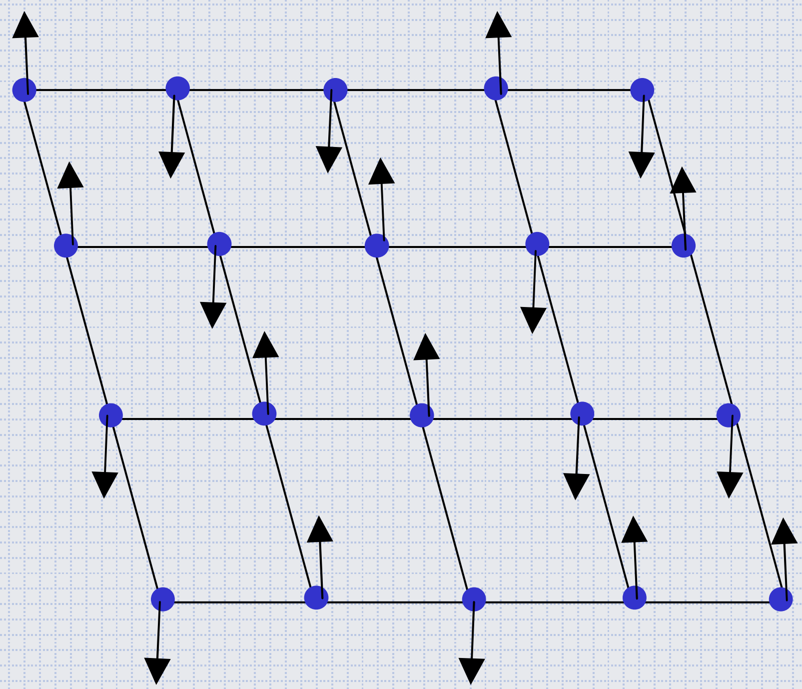
It has the property that at low temperatures it is magnetized, but as the temperature increases, the magnetism "melts away".

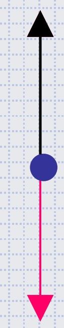
We would like to model this behavior. We make some simplifying assumptions to do so.

- The individual atoms have a "spin", i.e., they act like little bar magnets, and can either point up (a spin of +1), or down (a spin of –1).
- Neighboring atoms with different spins have an interaction energy, which we will assume is constant.
- The atoms are arranged in a regular lattice.

One possible state of the lattice

A choice of ‘spin’ at each lattice point.





$q = 2$

Ising Model has a choice of two possible spins at each point

The Kronecker delta function and the Hamiltonian of a state

Kronecker delta-function is defined as:

$$\delta_{a,b} = \begin{cases} 0 & \text{for } a \neq b \\ 1 & \text{for } a = b \end{cases}$$

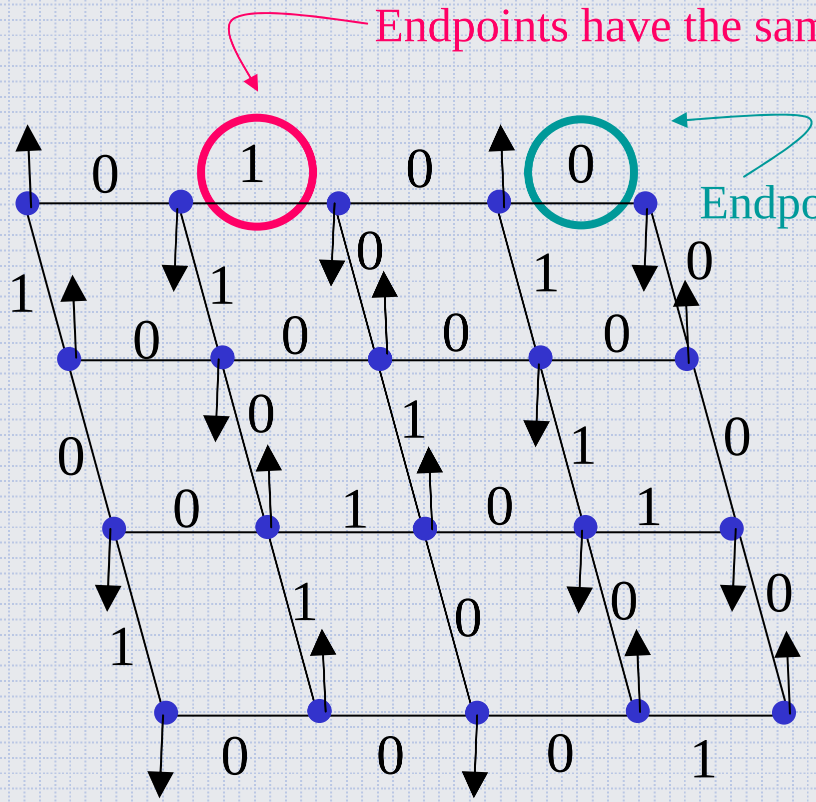
The *Hamiltonian* of a system is the sum of the energies on edges with endpoints having the same spins.

$$H = \sum_{edges} -J \; \delta(a,b)$$

where a and b are the endpoints of the edge, and J is the energy of the edge.

The energy (Hamiltonian) of the state

Endpoints have the same spins, so δ is 1.



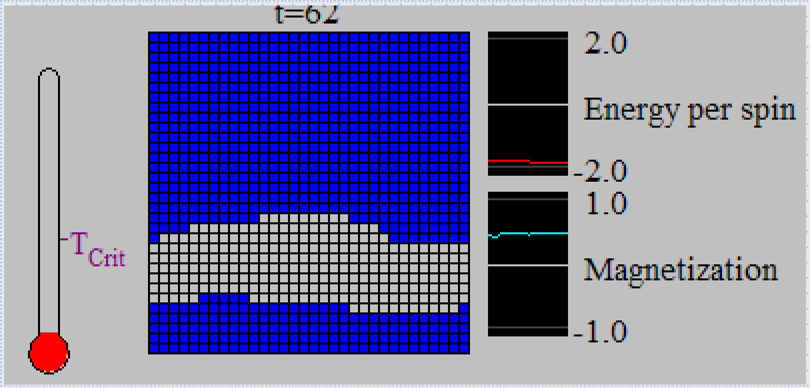
Endpoints have different spins, so δ is 0.

$$H(w) = \sum_{edges} -J\delta_{s_i, s_j}$$

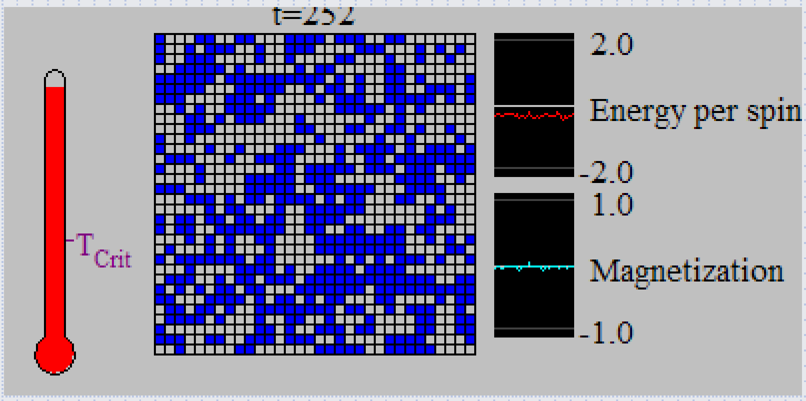
$H(w)$ of this system is $-11J$

A state w with the value of δ marked on each edge.

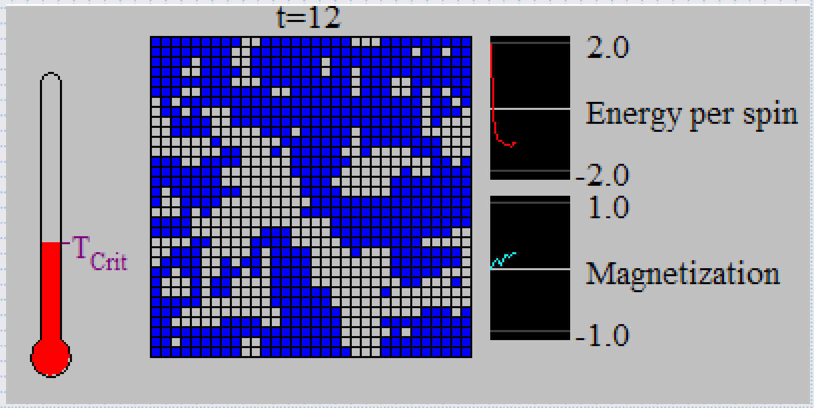
Ising Model at different temperatures



Cold Temperature



Hot Temperature



Critical Temperature

Images from http://bartok.ucsc.edu/peter/java/ising/keep/ising.html

Probability of a state occurring

$$\frac{e^{-\beta H(w)}}{\sum_{\text{all states } w} e^{-\beta H(w)}}$$

$\beta = \frac{1}{kT}$, where *T* is the temperature and *k* is the Boltzman constant 1.38×10^{-23} joules/Kelvin.

The numerator is easy. The denominator, called the *partition function,* is the interesting (hard) piece.

Effect of Temperature

- Consider two different states **A** and **B**, with ***H*(*A*) < *H*(*B*)**. The relative probability that the system is in the two states is:

$$\frac{P(A)}{P(B)} = \frac{e^{-\beta H(A)}}{\sum\limits_{\text{all states } w} e^{-\beta H(A)}} \Bigg/ \frac{e^{-\beta H(B)}}{\sum\limits_{\text{all states } w} e^{-\beta H(B)}}$$

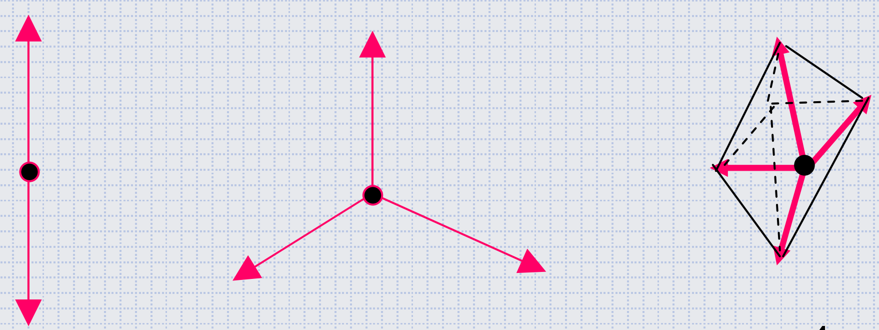
$$= \frac{e^{-\beta H(A)}}{e^{-\beta H(B)}} = e^{-\frac{D}{kT}} = e^{\frac{|D|}{kT}}, \text{ where } D = H(A) - H(B) < 0.$$

- At high temperatures (i.e., for ***kT*** much larger than the energy difference |**D**|), the system becomes equally likely to be in either of the states **A** or **B** - that is, randomness and entropy "win". On the other hand, if the energy difference is much larger than ***kT***, the system is far more likely to be in the lower energy state.

The Potts Model

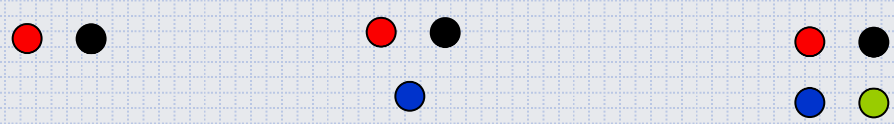
1952—(Domb)

Now let there be q possible states….



$q=2$ $q=3$ $q=4$

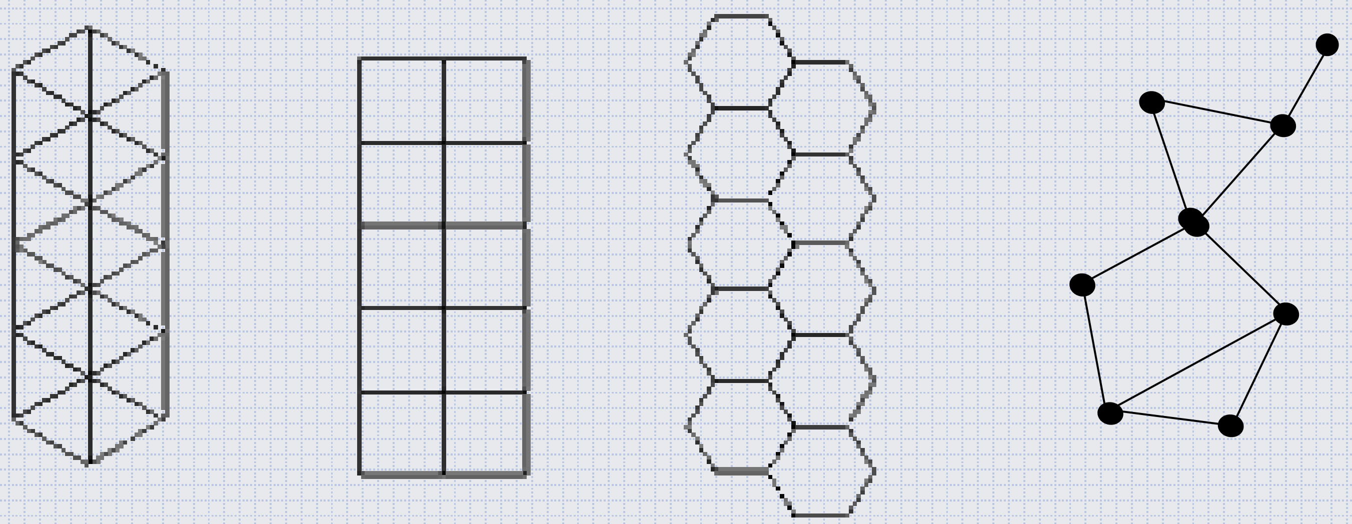
Orthogonal vectors, with δ replaced by dot product



Colorings of the points with q colors

Some extensions

- Let each edge have its own value— $J \to J_e$
- Change the lattice or even allow arbitrary graphs.



- Look at limits: infinite lattices or zero temperature.

Applications of the Potts Model

(about 1,000,000 Google hits…)

- **Liquid-gas transitions**
- **Foam behaviors**
- **Protein Folds**
- **Biological Membranes**
- **Social Behavior**
- **Separation in binary alloys**
- **Spin glasses**
- **Neural Networks**
- **Flocking birds**
- **Beating heart cells**

Nearest neighbor interactions….

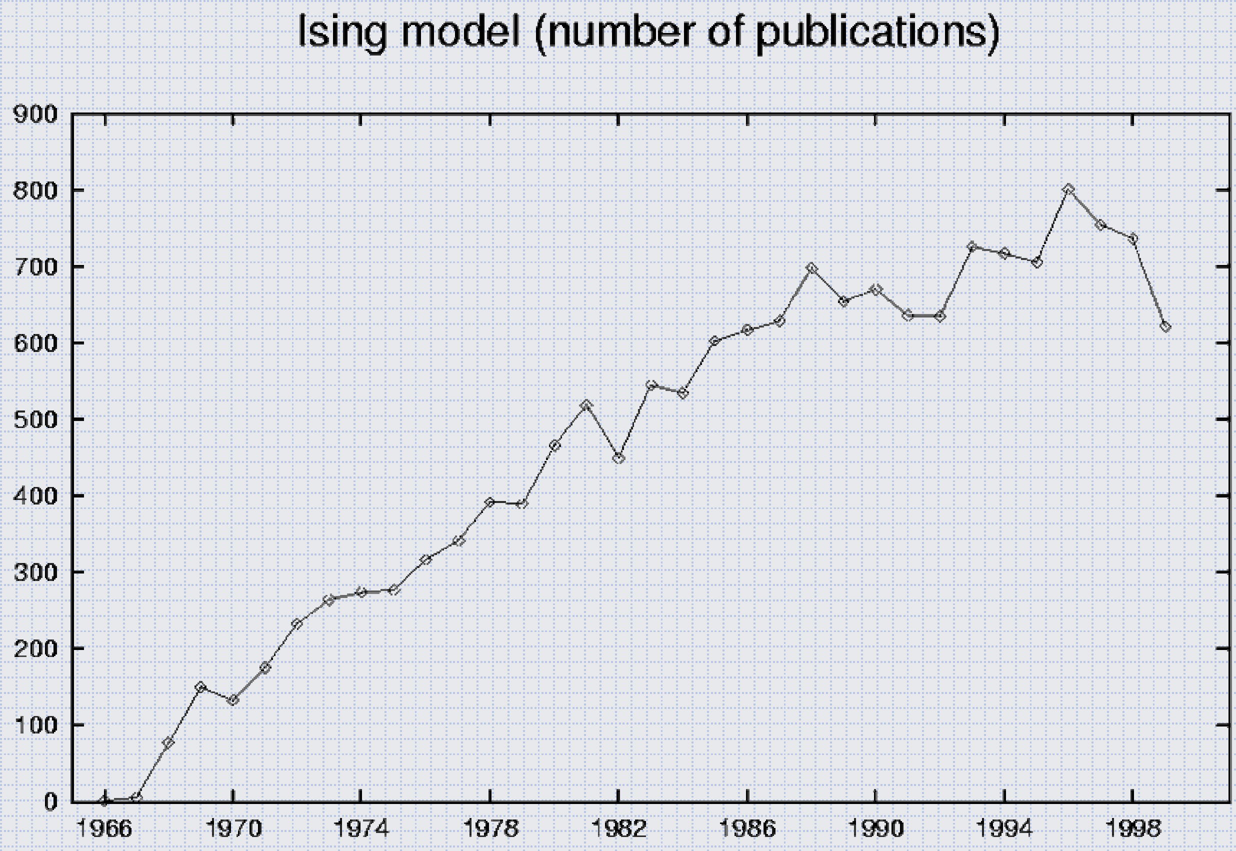
A personal favorite…

Y. Jiang, J. Glazier, *Foam Drainage: Extended Large-Q Potts Model Simulation*

We study foam drainage using the large-Q Potts model... profiles of draining beer foams, whipped cream, and egg white ...

3D model: http://www.lactamme.polytechnique.fr/Mosaic/images/ISIN.41.16.D/display.html

Ernst Ising 1900-1998



http://www.physik.tu-dresden.de/itp/members/kobe/isingconf.html

Potts Model Partition Function Equivalent Formulations

$$\sum_{\text{all states } w} e^{-\beta H(w)} = \sum_{\text{all states } w} e^{-\beta \sum_{edges} -J\delta(a,b)} =$$

$$\sum_{\text{all states } w} \left(\prod_{edges} e^{\beta J \delta(a,b)} \right) = \sum_{\text{all states } w} 1 - \left(e^{\beta J} - 1\right)\delta(a,b)$$

since $e^{\beta J \delta(a,b)} = 1$ if $\delta(a,b) = 0$ and $e^{\beta J \delta(a,b)} = e^{\beta J}$ if $\delta(a,b) = 1$

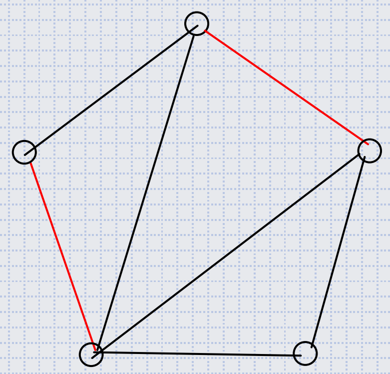
Letting $v = \left(e^{\beta J} - 1\right)$ gives that $\sum_{\text{all states } w} e^{-\beta H(w)} = \sum_{\text{all states } w} 1 - v\delta(a,b)$

Why would we want to do that??

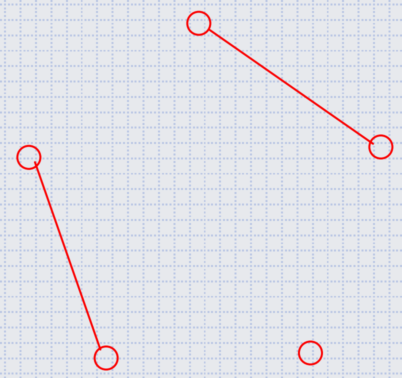
Theorem: The q – state Potts Model Partition function is a *polynomial* in q.

Motivation: Let w be a state, and let A be the set of edges in the state with endpoints the same color (spin). Thus, there are a $q^{k(A)}$ choices of ways to color the $k(A)$ components of the graph induced by A, and this gives a correspondence between states and subsets of the edges.

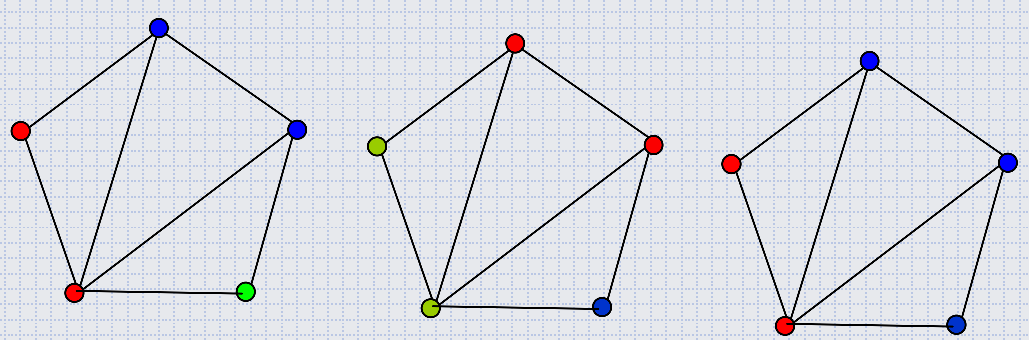
Example $q=3$



The edges of *A*



The components of the graph induced by *A*. Now color all vertices in the same component a single color (3^3 possibilities).



… plus 24 more possibilities

Potts is polynomial…

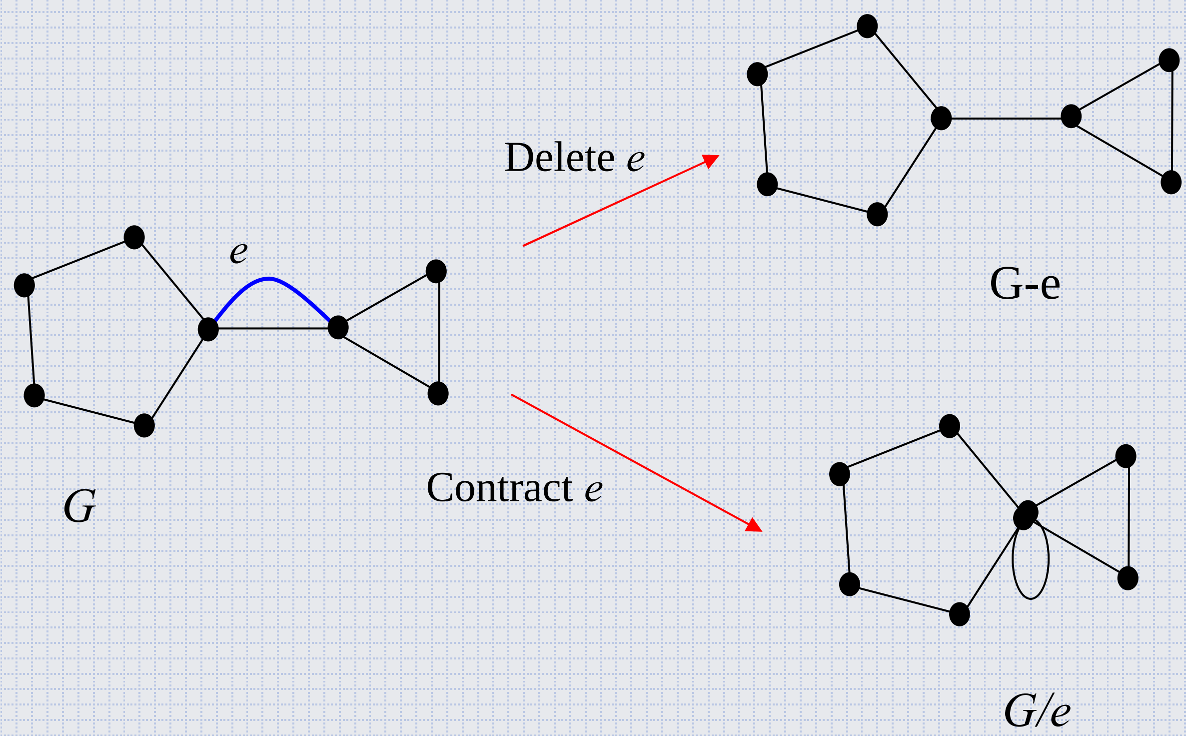
Thus, $$\sum_{\text{all states } w} e^{-\beta H(w)} = \sum_{\text{all states } w} 1 - v\delta(a,b) =$$

‘❁’ $$\sum_{A \subseteq E} q^{k(A)} v^{|A|}$$

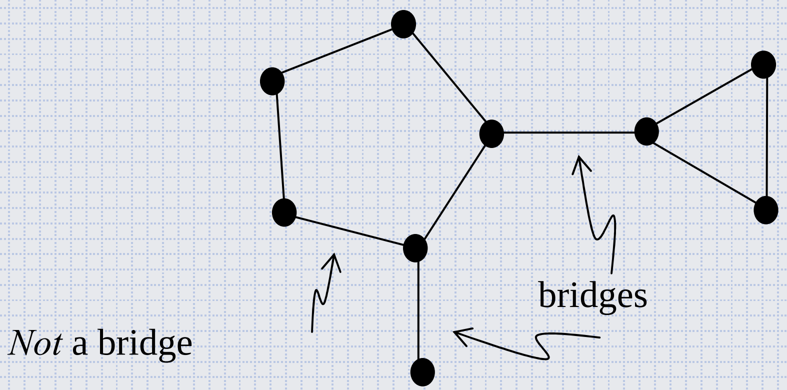
And now to Tutte…

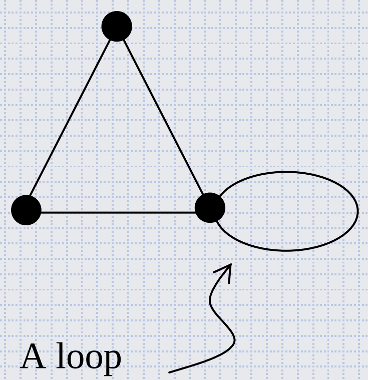
(with some preliminaries first)

Deletion and Contraction



Bridges and Loops





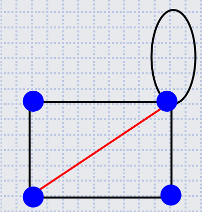
A *bridge* is an edge whose deletion separates the graph

A *loop* is an edge with both ends incident to the same vertex

Tutte Polynomial

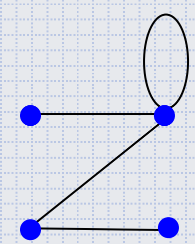
Let e be an edge of G that is neither an isthmus nor a loop. Then,

$$t(G;x,y) = t(G-e;x,y) + t(G \setminus e;x,y)$$

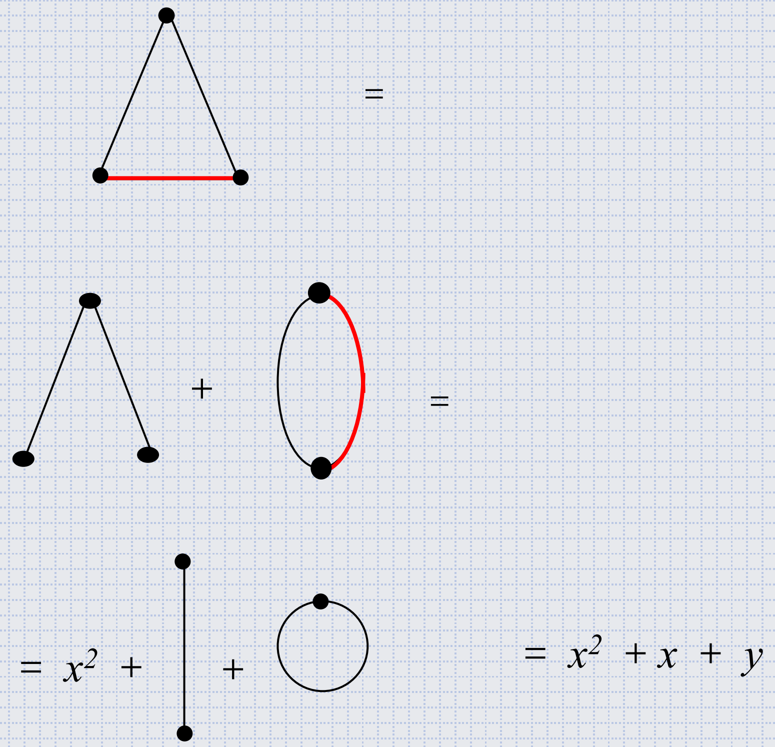


And if G consists of i bridges and j loops, then,

$$t(G;x,y) = x^i y^j$$



Example



Universality

THEOREM: (various forms—Brylawsky, Welsh, Oxley, etc.)
If f is a function of graphs such that

a) $f(G) = a\, f(G\text{-}e) + b\, f(G/e)$ whenever e is not a loop or an isthmus, and

b) $f(GH) = f(G)f(H)$ where GH is either the disjoint union of G and H or where G and H share at most one vertex.

Then,

$$f(G) = a^{|E|-|V|+k(G)} b^{|V|-k(G)} t\left(G; \frac{x_0}{b}, \frac{y_0}{a}\right),$$ where $|E|$, $|V|$, and $k(G)$

are the number of edges, vertices, and components of G, respectively, and where

$f($  $) = x_0$, and $f($  $) = y_0$.

Thus *any* graph invariant that reduces with a) and b) is an evaluation of the Tutte polynomial.

Proof: By induction on the number of edges.

A Slight Shift

The Dichromatic Polynomial:

$$Z(G;u,v) = \sum_{S \subseteq E(G)} u^{k(S)} v^{|S|}$$

Can show (by induction on the number of edges) that

$$u^{k(G)} v^{|V|-k(G)} t\left(G; \frac{u+v}{v}, v+1\right) = Z(G;u,v)$$

Note: this means that the Tutte polynomial is independent of the order the edges are deleted and contracted!

And back again….

The q-state Potts Model Partition Function is an evaluation of the Tutte Polynomial!

$$P\left(G;q,v\right)=q^{|V|}t\left(G;\frac{q+v}{v},v+1\right)$$

where $v=\left(e^{\beta J}-1\right)$ as before.

Fortuin and Kasteleyn, 1972

A reason to believe this…

Note that if an edge has end points with different spins, it contributes nothing to the Hamiltonian, so in some sense we might as well delete it.

On the other hand, if the spins are the same, the edge contributes something, but the action is local, so the end points might be coalesced, i.e., the edge contracted, with perhaps some weighting factor.

Thus, the Potts Model Partition Function has a deletion-contraction reduction, and hence by the universality property, must be an evaluation of the Tutte polynomial.

Another reason to believe this…

Recall we saw that the Potts Model Partition Function was polynomial:

‘❀’ $$\sum_{A \subseteq E} q^{k(A)} v^{|A|}$$

Compare this to the shifted expression for the Tutte polynomial:

$$Z(G;u,v) = \sum_{S \subseteq E(G)} u^{k(S)} v^{|S|}$$

Computational Complexity

If we let $x = \frac{e^{\beta}+1}{e^{\beta}-1}$ and $y = e^{\beta}$, the Potts Model Partition Function is the Tutte polynomial evaluated along the hyperbola $(x-1)(y-1) = q$

The Tutte polynomial is polynomial time to compute for planar graphs when $q = 2$ (Ising model).

The Tutte polynomial is also polynomial time to compute for all graphs on the curve $(x-1)(y-1)=1$ and 6 isolated points:

(1,1), (-1,-1), (j, j^2), (j^2, j), where $j = e^{\frac{2\pi i}{3}}$

But else where the Tutte polynomial is NP hard to compute (Jaeger, Vertigan, Welsh, Provan—1990's).

Thus the q-state Potts Model Partition Function is likewise computationally intractable.

Phase Transitions and the Chromatic Polynomial

Phase transitions (failure of analyticity) arise in the infinite volume limit.

Let $\{G\}$ be an increasing sequence of finite graphs (e.g. lattices).

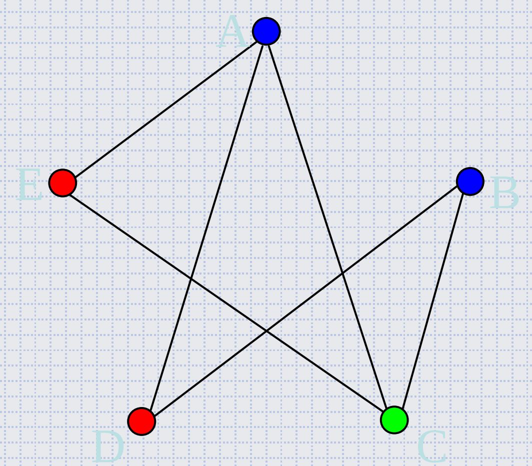
The (limiting) free energy per unit volume is:

$$f_{G_\infty}(q,v) = \lim_{n\to\infty} |V_n|^{-1} \log P(G_n; q, v)$$

Consider this at zero temperature

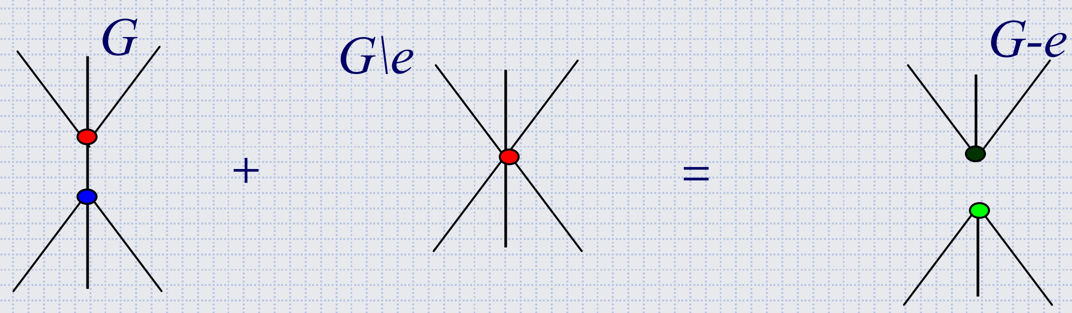
Recall that at zero temperature, high energy states prevail, i.e. we really need to consider states where the endpoints on *every* edge are different.

Such a state corresponds to a *proper coloring* of a graph:



Chromatic polynomial

The Chromatic Polynomial counts the ways to vertex color a graph: C(G, n) = # proper vertex colorings of G in n colors.

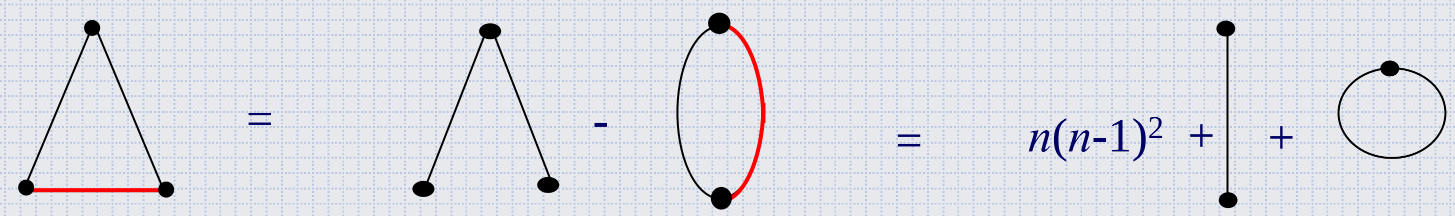


Recursively: Let e be an edge of G . Then,

$$C(G;n) = C(G-e;n) - C(G \setminus e;n)$$

$$C(\bullet;n) = n$$

Example



$$= \; n(n\text{-}1)^2 \; + n(n\text{-}1) \; + 0 \; = n^2 \; (n\text{-}1)$$

Since a contraction-deletion invariant, the chromatic polynomial

is an evaluation of the Tutte polynomial:

$$C(G;x) = \; (-1)^{|V|-k(G)} x^{k(G)} t(G;1-x,0)$$

Zeros of the chromatic polynomial

- phase transitions correspond to the accumulation points of roots of the chromatic polynolmial in the infinite volume limit

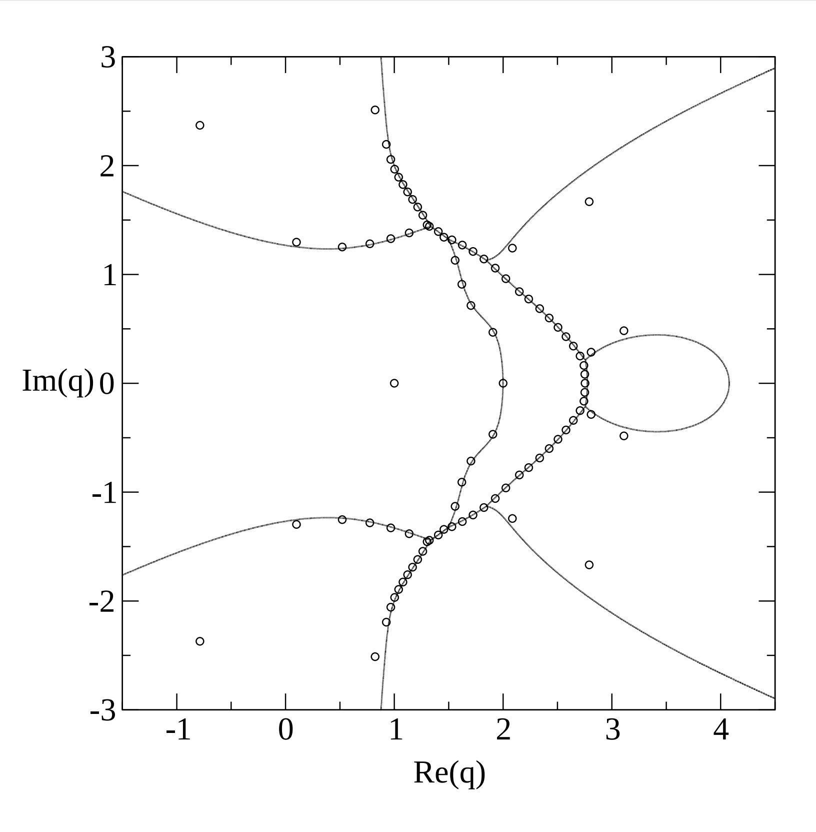
Locations of Zeros

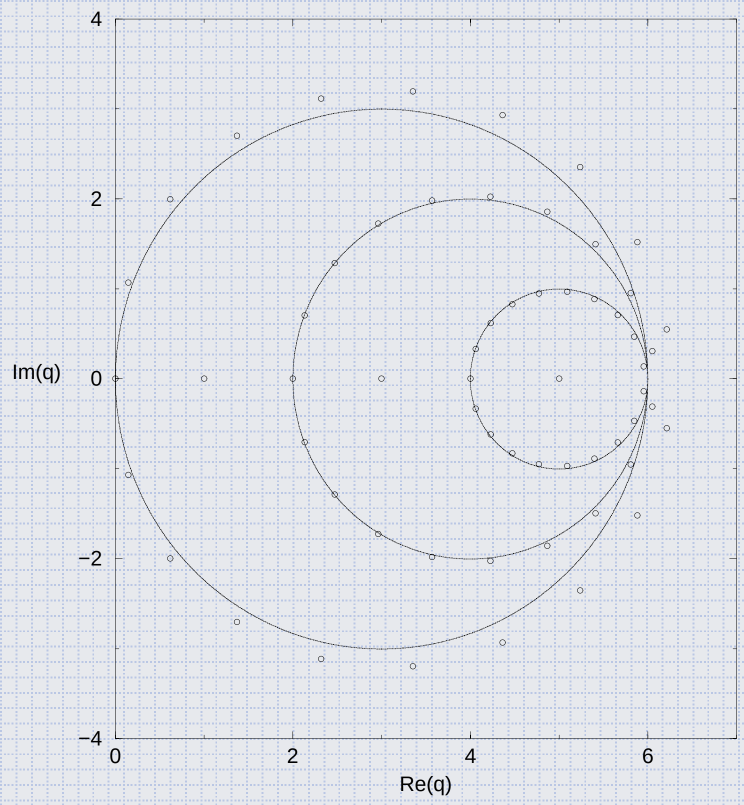
Mathematicians originally focused on the real zeros of the chromatic polynomial (the quest for a proof of the 4-color theorem…)

Physicists have changed the focus to the locations of complex zeros, because these can approach the real axis in the infinite limit.

Now an emphasis on ‘clearing’ areas of the complex plane of zeros.

Some zeros





(Robert Shrock)