On the study of the Potts model, Tutte and Chromatic Polynomials, and the Connections with Computation Complexity and Quantum Computing

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Abstract

The Tutte polynomial of a graph is revised and the chromatic polynomial is derived as a special case of the partition function of the Potts model. We introduce the calculations of the computational complexity for these polynomials and we derive some calculations on recursive families of graphs based on the literature, reproducing some of the simulations for the simple cases. Finally, we discuss some possible links of this theory to recent results on quantum algorithms and topological quantum computing.

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I. INTRODUCTION TO GRAPH THEORY

A. Graphs and Subgraphs

In mathematics and physics, there are several problems where one is interested in calculating a function on a graph,

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

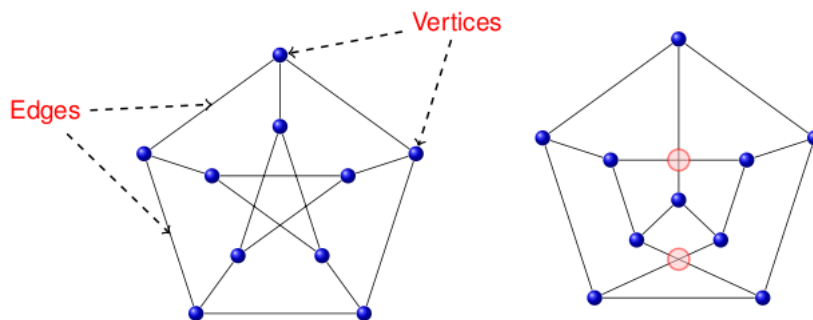where V is the set of *vertices* (sites) and E is the set of *edges* (bonds) [1].

FIG. 1: (Right) Petersen Graph is an example of a 3-regular graph, with 10 vertices, 15 edges, and where each vertex has 3 neighbors. (Left) It is also an example of a non-planar graph, *i.e.,* there are crossing edges [2].

Definition I.1 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 [1].

Definition I.2 A connected graph with no cycles is a *tree.*

Definition I.3 A spanning subgraph G' with no cycles is a spanning *forest* of G.

Definition I.4 The *complete graph* K_n is the graph with n vertices such that each pair of vertices is connected by an edge, so $E(K_n) = \binom{n}{2}$.

Definition I.5 A *loop* is an edge that connects a vertex to itself. $P(G, q)$ vanishes if G contains one or more loops.

Definition I.6 A *recursive family* of graphs G_m is a family for which the $(m+1)$'th member is obtained from the m'th member graph either by gluing on some fixed subgraph or by cutting through the m'th member, inserting the subgraph and gluing the graph together.

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B. Graph Coloring

Graphic coloring, i.e., vertex coloring, is the assignment of colors to the vertex of a graph in a such way that no two adjacent vertices share the same color.

Definition I.7 A q-coloring of a graph G is a function

$$\sigma : V(G) \rightarrow \{1, 2, ..., q\}$$

satisfying $\sigma(i) \neq \sigma(j)$ for any edge $E = i, j$. The graph is said to be q-colorable if such a function exists.

For instance, a graph is 2-colorable (*bipartite*) if it contains no odd cycle. The q-colorability for any q larger than 3 is **NP-complete** (*e.g.,* the question *Does G have a proper 3-coloring?*) and finding the chromatic number is **P-complete** , *i.e.,* it is unfeasible to calculate it in an efficient way [35].

C. The Chromatic Polynomial

George Birkhoff introduced the *chromatic polynomial* in 1912 as an attempt to prove the *four color theorem* [3]. He noticed the number of ways he could paint a map with at most q colors exhibits polynomial dependence on q yielding some conclusions on $q-$colorability (he hoped to be able to find an analytic proof that $P_G(4) > 0$ for any planar graph G).

Definition I.8 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.

Definition I.9 The *chromatic number* $\chi(G)$ is the minimal q for which the graph is q-colorable (*i.e.,* the minimum number of colors needed for a proper coloring of G) and G is q-chromatic if $\chi(G) = q$,

$$\chi(G) = \min\{P(G, q) > 0\}.$$

For example, the *path graph* P_3 on 3 vertices cannot be colored with 0 or 1 colors. With 2 colors, it can be colored in 2 ways. With 3 colors, it can be colored in 12 ways [5]. Another example is the *tree graph*, where there are q choices of colors for an arbitrary first vertex and then $q - 1$ choices for each subsequent vertex (see Fig. 3).
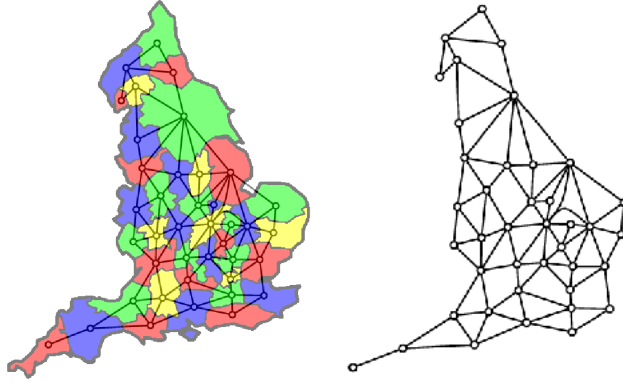
FIG. 2: In 1852, Guthrie noticed that he never needed more than 4 colors on any map (*planar graph*). The four color theorem was an open problem for almost a century until it was proven in 1976 by Appel and Haken [2].
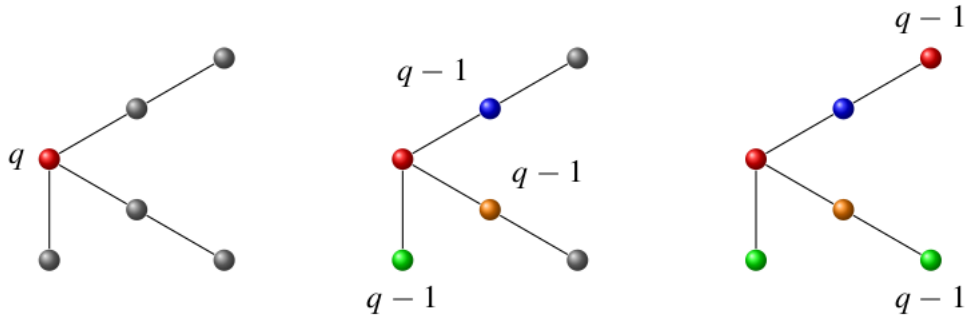
FIG. 3: Coloring a tree graph: for any tree T on n vertices, one has $P_T(q) = q(q-1)^{n-1}$ [4].

Definition I.10 Two non-isomorphic graphs may share the same chromatic polynomial. A graph that is determined by its chromatic polynomial is said to be a *chromatically unique graph*. Non-isomorphic graphs sharing the same chromatic polynomial are said to be *chromatically equivalent*.

Examples of classes of graphs and their chromatic polynomials are

- Complete graph can be obtained from the definition I.4, where we can write $P(K_n, q) = q(q-1)...(q-n+1) = \prod_{j=0}^{n-1}(q-j)$. For example, the triangle K_3, $P(K_3, q) = q(q-1)(q-2)$ and the chromatic number is $\chi(K_n) = n$.

- Tree with n vertices, $P(T_n, q) = q(q-1)^{n-1}$.

- Cycle of length n, $P(C_n, q) = (q-1)^n + (-1)^n(q-1)$.
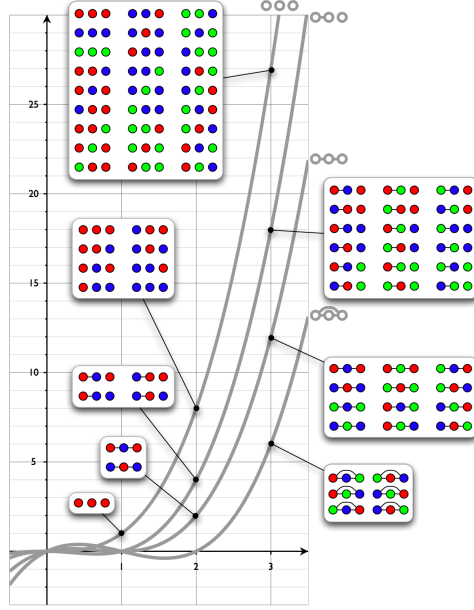
FIG. 4: All vertex colorings of vertex graphs with 3 vertices using q colors for $q = 0, 1, 2, 3$ [5].

D. Deletion-Contraction Property

A fundamental property of the chromatic polynomial is that it can be reduced to two smaller graphs, resulting from *deletion and contraction* of an edge E respectively, giving an algorithm to *recursively calculate the chromatic polynomial* for any graph.

Definition I.11 Let $G - E$ be the graph G with the edge E deleted and G/E the graph with E deleted and two vertices connected. The chromatic polynomial satisfies the recurrence relation,

$$P(G, q) = P(G - uv, q) - P(G, uv, q), \tag{1}$$

where u and v are adjacent vertices and $G - uv$ is the graph with the edge uv removed.

An example of recurrence relations for chromatic polynomials for simple classes of graphs is for the cycle graph,

$$P_n(C_n, q) = (1-2)P_{n-1}(q) + (q-1)P_{n-2}(q).$$

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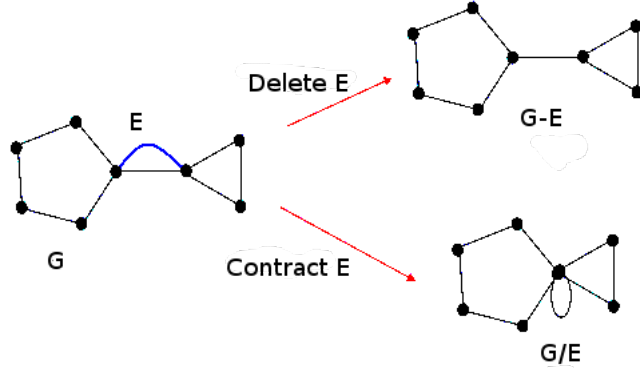FIG. 5: The deletion and contraction of an edge [6]. A *bridge* is an edge whose deletion separates the graph. A *loop* is an edge with both incident to the same vertex.

E. The Tutte Polynomial

Tutte defined his two-variable *dichromatic polynomial* as a generalization of the chromatic polynomial and the deletion-contraction argument.

Definition I.12 The *Tutte-Whitney* polynomial of a graph G and a spanning subgraph G' is

$$T(G, x, y) = \sum_{G' \subseteq G} (x - 1)^{k(G') - k(G)} (y - 1)^{c(G')}, \tag{2}$$

where $c(G')$ is the number of linearly independent cycles in G' and

$$c(G) = E(G) + k(G) - n(G). \tag{3}$$

Special cases of the Tutte polynomial yield the chromatic polynomial,

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

For a connected graph with vertices, the chromatic polynomial is related to the rank polynomial and Tutte polynomial by

$$\pi(x) = (-1)^{n-1} x T(1 - x, 0).$$

F. Chromatic Roots

A root (or zero) of a chromatic polynomial is a value where $P_G(x) = 0$. Chromatic roots have been very well studied, *e.g.,* recall that Birkhoffs original motivation for defining the

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chromatic polynomial was to show that for planar graphs, $P_G(x) > 0$, for $x > 3$. If G is an n-vertex graph then $P_G(z)$ has degree n and so this equation has n solutions over the complex numbers. Fundamental questions are related to the search for absolute bounds on the root-location and the search of this bounds in terms of graph parameters [2].

No graph can be 0-colored, so 0 is always a chromatic root. Only edgeless graphs can be 1-colored, so 1 is a chromatic root for every graph with at least an edge. On the other hand, except for these two points, no graph can have a chromatic root at a real number smaller than or equal to 32/27. This comes from a result of Tutte, connecting the golden ratio with the study of chromatic roots. He showed that if G is a planar triangulation of a sphere then

$$P(G_n, \phi) \leq \phi^{5-n}.$$

Later, Farell observed that some zeros are more "popular" than others, specifically the sequence $\{3/2 \pm i\sqrt{3}/2, 2 \pm i, 5/2 \pm i\sqrt{3}/2, ...\}$ [2].

For many years, it was thought that chromatic zeros were restricted to the right half-plane $\text{Re}(z) > 0$. In 1999, Alan Sokal proved that chromatic zeros are dense in the whole complex plane [10] [36].

While the real line thus has large parts that contain no chromatic roots for any graph, every point in the complex plane is arbitrarily close to a chromatic root in the sense that there exists an infinite family of graphs whose chromatic roots are dense in the complex plane.

In the case of **complex** zeros, *generalized theta graphs* are graphs with two end points connected via paths of varying lengths. Sokal also analytically proved that all the chromatic roots of these graphs lie within a certain disc [10].

Recently, progress has been made in the theory of zeros of recursive families (recall from Definition I.6 that a sequence of graphs $\{G_1, ..., G_m\}$ is a recursive family if $P(G_m, m) = f(P(G_{m-1}), ..., P(G_1))$, where f is some simple linear function). Chromatic zeros of recursive families of graphs obey a limiting process and Shrock and Tsai [11] proved that a certain family of graphs have zeros lying on circles and relate the results to a certain *Potts model* (described in the next session). This paper provides an interesting link between chromatic zeros and the Potts model on a certain class of graphs.

G. Algorithm to Chromatic Roots

Computational problems associated with the chromatic polynomial are related to finding the chromatic polynomial of a given graph P_G, *e.g.,* finding its coefficients evaluating $P_G(q)$ at a fixed point q. When q is a natural number, this problem is viewed as computing the number of q-colorings of a given graph. The time required for this classical calculation grows exponentially with the number of vertices, $n = |V|$, *i.e.,* $\mathcal{O}(2^n)$. Quantum computing may be able to reduce the calculations time to polynomial time [13].

The chromatic polynomial of a general graph can also be calculated with the deletion-contraction recursion. In the worst case running time the algorithm runs in time within a polynomial factor of

$$\mathcal{O}(\phi^{n+m}) = \mathcal{O}\Big(\frac{1 + \sqrt{5}}{2}\Big)^{n+m} = \mathcal{O}(1.6180)^{n+m},$$

where ϕ is the golden ratio and n and m are the number of nodes and edges respectively. This algorithm also has an exponential complexity and is only practical for small graphs [37]. The analysis can be improved to a polynomial time in some cases, with some spanning trees as the the input graphs [12].

Another calculation methods include high and low temperature series expansions, which enable one to calculate these quantities exactly for arbitrary large n for certain families of graphs [1].

II. INTRODUCTION TO THE POTTS MODEL

A.   A Model for Interacting Spins

In Physics, ferromagnets can be thought of as a set of interacting spins on a crystalline lattice. In the *Potts model*, each spin can assume one of the q possible states. If two neighboring spins (joined by an edge E) are in the same state, it adds some value J to the energy given by the Hamiltonian, $\mathcal{H}$, of the system.
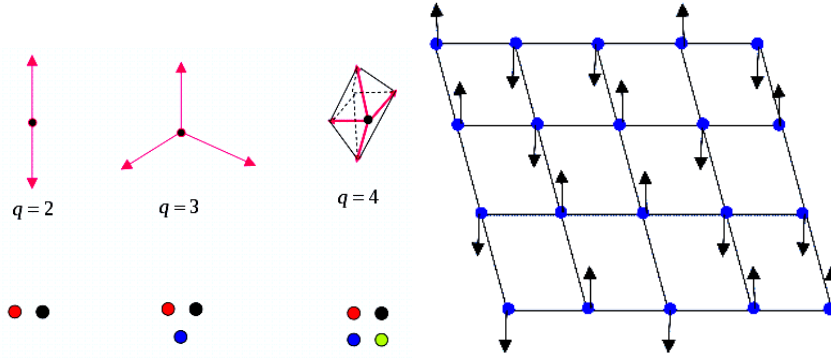

FIG. 6: (Left) The q-state Potts model, with $q = 2, 3, 4$ states and the coloring of the points with q colors. (Right) The $q = 2$-state Potts model is known as the *Ising Model*. A sheet of metal at low temperature is magnetized and when the temperature increases the magnetism decreases. To model this behavior one assumes that (i) individual atoms have a spin (*e.g.,* up and down), (ii) neighboring atoms with different spins have an interaction energy (assumed constant), (iii) the atoms are arranged in a regular lattice. [6]

Definition II.1 The *Boltzmann weight* of a configuration (assignments of states to spin) is $e^{-\beta \mathcal{H}}$, where the probability of the configuration is proportional to its Boltzmann weight.

To form a probability distribution, one normalizes with the sum of the Boltzmann weights of all configurations, *i.e.,* the partition functions of the Potts model, which is a polynomial in terms of q.

The behavior of the coupling J is determined by the willingness of spins to become aligned, being ferromagnetic if $J > 0$ and antiferromagnet if $J < 0$. The interaction is strengthened by decreasing the temperature to the limit $T = 0$, where only **configurations with no**

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adjacent spins sharing common state will have nonzero energy. The connection to the chromatic polynomial is natural in this sense. Moreover, *phase transitions* are closely related to the roots of this partition function, and therefore to the roots of the chromatic polynomial.

B.   The Potts Model Partition Function

Definition II.2 Let G be a graph and S the set of q elements called spins. A *state* of a graph G is an assignment of a single spin to each vertex of the graph, where the Hamiltonian measures the energy of this state.

Definition II.3 The Potts model on a graph G at temperature T ($\beta = 1/k_B T$) is related to classical spin variables σ_i on each vertex i in V that can take values in $\{1, 2, ...q\}$, with an interaction Hamiltonian,

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

and

$$- \beta\mathcal{H} = K \sum_{E_{ij}} \delta_{\sigma_i \sigma_j}. \tag{4}$$

Definition II.4 The Potts model partition function is,

$$Z = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}} = \sum_{\{\sigma_i\}} e^{K \sum_{E_{ij}} \delta_{\sigma_i \sigma_j}}. \tag{5}$$

Writing $\nu = e^K - 1$ such that

$$
\begin{aligned}
e^{K\delta_{\sigma_i \sigma_j}} &= 1 + (e^K - 1)\delta_{\sigma_i \sigma_j}, \\
&= 1 + \nu\delta_{\sigma_i \sigma_j}, \tag{6}
\end{aligned}
$$

one has

$$
\begin{aligned}
Z(G, q, \nu) &= \sum_{\{\sigma_i\}} \prod_{E_{ij}} (1 + \nu\delta_{\sigma_i \sigma_j}), \\
&= \sum_{G' \subseteq G} q^{k(G')} v^{E(G')}, \tag{7}
\end{aligned}
$$

where k and E are the number of connected components and edges in G'. This is the *Fortuin-Kasteleyn cluster representation* and it shows that $Z(G, q, \nu)$ is a polynomial in q and ν, since there is a $1 - 1$ correspondence between Z and the spanning subgraph G'.

Example II.1: The Cyclic Group C_n

Let us see the case of the cyclic group, taking C_3 as an example [1],

$$
\begin{aligned}
Z(C_3, q, \nu) &= \sum_{\{\sigma_i\}} \prod_{E_{ij}} (1 + \nu \delta_{\sigma_i \sigma_j}), \\
&= \sum_{\sigma_i} (1 + \nu \sigma_{\sigma_1 \sigma_2})(1 + \nu \sigma_{\sigma_2 \sigma_3})(1 + \nu \sigma_{\sigma_3 \sigma_1}) \\
&= 1 + \nu(\delta_{\sigma_1 \sigma_2} + \delta_{\sigma_2 \sigma_3} + \delta_{\sigma_3 \sigma_1}) + \nu^2(\delta_{\sigma_1 \sigma_2} \delta_{\sigma_2 \sigma_3} + \delta_{\sigma_2 \sigma_3} \delta_{\sigma_3 \sigma_1} + \delta_{\sigma_3 \sigma_1} \delta_{\sigma_1 \sigma_2}) \\
&+ \nu^3(\delta_{\sigma_1 \sigma_2} \delta_{\sigma_2 \sigma_3} \delta_{\sigma_3 \sigma_1}), \\
&= q^3 + 3q^2\nu + 3q\nu^2 + q\nu^3, \\
&= (q + \nu)^3 + (q - 1)\nu^3.
\end{aligned}
\tag{8}
$$

The generalization proceeds naturally,

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

C. The Potts Model Partition Function and the Tutte Polynomial

If we generalize the regular lattice to an abstract, the q-state Potts model partition function is an evaluation of the Tutte Polynomial, and the Potts is equivalent to the Tutte polynomial if both q and the temperature are viewed as indeterminate variables [7]. Let

$$
x = 1 + \frac{q}{\nu},
$$

and

$$
y = \nu + 1 = e^K,
$$

so

$$
q = (x - 1)(y - 1),
$$

and

$$
\nu = y - 1.
$$

We use $n(G') = n(G)$ and similar relation given in Eq. 3,

$$
c(G') = E(G') + k(G') - n(G),
$$

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to write the Tutte polynomial of a graph G, from Eq. 2,

$$
\begin{aligned}
T(G, x, y) &= (x-1)^{-k(G)} \sum_{G' \subseteq G} (x-1)^{k(G')}(y-1)^{c(G')}, \\
&= (x-q)^{-k(G)} \sum_{G' \subseteq G} \left(\frac{q}{\nu}\right)^{k(G')} \nu^{E(G')+k(G')-n(G)}, \\
&= (x-1)^{-k(G)}(y-1)^{-n(G)} \sum_{G' \subseteq G} q^{k(G')} \nu^{E(G')}, \\
&= (x-1)^{-k(G)}(y-1)^{-n(G)} Z(G, q, \nu). \qquad (9)
\end{aligned}
$$

This equivalence connects statistical mechanics and mathematical graph theory [1].

Definition II.5 The Potts parameters ν and q are physical parameters when [18]:

- q is an integer larger than 0, and for all edges $\nu_E > 1$; or

- $q > 0$ and for all edges $\nu_E > 0$.

Example II.2: Partition function and Tutte Polynomial for a Tree Graph with n vertices.

From Eq. 7, we can write for T_n,

$$
\begin{aligned}
Z(T_n, q, \nu) &= q(q+\nu)^{n-1}, \\
&= \left(\frac{q}{\nu}\right)^{k(G)} \nu^n T(G, x, y), \\
&= q\nu^{n-1} T(G, x, y), \\
&= q\nu^{n-1}\left[1 + (q/\nu)\right]^{n-1}, \\
&= q\nu^{n-1} x^{x-1},
\end{aligned}
$$

and

$$
T(T_n, x, y) = x^{n-1},
$$

where from the Definition I.10, we observe that two different graphs can have the same Tutte polynomial and Potts partition function. Setting $\nu = -1$, gives back the chromatic polynomial,

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

Example II.3: Partition function and Tutte Polynomial for a Cycle Graph with n vertices.

Following the same steps as the previous example, now for C_n, with $x - 1 = q/\nu$ and $q = (x-1)(y-1)$, one has

$$
\begin{aligned}
Z(C_n, q, \nu) &= (q + \nu)^n + (q-1)\nu^n, \\
&= \nu^n \left[\left(1 + \frac{q}{\nu}\right)^n + (q-1) \right], \\
&= \nu^n \left[x^n + q - 1 \right], \\
&= q\nu^{n-1} \left[\frac{x^n + q - 1}{x - 1} \right],
\end{aligned}
$$

and using the expansion

$$
\sum_{j=1}^{n-1} x^j = \frac{x^n - x}{x - 1}
$$

the Tutte polynomial is

$$
\begin{aligned}
T(C_n, x, y) &= \left[\frac{x^n + xy - y - x}{x - 1} \right], \\
&= y + \sum_{j=1}^{n-1} x^j,
\end{aligned}
$$

and we can recover its chromatic polynomial setting again $\nu = -1$.

D. The Antiferromagnetic Potts Model

Special cases of the Tutte polynomial yield some graph-theoretic functions of interest in Physics, such as when $\nu = -1$ ($y = 0$) and one recovers the chromatic polynomial of the antiferromagnet Potts model (see Fig. 7).

For this case, one considers the limit $T \to 0$ and $K \to -\infty$ (with $K = \beta J$ and $J < 0$) and $\nu = e^K - 1 \to -1$. The only spin configuration that contributes is the one having an adjacent spin with different value. This results on the $T = 0$ limit of the Potts antiferromagnetic partition function given by the following chromatic polynomial

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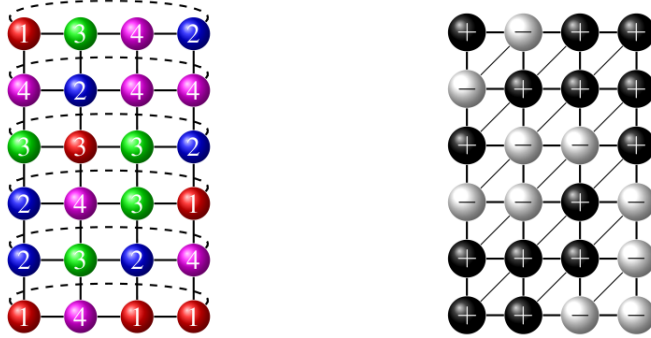Z(G, q, -1) = P(G, q) = (-1)^{k(G)} (-1)^{n(G)} T(G, 1 - q, 0).
$$

FIG. 7: The q-state Potts model models a physical system as collection of interacting spins, each taking on one of q distinct values, and in this case, located on a regular lattice grid. Every edge E contributes with $1 + \nu$ if it joins equal spins. If one writes $\nu = -1$ for every edge, one gets the *zero temperature limit of the antiferromagnetic Potts model*, $Z_G(q, -1) = P_G(q)$. (Left) The lattice may be periodic. (Right) The $q = 2$ case is known as the *Ising Model* [5]

E.   Exact Calculations on Recursive Graphs for the Potts Partition Function

In the end of the last session we have learned that we can use the deletion-contraction recursion to calculate family of graphs. It is possible to use the same logic to rewrite the Eq. 1 for the Potts partition function from Eq. 5,

$$Z(G, q, \nu) = Z(G - E, q\nu) + \nu Z(G/E, q, \nu),$$

with two possibilities for the two spins on the vertices joined by the edge E: (i) either they are different, so Z is the same as if the edge was moved, (ii) or they are the same so it is summed by the term $\nu \delta_{\sigma_i \sigma_j}$, (see Fig. 8).

The general calculation of $Z(G, q, v)$ for an arbitrary graph G and arbitrary values of q and ν, which is the calculation of $T(G, x, y)$ for an arbitrary graph G and values of x and y, takes a time $\propto \mathcal{O}(e^{n(G)})$ or $\propto \mathcal{O}(e^{e(G)})$. Although $Z(G, q, \nu)$ satisfies the above deletion-contraction relation, this again does not reduce the complexity of the calculation, but for some graphs, this enables to calculate exactly in the closed form, avoiding exponential growth of the time required [1].
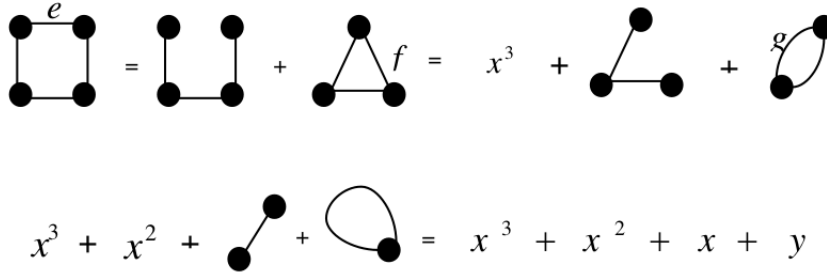
FIG. 8: Calculation of the Tutte polynomial for C_4 using the deletion-contraction propriety [7]. First we start with $G = C_4$ and $Z(C_4, q, \nu) = (q + \nu)^4 + (q - 1)\nu^4$. Subtracting any edge gives $C_4 - E = T_4$, where $T(T_4, x, y) = x^3$, and $Z(T_4, q, \nu) = q(q + 3)^3$. Contracting on E gives $C_4/E = C_3$, where $T(C_3, x, y) = x + x^2 + y$, and $Z(C_3, q, \nu) = (q + \nu)^3 + (q - 1)\nu^3$. Summing these two results returns the the Tutte polynomial of C_4, *i.e.*, $T(C_4, x, y) = x + x^2 + x^3 + y$.

F.   Thermodynamics Functions and Phase Transition

The thermodynamic functions, *e.g.*, internal energy, specific heat, entropy, free energy, can be derived from the Potts model partition function, $Z(G, q, \nu)$ [8].

A *phase transition* in a physical system occurs when continuous variation in a control parameter yields a discontinuity in its observed behavior. Statistical physicists are interested in complex zeros because a phase transition can only occur at a real limit point of the complex zeros of the partition function. Hence a zero-free region for a family of graphs provides evidence that phase-transitions cannot occur in that region of parameter space - such theorems are called *Lee-Yang theorems* [5]. Phase transitions correspond to the accumulation points of roots of the chromatic polynomial in the infinite volume limit.

We consider connected graphs G without loops or multiple bonds and denote the number of vertices as $n = V(G)$, the edges as $E(G)$, and the chromatic number as $\chi(G)$. Based on many results from the literature, we consider the infinite length of a strip graph, denoted as $\{G\} = \lim_{n \to \infty} G$ [12] [31] [32] [33]. For arbitrary strip length $L_x = m$, we consider the limit $n \to \infty$ obtained by taking the length $L_x \to \infty$. For a given type of strip graph, we can denote this as G and define a reduced free energy (per site) of the Potts model,

$$f(G, q, \nu) = \lim_{n \to \infty} \frac{1}{n} \ln Z.$$

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The ground state degeneracy (per site) of the Potts antiferromagnet is given by

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

with associated ground state entropy $S = k_B \ln W$.

As we have seen in the section I F, since $P(G,q)$ is a polynomial, it is of interest to analyze its real and complex zeros (chromatic zeros). Moreover, important results comes from analyzing the zeros of $Z(G,q,\nu)$ in the q plane for fixed ν, and in the v plane for fixed q, such as the study of the behavior of these zeros in the limit $n \to \infty$. We find that in this limit zeros accumulate to form certain curves and line segments, generically denoted as the loci $\mathcal{B}_q$ [38]. These are determined by the condition that two dominant λs are equal in magnitude, which defines algebraic curves.

Following some of the *Mathematica's notebooks* with the transfers matrices given by the above literature (arxiv files), we reproduced one case of $\mathcal{B}_q$ for one familiy of graphs, for the square lattice (the code source is attached in the end of this paper). The families of graphs may depend on several parameters (*e.g.,* width, length, number of homeomorphic expansions, etc.), and there can be several ways in which one can obtain the limit $n \to \infty$. We concentrate on one parameter, such as the length of a strip of a regular lattice, so that n is a linear function of m. We take the width to be fixed and the length to be variable and arbitrarily great.

FIG. 9: Locus $\mathcal{B}_q$ in the q plane for $n \to \infty$ limit for the square lattice with $L_y = 5$ strip.

III. SOME CONNECTIONS TO QUANTUM COMPUTING

A. Partition Function Algorithm (Superpolynomial Speed)

As we have seen in the last section, the computation of Tutte polynomials is a $\#P$-hard problem [39]. This problem cannot be confronted using standard Turing machines and the corresponding classical computers. It is believed that quantum computers and specifically *topological quantum computers* [15] [16] are more efficient than classical computers when Tutte computations are involved.

For a *classical system* with a finite set of states S the partition function is given by the general (statistical mechanics) form of equation 4,

$$Z = \sum_{s \in S} e^{-E(s)/k_B T},$$

where T is the temperature and k_B is Boltzmann constant. Every thermodynamic quantity can be calculated by taking an appropriate partial derivative of the partition function. As we have seen in the last sessions, the partition function of the Potts model is a special case of the Tutte polynomial.

In 2007, a topological quantum algorithm, the *Aharonov-Arab-Ebal-Landau* (AAEL algorithm), was proposed for the approximated computation of numerical evaluations of the Tutte polynomial for any given network [17]. This includes an additive approximation of the partition function of the Potts model for any weighted planer graph at any temperature, as well as approximations to many other combinatorial graph properties described by the Tutte polynomial [18].

They make the following claim: *There exists an efficient quantum mechanical algorithm for the following problem. The input is a planar graph, with (complex) weights on the edges, and a (complex) number q. The output is an additive approximation of the (multivariate) Tutte polynomial of the graph with those weights.* However, their methods of proving universality seem to be not applicable for a physical Potts model (see Definition II.5) and they claim that the characterization of the quality of the algorithm for the Potts parameters is still an open problem, together with finding other non-unitary [40] representations of algebras to derive efficient quantum algorithms for combinatorial problems.

B. Knot Invariants Algorithms (Superpolynomial Speed)

A special case of the previous session was the work by of Aharonov, Jones and Landau regarding the *Jones polynomial* [18]. A special case of the multivariate Tutte polynomial of planar graphs is the Jones polynomial, where one can translate a planar graph to a knot in the 3D space. For a particular choice of weights and q, there is a simple connection between the Tutte polynomial of the original graph and the Jones polynomial of the knot, *i.e.,* Jones polynomial is a partition function in Potts model.

Consider a *braid* and represent it in an algebra spanned by objects similar to braids but with *no crossings*. This algebra is called the *Temperley Lieb algebra* [20] (in 1970, Temperley and Lieb also claimed that low temperature solutions of 2D-Potts model are related to the chromatic polynomial). The works results in an efficient quantum algorithm that approximates the Tutte Polynomial to an additive approximation (the norm of the overall product of operators is equal to the value of the Tutte polynomial). In [18], a quantum algorithm was developed to approximate the overall norm, to *inverse polynomial times the scale.*

Mike Freedman et al. showed that finding a certain additive approximation to the Jones polynomial of a braid at $e^{i2\pi/5}$ is a BQP-complete problem [14] [41]. Some connections between these approaches are discussed in by D. Lidar [21]. In *knot theory* one seeks to construct a topological invariant which is independent of the knot shape, lending to a number of *knot polynomials* (*e.g.,* the Jones polynomials). Two knots are topologically equivalent if they have the same knot polynomial. There is a connection between knot polynomials and the partition function of the Potts model. Considering a knot in 3D-space (*e.g.,* a piece of rope). The knot can be projected onto the 2D plane where the topological information is contained in the pattern of *crossings*, which is given by the *Betti number*, $b_k = \pm 1$, (see Fig. 10).

The connection to the Potts model is made by assigning random values to the crossing variables, b_k. In this case, the *Kauffman polynomial* is identical to the Potts Model partition function [22] (and the Jones and Kauffman polynomials coincide with the polynomial variable $q_{Jon} = q_{Kau}^{1/4}$). Therefore, the equivalence of the Kauffman polynomial to the Potts partition function is established when one assigns the Potts variables q and βJ_{ij} the values

$$q = (q_{Kau}^2 + q_{Kau}^{-2})^2,$$
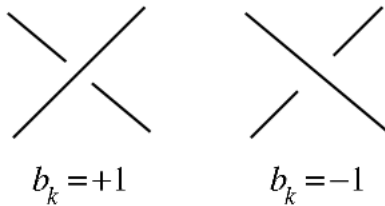
$$b_k = +1 \qquad b_k = -1$$

FIG. 10: The definition of crossing variables for knots, given by the Betti number [21].

and

$$\beta J_{ij} = \ln(-q_{Kau}^{4b_{ij}}).$$

Solving for q_{Kau} give

$$q_{Kau} = \pm[(q^{1/2} \pm (q-4)^{1/2})/2]^{1/2}.$$

Thus βJ_{ij} can be real only for $q \geq 4$. In the Ising case ($q = 2$), this value is complex, which implies complex-valued estimation of the polynomial.

Again, a physically unsatisfactory aspect of the knots-Potts connection is that the (complex-valued) temperature cannot be tuned independently from the bonds J_{ij}, which however does not matter from the computational complexity perspective.

Additional algorithms for estimating partition functions on quantum computers are given in [23], [24], [25], and [26]. In [24] a BQP-completeness result is presented, where the energies are allowed to be complex. In addition, an efficient quantum algorithm for the exact evaluation of either the fully ferromagnetic or anti-ferromagnetic q-state Potts partition function Z for a family of graphs is related to irreducible cyclic codes (which is related to the evaluation of the Jones and Tutte polynomials).

C. Applications on Topological Quantum Computing

A 2D quantum system with anyonic excitations can be considered as a quantum computer. Unitary transformations can be performed by moving the excitations around each other. Measurements can be performed by joining excitations in pairs and observing the result of fusion. Such computation is fault-tolerant by its physical nature. (Kitaev, 2008)

The great promise of quantum computers has to be worked against the difficulty of

building them. A fundamental challenge is to defeat decoherence and errors. Topological quantum computation is an approach that employs many-body physical systems with the unique property of encoding and processing quantum information in a naturally *fault-tolerant way* [28] [15] [16].

A topological quantum computer employs 2D quasiparticles, *i.e.,* anyons, whose world lines cross over one another to form braids in a 3D spacetime. The application of topology theory is seen in many cases such as the non-trivial example of the Temperle-Lieb recoupling, the so-called Fibonacci model, and the quantum computation of colored Jones polynomials and the Witten-Reshetikhin-Turaev Invariants [16] [27].

IV. DISCUSSION

In section I, we have introduced some aspects of the graph theory and discussed the chromatic and Tutte polynomials. In section II, the Potts Model were introduced and the exact calculations of the Potts model partition function $Z(G, q, v)$ for arbitrary q and temperature variable and equivalent Tutte polynomial $T(G, x, y)$ for arbitrary x and y on recursive families of graphs.

In section III, we proceed with an attempt of connecting the above theory to some recent results on quantum computing. In any of these subjects, the literature available is very extensive and dense. The discussion here intends to only give a very general idea of the field. Much more study and further derivations must be done before one acquires a reasonable understanding of the subject. Due to its scope, some of the following aspects were left for future studies:

- expanding the simulations for the exact calculations of the Potts model partition for arbitrary q and temperature variable, and equivalent Tutte polynomial, on recursive families of graphs;

- developing the mathematical aspects on graph theory regarding the Tutte Polynomials and the Chromatic Polynomials and relations to other invariants such as the Jones and Kaufman;

- explicitly deriving detailed proves of the complexity time relation for many of the cited quantum algorithms.

An interesting subject left out of this paper is, for instance, the study of the *Kramers-Wannier duality* of two-dimensional classical lattice models and the *topological symmetry* of interacting anyonic chains. This has applications to both classical and quantum lattice models. In classical models, this allows one to generalize duality to essentially any lattice (restricted) height model with an integrable critical point. In quantum models, this allows one to find ground states with non-abelian topological order, and moreover construct relatively simple local Hamiltonians with such ground states. Such models are also of interest for topological quantum computation.

Another current related field of studies is the *categorification* of the chromatic polynomial and its relations to relationship to the *Yamada polynomial* [34]. A very special case of spin networks (2-colored spin networks) is closely related to the chromatic polynomial for graphs. The study of the categorification of the chromatic polynomial is the simplest case for a quantum 3-manifold invariant.

The study of categories, and the possibility of developing higher dimension categories [30], have also implications in topological quantum computing. Examples of the connection of the field can be seen at [29], for example.

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[35] The term efficient or inefficient for algorithms is precisely defined by the computational complexity theory. An efficient algorithm runs in polynomial time to the size of the problem. An inefficient algorithm runs in superpolynomial (*e.g.,* exponential) time.

[36] Questions such as *which cubic graph has the largest real chromatic root?* are still open. Computation shows that among cubic graphs on up to 20 vertices (half million), the record holder has a real chromatic root at about 2.7712.

[37] A very exciting mathematical byproduct is that using quantum topology we find new algebraic proofs of the golden identity for the chromatic polynomial [9].

[38] A further analysis of many questions regarding to the properties of $\mathcal{B}$ can be discussed, regarding its symmetries, dimensionality in the q plane, topology of its curve, etc, can be seen in [12].

[39] A problem is polynomial time if there exists an algorithm which computes this function in a length of time (number of steps) bounded by a polynomial in the size of the problem. The class $\#P$ can be described as the class of enumeration problems in which the structures are recognizable in polynomial time. [17].

[40] A group representation is unitary if all matrices $D(g)$ are unitary. Every representation of a

compact finite group is equivalent to a unitary representation, $D^\dagger = D^{-1}$ [19].

[41] BQP (bounded error quantum polynomial time) is the class of decision problems solvable by a quantum computer in polynomial time, with an error probability of at most 1/3 for all instances.