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The Tutte–Potts connection in the presence of an external magnetic field

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A B S T R A C T

The classical relationship between the Tutte polynomial of graph theory and the Potts model of statistical mechanics has resulted in valuable interactions between the disciplines. Unfortunately, it does not include the external magnetic fields that appear in most Potts model applications. Here we define the $\boldsymbol{V}$-polynomial, which lifts the classical relationship between the Tutte polynomial and the zero field Potts model to encompass external magnetic fields. The $\boldsymbol{V}$-polynomial generalizes Noble and Welsh's W-polynomial, which extends the Tutte polynomial by incorporating vertex weights and adapting contraction to accommodate them. We prove that the variable field Potts model partition function (with its many specializations) is an evaluation of the $\boldsymbol{V}$-polynomial, and hence a polynomial with deletion–contraction reduction and Fortuin–Kasteleyn type representation. This unifies an important segment of Potts model theory and brings previously successful combinatorial machinery, including complexity results, to bear on a wider range of statistical mechanics models.

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1. Introduction

The classical relationship between the Tutte polynomial, $T(G; x, y)$, and the zero-field Potts model partition function, $Z(G; q, v)$, given by

$$Z(G; q, v) = q^{k(G)} v^{|V(G)|-k(G)} T\big(G; (q+v)/v, v+1\big), \tag{1}$$

where $v = e^{\beta J} - 1$, has resulted in valuable interactions between graph theory and statistical physics. This relation assumes a zero-field Hamiltonian (Eq. (2)). However, many applications of the Potts model depend on additional terms in the Hamiltonian corresponding to the presence of additional influences (for example the standard models of magnetism, the cellular Potts model of [4], and also see [11] for examples in the life sciences). Many of these models involve edge-dependent interaction energies and site dependent external fields. The classical Tutte–Potts connection, of Eq. (1), does not apply to these situations. Here we extend the Tutte–Potts connection so that it includes the influence of external fields.

Our main result is the assimilation of the following generic form of the Hamiltonian into the theory of the Tutte–Potts connection:

$$h(\sigma) = -\sum_{\{i,j\} \in E(G)} J_{i,j} \delta(\sigma_i, \sigma_j) - \sum_{v_i \in V(G)} \sum_{\alpha=1}^{q} M_{i,\alpha} \delta(\alpha, \sigma_i),$$

where a magnetic field vector $\boldsymbol{M}_i := \{M_{i,1}, M_{i,2}, \dots, M_{i,q}\}$ is associated to each vertex v_i. From this generic form we are able to specialize to various forms of the Hamiltonian with external fields that are common in the physics literature. To do this, we introduce the $\boldsymbol{V}$-polynomial, which is an extension of the Tutte polynomial to vertex-weighted graphs motivated by Noble and Welsh's W-polynomial from [10]. We prove that the Potts model partition function with an external field is an evaluation of the $\boldsymbol{V}$-polynomial. This gives the desired deletion–contraction reduction for the external field Potts model. The various partition functions may now be expressed as polynomials with Fortuin–Kasteleyn-type representations for them. Furthermore, this new relationship for the variable field Potts model extends the computational and analytic tools available to statistical mechanics applications. In particular, we are able to immediately transfer computational complexity results for the W- and U-polynomials to Potts model partition functions in broader settings.

2. Conventions

We assume that the reader is familiar with the connections between the Potts model and graph theory, surveyed, for example, in [1], [13] or [15]. We also assume a familiarity with Noble and Welsh's W-polynomial from [10].

2.1. The q-state Potts model

A *state* of a graph G is an assignment $\sigma : V(G) \to \{1, \dots, q\}$, for $q \in \mathbb{Z}^+$. We let $\mathcal{S}(G)$ denote the set of states of G, and $\sigma_i := \sigma(v_i)$, for $\sigma \in \mathcal{S}(G)$. At times we will use the indices $i = 1, \dots, n$ of the vertices in place of the vertices. We denote the interaction energy on an edge $e = \{v_i, v_j\}$ by $J_e := J_{i,j} (= J_{v_i,v_j})$, and let $j(\sigma) := -\sum_{e \in E(G)} J_e \delta(\sigma_i, \sigma_j)$. The *zero field Hamiltonian* is

$$h(\sigma) = -J \sum_{\{i,j\} \in E(G)} \delta(\sigma_i, \sigma_j), \tag{2}$$

where σ is a state of a graph G, where σ_i is the spin at vertex i, and where δ is the Kronecker delta function. To encompass various external fields and variable interaction energies, a more general form of the Hamiltonian is used.

If G is a graph with an interaction energy of J_e at each edge e, and a magnetic weight vector $\boldsymbol{M}_i := (M_{i,1}, M_{i,2}, \dots, M_{i,q})$ at each vertex v_i, then the *Hamiltonian of the Potts model with variable edge interaction energy and variable magnetic field* is

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i, \sigma_j) - \sum_{v_i \in V(G)} \sum_{\alpha=1}^{q} M_{i,\alpha}\delta(\alpha, \sigma_i). \tag{3}$$

Regardless of the choice of Hamiltonian, the *Potts model partition function* is the sum over all possible states of an exponential function of the Hamiltonian:

$$Z(G) = \sum_{\sigma \in \mathcal{S}(G)} \mathrm{e}^{-\beta h(\sigma)}, \tag{4}$$

where $\beta = 1/(\kappa T)$, where T is the temperature of the system, and where $\kappa = 1.38 \times 10^{-23}$ joules/Kelvin is the Boltzmann constant.

2.2. Deletion and contraction in vertex weighted graphs

We use standard notation for graphs. $E(G)$ and $V(G)$ denote the edge set and vertex set, respectively, of a graph G. If $A \subseteq E(G)$, then $n(A)$, $r(A)$, and $k(A)$ are, respectively, the nullity, rank, and number of components of the spanning subgraph of G with edge set A. Here, a *vertex weighted graph* consists of a graph G, with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ equipped with a weight function ω mapping $V(G)$ into a torsion-free commutative semigroup. The *weight* of the vertex v_i is the value $\omega(v_i)$. We will often write ω_i rather than $\omega(v_i)$, and $\boldsymbol{x}$ for an indexed set of variables. An *edge weighted* graph G is a graph equipped with a mapping γ from its edge set $E(G)$ to a set $\boldsymbol{\gamma} := \{\gamma_e\}_{e\in E(G)}$. We use the standard convention $\gamma : e \mapsto \gamma_e$, for $e \in E(G)$.

If G is a vertex weighted graph with weight function ω, and e is an edge of G, then $G - e$ is the graph obtained from G by deleting the edge e and leaving the weight function unchanged. If e is any non-loop edge of G, then G/e is the graph obtained from G by contracting the edge e and changing the weight function as follows: if v_i and v_j are the vertices incident to e, and v is the vertex of G/e created by the contraction, then $\omega(v) = \omega(v_i) + \omega(v_j)$. Loops are not contracted.

3. The $\boldsymbol{V}$-polynomial

Here we introduce the $\boldsymbol{V}$-polynomial, which is an extension of the W-polynomial of Noble and Welsh [10] to graphs that have both edge weights and more general vertex weights.

Definition 3.1. Let S be a torsion-free commutative semigroup, let G be a graph equipped with vertex weights $\boldsymbol{\omega} := \{\omega_i\} \subseteq S$ and edge weights $\boldsymbol{\gamma} := \{\gamma_e\}$, and let $\boldsymbol{x} = \{x_k\}_{k\in S}$ be a set of commuting variables. Then the *$\boldsymbol{V}$-polynomial*, $\boldsymbol{V}(G) = \boldsymbol{V}(G, \omega; \boldsymbol{x}, \boldsymbol{\gamma}) \in \mathbb{Z}[\{\gamma_e\}_{e\in E(G)}, \{x_k\}_{k\in S}]$, of the vertex and edge weighted graph G, is defined recursively by:

1. $\boldsymbol{V}(G) = \boldsymbol{V}(G - e) + \gamma_e \boldsymbol{V}(G/e)$, if e is a non-loop edge of G;
2. $\boldsymbol{V}(G) = (\gamma_e + 1)\boldsymbol{V}(G - e)$, if e is a loop;
3. $\boldsymbol{V}(E_m) = \prod_{i=1}^{m} x_{\omega_i}$, if E_m consists of m isolated vertices of weights $\omega_1, \dots, \omega_m$.

We now state several basic results about the $\boldsymbol{V}$-polynomial. The proofs of most of these results are straight-forward adaptations of Noble and Welsh's proofs of the corresponding results about the W-polynomial from [10], and hence we omit the details. Full details may be found in an expanded version of this paper at http://arxiv.org/abs/1005.5470.

Proposition 3.2. *The polynomial $\boldsymbol{V}$ is well defined in the sense that the polynomial is independent of the order in which the deletion–contraction relation is applied to the edges.*

Sketch of Proof. The proof is by induction on the number of edges of G. The result clearly holds for all graphs with fewer than two edges. Calculate $\boldsymbol{V}(G)$ by applying the deletion–contraction relation to the edge e first, and f second; then showing that the same expression results when the order is reversed completes the proof. □

Theorem 3.3. *$\boldsymbol{V}(G)$ can be represented as a sum over spanning subgraphs*:

$$\boldsymbol{V}(G) = \sum_{A \subseteq E(G)} x_{c_1} x_{c_2} \cdots x_{c_{k(A)}} \prod_{e \in A} \gamma_e,$$

where c_l is the sum of the weights of all of the vertices in the l-th connected component of the spanning subgraph $(V(G), A)$.

Sketch of Proof. Again the result follows by induction: fix a non-loop edge e, split the sum into A with $e \in A$, and A with $e \notin A$, then use the natural bijection between the spanning subgraphs of G that contain the edge e and the spanning subgraphs of G/e, and the obvious correspondence between the spanning subgraphs of $G - e$ and the spanning subgraphs of G that do not contain e. □

Theorem 3.4. *Let f be a function on vertex and edge weighted graphs defined recursively by the following conditions* (*where each $\alpha_e \neq 0$*):

1. $f(G) = \alpha_e f(G - e) + \beta_e f(G/e)$, *when e is a non-loop edge*;
2. $f(G) = (\alpha_e + \beta_e) f(G - e)$, *when e is a loop*;
3. $f(E_m) = \prod_{i=1}^{m} x_{\omega_i}$, *when E_m consists of m isolated vertices with weights $\omega_1, \ldots, \omega_m$*.

Then $f(G) = (\prod_{e \in E(G)} \alpha_e) \boldsymbol{V}(G, \omega; \boldsymbol{x}, \{\beta_e/\alpha_e\}_{e \in E(G)})$.

Proof. Let $\tilde{f} := f/(\prod_{e \in E(G)} \alpha_e)$, and let $\gamma_e := \beta_e/\alpha_e$. Then $\tilde{f}(G) = \tilde{f}(G - e) + \gamma_e \tilde{f}(G/e)$, when e is a non-loop edge of G, and $\tilde{f}(G) = (1 + \gamma_e)\tilde{f}(G - e)$, when e is a loop. So $\tilde{f}$ is equal to the $\boldsymbol{V}$-polynomial and the result follows. □

The $\boldsymbol{V}$-polynomial extends both the multivariate Tutte polynomial, Z_T (see [13] and [14]), and Noble and Welsh's W-polynomial [10] as described in the following theorem.

Theorem 3.5. *The $\boldsymbol{V}$-polynomial generalizes both the W-polynomial and the multivariate Tutte polynomial.*

1. *If $\omega : V(G) \to \mathbb{Z}^+$ and $\gamma_e = (y - 1)$ for each $e \in E(G)$, then*

$$\boldsymbol{V}\big(G, \omega; \boldsymbol{x}, \gamma_e = (y-1)\big) = (y-1)^{|V(G)|} W\big(G, \omega; \boldsymbol{x}/(y-1), y\big).$$

2. *If $x_i = \theta$, for each $i \in \mathbb{Z}^+$, then, independently of the weights ω,*

$$\boldsymbol{V}(G, \omega; x_i = \theta, \boldsymbol{\gamma}) = Z_T(G; \theta, \boldsymbol{\gamma}).$$

Proof. The first item follows from the recipe theorem for $\boldsymbol{V}$ (Theorem 3.4) using $f(G) = (y-1)^{|V(G)|} W(G; \boldsymbol{x}/(y-1), y)$. The second item follows by comparing the state sum for the $\boldsymbol{V}$-polynomial and the multivariate Tutte polynomial. □

It follows from Theorem 3.5 that the $\boldsymbol{V}$-polynomial also extends the classical Tutte polynomial.

4. The *V*-polynomial and the Potts model in an external field with edge dependent interaction energies

We now come to our reason for creating the ***V***-polynomial. Here we show that the Potts model partition function with the Hamiltonian $h(\sigma)$ from Eq. (3) is an evaluation of the ***V***-polynomial. This provides a recursive deletion–contraction definition for the full Potts partition function with variable edge interaction energy and variable magnetic field, and also shows that it is a polynomial.

Theorem 4.1. *Let G be a graph equipped with a magnetic field vector $\boldsymbol{M}_i = (M_{i,1}, \dots, M_{i,q}) \in \mathbb{C}^q$ at each vertex v_i, and let $h(\sigma)$ be the Hamiltonian given in Eq.* (3)*. Then*

1. $Z(G) = Z(G-e) + (\mathrm{e}^{\beta J_{i,j}} - 1)Z(G/e)$, *if $e = \{v_i, v_j\}$ is a non-loop edge of G;*
2. $Z(G) = \mathrm{e}^{\beta J_{i,i}} Z(G-e)$, *if $e = \{v_i, v_i\}$ is a loop;*
3. $Z(E_n) = \prod_{i=1}^n X_{\boldsymbol{M}_i}$, *where E_n consists of n isolated vertices of vector valued weights $\boldsymbol{M}_1, \boldsymbol{M}_2, \dots, \boldsymbol{M}_n$, and, for any weight $\boldsymbol{M}_i$, we write $X_{\boldsymbol{M}_i} := \sum_{\alpha=1}^q \mathrm{e}^{\beta M_{i,\alpha}}$.*

Proof. For item 1, let $e = \{v_a, v_b\}$ be a non-loop edge of G. By simplifying and collecting together the states in which $\sigma_a \neq \sigma_b$, and in which $\sigma_a = \sigma_b$, we can write

$$Z(G) = \sum_{\substack{\sigma \in \mathcal{S}(G) \\ \sigma_a \neq \sigma_b}} \mathrm{e}^{-\beta j(\sigma)} \prod_{v_i \in V(G)} \mathrm{e}^{\beta M_{i,\sigma_i}} + \sum_{\substack{\sigma \in \mathcal{S}(G) \\ \sigma_a = \sigma_b}} \mathrm{e}^{-\beta j(\sigma)} \prod_{v_i \in V(G)} \mathrm{e}^{\beta M_{i,\sigma_i}}. \tag{5}$$

If σ is any state of G, then there is a unique state σ' of $G-e$ where each vertex has the same spin as it has in σ. Using this correspondence, we can index the sums in Eq. (5) over $\mathcal{S}(G-e)$, instead of $\mathcal{S}(G)$, provided that we multiply the right-hand sum by $\mathrm{e}^{\beta J_e}$. The left-hand sum, which is over states of $G-e$ with $\sigma_a \neq \sigma_b$ is nearly $Z(G-e)$, but we are missing the states where $\sigma_a = \sigma_b$. Add and subtract these states to the expression, so that the left-hand sum becomes $Z(G-e)$, and the factor in front of the right-hand sum becomes $(\mathrm{e}^{\beta J_e} - 1)$.

For the right-hand sum, if $\sigma \in \mathcal{S}(G-e)$ with $\sigma_a = \sigma_b$, then there is a unique state $\sigma'' \in \mathcal{S}(G/e)$, where the vertex v_c resulting from identifying v_a and v_b has the spin $\sigma_c = \sigma_a = \sigma_b$, and each remaining vertex has the same spin as in σ. We immediately have $j(\sigma) = j(\sigma'')$. Now, for a state σ with $\sigma_a = \sigma_b$, we have

$$\prod_{v_i \in V(G-e)} \mathrm{e}^{\beta M_{i,\sigma_i}} = \left(\mathrm{e}^{\beta(M_{a,\sigma_a} + M_{b,\sigma_a})}\right) \prod_{\substack{v_i \in V(G-e) \\ i \neq a \text{ or } b}} \mathrm{e}^{\beta M_{i,\sigma_i}} = \prod_{v_i \in V(G/e)} \mathrm{e}^{\beta M_{i,\sigma_i}}.$$

Here the first equality uses the fact that $\sigma_a = \sigma_b$, and the second equality uses the fact that $\boldsymbol{M}_c = \boldsymbol{M}_a + \boldsymbol{M}_b$, and so $M_{a,\sigma_a} + M_{b,\sigma_a} = M_{c,\sigma_a}$. This allows us to express the right-hand sum in Eq. (5) as $Z(G/e)$. Remembering the factors, this gives $Z(G) = Z(G-e) + (\mathrm{e}^{\beta J_e} - 1)Z(G/e)$, as required.

Item 2 can be proved by following the proof of item 1 and noting that the left-hand sum in Eq. (5) is empty.

Finally, if G consists of a single isolated vertex, it is easily checked that $Z(G) = \sum_{\alpha=1}^q \mathrm{e}^{\beta M_{1,\alpha}}$. Item (3) then follows by the multiplicativity of the partition function. $\square$

The following theorem is the main result of this paper. It states that the Potts model partition function with a variable external magnetic field and variable edge interaction is an evaluation of the ***V***-polynomial.

Theorem 4.2. *Let G be a graph equipped with a magnetic field vector $\boldsymbol{M}_i = (M_{i,1}, \dots, M_{i,q}) \in \mathbb{C}^q$ at each vertex v_i, and let $h(\sigma)$ be the Hamiltonian given in Eq.* (3)*. Then*

$$Z(G) = \boldsymbol{V}\big(G, \omega; \{X_{\boldsymbol{M}}\}_{\boldsymbol{M}\in\mathbb{C}^q}, \big\{e^{\beta J_{i,j}} - 1\big\}_{\{i,j\}\in E(G)}\big),$$

where the vertex weights are given by $\omega(v_i) = \boldsymbol{M}_i$ *and, for any* $\boldsymbol{M} = (M_1, \ldots, M_q) \in \mathbb{C}^q$*, we have* $X_{\boldsymbol{M}} = \sum_{\alpha=1}^{q} e^{\beta M_\alpha}$.

Proof. The equality of $Z(G)$ and the $\boldsymbol{V}$-polynomial follows immediately from Theorem 4.1 and the recipe theorem for the $\boldsymbol{V}$-polynomial (Theorem 3.4). □

As a corollary to this theorem we obtain a Fortuin–Kasteleyn-type representation for the Potts model with variable external magnetic field and variable edge interaction.

Corollary 4.3. *Let G be a graph equipped with a magnetic field vector* $\boldsymbol{M}_i = (M_{i,1}, \ldots, M_{i,q}) \in \mathbb{C}^q$ *at each vertex* v_i*, and Hamiltonian* $h(\sigma)$ *as in Eq.* (3)*. Then*

$$Z(G) = \sum_{A\subseteq E(G)} X_{\boldsymbol{M}_{C_1}} \cdots X_{\boldsymbol{M}_{C_{k(A)}}} \prod_{e\in A}\big(e^{\beta J_e} - 1\big),$$

where $\boldsymbol{M}_{C_l}$ *is the sum of the weights,* $\boldsymbol{M}_i$*, of all of the vertices* v_i *in the l-th connected component of the spanning subgraph* $(V(G), A)$*, and* $X_{\boldsymbol{M}} = \sum_{\alpha=1}^{q} e^{\beta M_\alpha}$.

Proof. The result follows immediately from Theorem 4.2 and Theorem 3.3. □

Since the $\boldsymbol{V}$-polynomial of a graph G is a polynomial in $\mathbb{Z}[\{x_k\}, \{\gamma_e\}]$, we can use the relation between the $\boldsymbol{V}$-polynomial and the Potts model to express the q-state Potts model partition function with variable edge interaction energy and variable magnetic field as a polynomial.

Corollary 4.4. *For a connected graph G equipped with a magnetic field vector* $\boldsymbol{M}_i = (M_{1,1}, \ldots, M_{i,q}) \in \mathbb{C}^q$ *at each vertex* v_i*, the q-state Potts model partition function with variable edge interaction energy and variable magnetic field is a polynomial in the variables* $\{\boldsymbol{v}, X_{\boldsymbol{M}} \mid \boldsymbol{M} \in \mathcal{M}\}$*, where* $\boldsymbol{v} = \{e^{\beta J_e} - 1\}_{e\in E(G)}$*, and* $X_{\boldsymbol{M}} = \sum_{\alpha=1}^{q} e^{\beta M_\alpha}$ *for* $\mathcal{M} := \{\sum_{i=1}^{|V(G)|} \varepsilon_i \boldsymbol{M}_i \mid \varepsilon_i = 0 \text{ or } 1\}$.

5. Hamiltonians and a hierarchy of graph polynomials

The $\boldsymbol{V}$-polynomial provides a unifying framework for Potts models with various Hamiltonians. We show how Theorem 4.2 can be applied to various forms of Hamiltonian to provide a hierarchy of relations among the resulting partition functions, $Z(G)$, and the W-, U-, multivariate Tutte, and Tutte polynomials.

The following result says that if we restrict to the Potts model with constant interaction energies and where all the magnetic field vectors are positive integer multiples of a given magnetic field vector, then the partition function is described by the W-polynomial.

Theorem 5.1. *Let* $\boldsymbol{B} \in \mathbb{C}^q$*, and let G be a graph equipped with constant edge weights* J*, and a magnetic field vector* $\boldsymbol{M}_i := k_i\boldsymbol{B} = k_i(B_1, \ldots, B_q)$ *at each vertex* v_i*, where* $k_i \in \mathbb{Z}^+$*. If the Hamiltonian* $h(\sigma)$ *is as in Eq.* (3)*, then*

$$Z(G) = \big(e^{\beta J} - 1\big)^{|V(G)|} W\big(G, \omega; \{x_k\}_{k\in\mathbb{Z}^+}, e^{\beta J}\big),$$

where $x_k = (\sum_{\alpha=1}^{q} e^{\beta k B_\alpha})/(e^{\beta J} - 1)$*, and* B_α *is the* α*-entry of* $\boldsymbol{B}$.

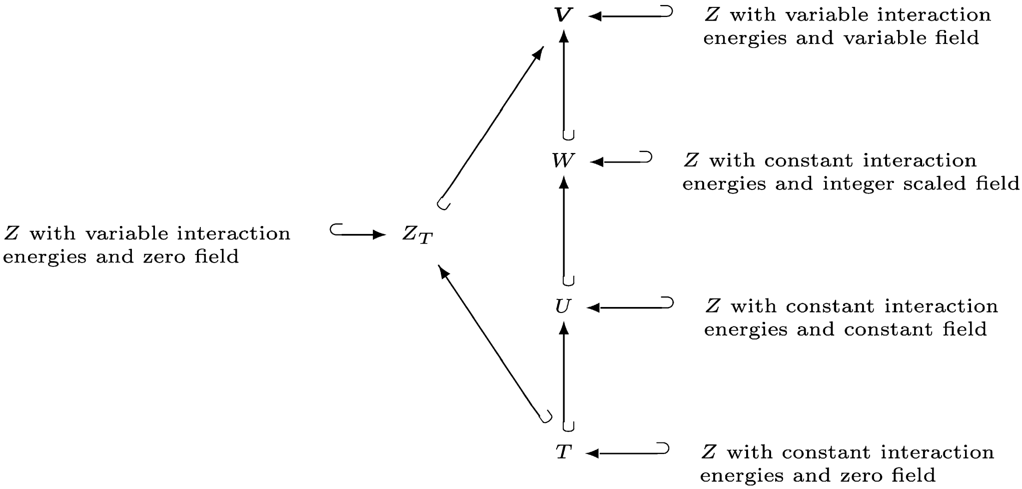

Fig. 1. A hierarchy of graph polynomials and Hamiltonians.

Proof. Setting each $J_{i,j} = J$ in Theorem 4.2 gives $Z(G) = \boldsymbol{V}(G, \omega; \{X_{\boldsymbol{M}}\}_{\boldsymbol{M}\in\mathbb{Z}^{+q}}, \gamma_e = \mathrm{e}^{\beta J} - 1)$, where the $X_{\boldsymbol{M}}$ are defined in Theorem 4.2. Each index $\boldsymbol{M}$, of $X_{\boldsymbol{M}}$, is then of the form $k\boldsymbol{B}$ for some $k \in \mathbb{Z}^+$. Therefore $X_{\boldsymbol{M}} = X_{k\boldsymbol{B}} = \sum_{\alpha=1}^{q} \mathrm{e}^{\beta k B_\alpha}$, where B_α is the α-entry of $\boldsymbol{B}$. Since every index is of the form $k\boldsymbol{B}$, the indexing set is isomorphic to $\mathbb{Z}^+$. Thus, we can choose our indexing set to be $\mathbb{Z}^+$, letting $X_k = \sum_{\alpha=1}^{q} \mathrm{e}^{\beta k B_\alpha}$. Applying Theorem 3.5 then gives $Z(G) = (\mathrm{e}^{\beta J} - 1)^{|V(G)|} W(G, \omega; \{x_k\}_{k\in\mathbb{Z}^+}, \mathrm{e}^{\beta J})$, where $x_k = (\sum_{\alpha=1}^{q} \mathrm{e}^{\beta k B_\alpha})/(\mathrm{e}^{\beta J} - 1)$. □

The U-polynomial [10] is an adaptation of the W-polynomial to unweighted graphs. The U-polynomial is defined simply by assigning the weight 1 to each vertex and then taking the W-polynomial of the resulting weighted graph. The U-polynomial describes the Potts model for constant edge interaction energy and fixed magnetic field vectors.

Theorem 5.2. *Let G be a graph equipped with a fixed magnetic field vector $\boldsymbol{B} = (B_1, \ldots, B_\alpha)$ at each vertex, and constant edge weights J. If the Hamiltonian $h(\sigma)$ is as in Eq.* (3) *then*

$$Z(G) = \left(\mathrm{e}^{\beta J} - 1\right)^{|V(G)|} U\left(G, \omega; \{x_k\}_{k\in\mathbb{Z}^+}, \mathrm{e}^{\beta J} - 1\right),$$

where $x_k := (\sum_{\alpha=1}^{q} \mathrm{e}^{\beta k B_\alpha})/(\mathrm{e}^{\beta J} - 1)$, and B_α is the α-entry of $\boldsymbol{B}$.

Proof. The result follows easily from Theorem 5.1 upon noting that the vector $1\boldsymbol{B}$ is the vertex weight of each vertex of G. □

The classic result of Eq. (1) relating the Potts model and the Tutte polynomial, as well as the edge weighted version that if $h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i, \sigma_j)$, then $Z(G) = Z_T(G; q, \{\mathrm{e}^{\beta J_{i,j}} - 1\}_{\{i,j\}\in E(G)})$, can also be recovered from Theorem 4.1 and Theorem 3.5.

From the preceding theorems, we have a hierarchy (shown in Fig. 1) of relations among the $\boldsymbol{V}$-, W-, U-, and Tutte polynomials, and the partition functions with Hamiltonians of various degrees of generality. This hierarchy also adapts to the single preferred spin models of Theorems 6.1 and 6.2 below.

6. Applications to common models

Here we highlight some special forms of the magnetic weight vectors and resulting Hamiltonians that are frequently studied in the physics literature. We show how the associated partition functions are evaluations of the $\boldsymbol{V}$-polynomial and its specializations. This implies that these important models are also polynomials with deletion–contraction reductions. Our results can also be used to find Fortuin–Kasteleyn-type representations for these common models.

Our first example of a Hamiltonian that is of particular interest in the physics literature models a system with an external field in which one particular spin is preferred (see for example the surveys [2,16]). Here again, variable interaction energies and magnetic field values are allowed. In this case we have the following relation with the $\boldsymbol{V}$-polynomial.

Theorem 6.1. *Suppose a complex value z_i is associated to each vertex v_i of a graph G, and the Hamiltonian is given by*

$$h(\sigma) = -\sum_{\{i,j\}\in E} J_{i,j}\delta(\sigma_i,\sigma_j) - \sum_{v_i\in V(G)} z_i\delta(1,\sigma_i). \tag{6}$$

Then

$$Z(G) = \boldsymbol{V}\big(G,\omega;\{X_z\}_{z\in\mathbb{C}},\big\{\mathrm{e}^{\beta J_e}-1\big\}_{e\in E(G)}\big),$$

where the vertex weights are given by $\omega(v_i)=z_i$ and $X_z=\mathrm{e}^{\beta z}+q-1$.

Sketch of Proof. Associate a magnetic field vector, $\boldsymbol{M}_i=(z_i,0,\dots,0)$, with each vertex v_i of G. Set $\hat{h}(\sigma) := -\sum_{\{i,j\}\in E(G)} J_{i,j}\delta(\sigma_i,\sigma_j) - \sum_{v_i\in V(G)}\sum_{\alpha=1}^{q} M_{i,\alpha}\delta(\alpha,\sigma_i)$, so $Z(G)=\sum_{\sigma\in\mathcal{S}(G)}\mathrm{e}^{-\beta h(\sigma)} = \sum_{\sigma\in\mathcal{S}(G)}\mathrm{e}^{-\beta\hat{h}(\sigma)}$. Theorem 4.2 with the Hamiltonian $\hat{h}$ yields that $Z(G)=\boldsymbol{V}(G,\omega;\{X_{\boldsymbol{M}}\}_{\boldsymbol{M}\in\mathbb{C}^q}, \{\mathrm{e}^{\beta J_e}-1\}_{e\in E(G)})$, where the vertex weights are given by $\omega(v_i)=\boldsymbol{M}_i$ and, for any $\boldsymbol{M}\in\mathbb{C}^q$, $X_{\boldsymbol{M}}=\sum_{\alpha=1}^{q}\mathrm{e}^{\beta M_\alpha}$, where M_α is the α-entry of $\boldsymbol{M}$. However, the only indices $\boldsymbol{M}\in\mathbb{C}^q$ that actually appear are of the form $(z,0,\dots,0)$ for some $z\in\mathbb{C}$, and if $\boldsymbol{M}$ has this form, then $X_{\boldsymbol{M}}=\mathrm{e}^{\beta z}+q-1$. Thus, we can choose our indexing set to be $\mathbb{C}$ instead of $\mathbb{C}^q$, so that $Z(G)=\boldsymbol{V}(G,\omega;\{X_z\}_{z\in\mathbb{C}},\{\mathrm{e}^{\beta J_e}-1\}_{e\in E(G)})$, where $X_z=\mathrm{e}^{\beta z}+q-1$, as claimed. □

When the Hamiltonian is that of Eq. (6), a Fortuin–Kasteleyn-type representation for the Potts model is well known. This Fortuin–Kasteleyn-type representation can be immediately recovered from Corollary 4.3 and Theorem 6.1.

In [12], Sokal studied the Potts model partition function in the case where the magnetic field vectors are of the form $\boldsymbol{M}_i=(M_{i,1},M_{i,2},\dots,M_{i,r},0,\dots,0)$, where $0\leqslant r\leqslant q$ is fixed. With these magnetic field vectors, Theorem 4.2 immediately gives the following result.

Theorem 6.2. *Let G be a graph where each vertex v_i is equipped with a magnetic field vector $\boldsymbol{M}_i = (M_{i,1},M_{i,2},\dots,M_{i,r},0,\dots,0)$, and let $h(\sigma)$ be the Hamiltonian given in Eq.* (3). *Then*

$$Z(G) = \boldsymbol{V}\big(G,\omega;\{X_{\boldsymbol{M}}\}_{\boldsymbol{M}\in\mathbb{C}^q},\big\{\mathrm{e}^{\beta J_{a,b}}-1\big\}_{\{a,b\}\in E(G)}\big),$$

where the vertex weights are given by $\omega(v_i)=\boldsymbol{M}_i$, and, for any $\boldsymbol{M}\in\mathbb{C}^q$, $X_{\boldsymbol{M}}=q-r+\sum_{\alpha=1}^{r}\mathrm{e}^{\beta M_\alpha}$, where M_α is the α-entry of $\boldsymbol{M}$.

In [12], Sokal found a Fortuin–Kasteleyn-type representation for the partition function used in the above theorem. We observe that his Fortuin–Kasteleyn-type representation can be immediately recovered from Corollary 4.3 and Theorem 6.2.

Our final example relates to the Ising model used to study glassy behaviors. We show that the $\boldsymbol{V}$-polynomial assimilates both the Ising spin glass model (which has edge dependent random bond strengths J_e, but no external field), and the Random Field Ising Model (RFIM) (which has a random magnetic field in that the z_i's are randomly chosen local magnetic fields that each affect only a single site). To avoid redundancy of proof, we merge the two models in the following theorem (this generalization is also sometimes called the RFIM), from which each may be recovered.

The RFIM takes spin values in $\{-1, 1\}$. We will let τ denote a state for the RFIM, which is a map $\tau : V(G) \to \{-1, +1\}$. As usual we set $\tau_i := \tau(v_i)$. Also we will let $\mathcal{T}(G)$ be the set of states for the Ising model.

Theorem 6.3. *Let G be a graph with a vertex weight $\omega(v_i) = z_i \in \mathbb{C}$ associated to each vertex v_i, and suppose the Hamiltonian and partition function are given by*

$$h(\tau) = -\sum_{\{i,j\}\in E(G)} J_{i,j}\tau_i\tau_j - \sum_{v_i\in V(G)} z_i\tau_i \quad \text{and} \quad Z(G) = \sum_{\tau\in\mathcal{T}(G)} \mathrm{e}^{-\beta h(\tau)}. \tag{7}$$

Then

$$Z(G) = \mathrm{e}^{-\beta\eta(G)} \boldsymbol{V}\left(G, \omega; \{x_z\}_{z\in\mathbb{C}}, \left\{\mathrm{e}^{2\beta J_e} - 1\right\}_{e\in E(G)}\right) = \sum_{A\subseteq E(G)} x_{z_{C_1}} \cdots x_{z_{C_{k(A)}}} \prod_{e\in A}\left(\mathrm{e}^{\beta J_e} - 1\right),$$

where for any $z \in \mathbb{C}$, $x_z = \mathrm{e}^{2z} + \mathrm{e}^{4z}$; $\eta(G) = \sum_{e\in E} J_e + 3\sum_{i\in V(G)} z_i$; and in the Fortuin–Kasteleyn-type representation, z_{C_l} is the sum of the weights, z_i, of all of the vertices v_i in the l-th connected component of the spanning subgraph $(V(G), A)$.

Proof. There is a natural bijection between $\mathcal{T}(G)$ and $\mathcal{S}(G) = \{\sigma : V(G) \to \{1, 2\}\}$, which, given $\tau \in \mathcal{T}(G)$, is determined by setting $\sigma_i = 1$ if $\tau_i = -1$, and $\sigma_i = 2$ if $\tau_i = +1$. Under this bijection, observe that $\tau_i = 2\sigma_i - 3$ and $\tau_i\tau_j = 2\delta(\sigma_i, \sigma_j) - 1$, and so we may write the Hamiltonian in Eq. (7) as

$$h(\sigma) = -2\sum_{\{i,j\}\in E(G)} J_{i,j}\delta(\sigma_i, \sigma_j) - 2\sum_{i\in V(G)} z_i\sigma_i + \sum_{\{i,j\}\in E} J_{i,j} + 3\sum_{i\in V(G)} z_i. \tag{8}$$

With this Hamiltonian, $Z(G) = \sum_{\tau\in\mathcal{T}(G)} \mathrm{e}^{-\beta h(\tau)} = \sum_{\sigma\in\mathcal{S}(G)} \mathrm{e}^{-\beta h(\sigma)}$. Let $\tilde{h}(\sigma)$ denote the first two terms on the right of Eq. (8), and $\eta(G)$ denote the last two. Then $Z(G) = \mathrm{e}^{-\beta\eta(G)} \sum_{\sigma\in\mathcal{S}(G)} \mathrm{e}^{-\beta\tilde{h}(\sigma)}$. Theorem 4.2 then gives

$$Z(G) = \mathrm{e}^{-\beta\eta(G)} \boldsymbol{V}\left(G, \omega; \{X_{\boldsymbol{M}}\}_{\boldsymbol{M}\in\mathbb{C}^2}, \left\{\mathrm{e}^{2\beta J_e} - 1\right\}_{e\in E(G)}\right),$$

where the weight function ω is now $\omega_i = \boldsymbol{M}_i := 2z_i(1, 2) \in \mathbb{C}^2$, and, if $\boldsymbol{M} = z(1, 2)$ then $X_{\boldsymbol{M}} = \sum_{\alpha=1}^{2} \mathrm{e}^{\beta M_\alpha} = \mathrm{e}^{2z} + \mathrm{e}^{4z}$. The theorem then follows by observing that since each $\boldsymbol{M} = z(1, 2)$, for some $z \in \mathbb{C}$, we can take $\mathbb{C}$ as the indexing set instead of $\mathbb{C}^2$. $\square$

While we have given examples of several Potts models that may be unified by the $\boldsymbol{V}$-polynomial, this list is not exhaustive, being only intended to illustrate the applications and techniques. Because of the generality of the indexing set, even Theorem 4.2 might be adapted to other applications. A more ambitious direction would be determining if non-linear terms in the Hamiltonian, such as the squared differences that appear in some biological models (see [4,11] for example), might be assimilated into this theory in some way.

7. Computational complexity

Realizing the Potts model partition function as an evaluation of the $\boldsymbol{V}$-polynomial now means that the computational complexity results for the W-polynomial apply directly to partition functions with an external field. We collect some of these here, drawing on the work of Noble and Welsh [10], and Noble [9].

It is not surprising that the computational complexity consequences of Theorem 4.1 for the variable field Potts model are somewhat bleak. Noble and Welsh [10] have shown that computing any coefficient of the W-polynomial is $\sharp$P-hard even for trees, and specific coefficients are $\sharp$P-hard for complete graphs. Thus the complexity of the variable field Potts model is at least as problematic (presumably more so if variable interaction energies are also used). Additionally, Noble and Welsh [10] have shown that computing evaluations of the W-polynomial, and hence the Potts model partition function with external field, is $\sharp$P-hard not only for trees, but even just for stars.

The prognosis in the case of a constant, but non-zero, magnetic field, is somewhat better. As noted above, the U-polynomial corresponds to a constant magnetic field vector. Noble [9] has shown that if G is a graph with tree-width at most K, then the U-polynomial, and hence the partition function of G, may be evaluated at any point in roughly $O(a_K n^{2K+3})$ arithmetic operations.

Complexity results for the Ising model, essentially the $q = 2$ Potts model, differ significantly from the general Potts model. In particular, the partition function for the Ising model with zero field and constant interaction energies can be reformulated as a tractable problem for planar graphs (see [3,8,6]). Considerable work has been done investigating the computational complexity of the variable field Ising model under several conditions, notably by Goldberg and Jerrum [5], and Jerrum and Sinclair [7]. These include complexity classifications and, where possible, approximation algorithms for the Ising model with different restrictions on the interaction energies and magnetic fields. In particular there is no fully polynomial randomized approximation scheme (FPRAS) in the antiferromagetic case, but there is a FPRAS in the ferromagnetic case provided that all the local magnetic field values have the same sign. Without this restriction on the magnetic field values, the problem again becomes intractable.

However, Theorems 5.1 and 6.3 imply that the Ising model with constant interaction energies and a constant magnetic field vector (without all entries necessarily having the same sign), is an evaluation of the U-polynomial. Thus, by the results of Noble [9], it may be computed in polynomial time for graphs with bounded tree-width. It is very likely that this result may be improved by restricting to the $q = 2$ case of the Ising model, and also likely that these results might be extended to variable interaction energies. Applying the theory in the other direction, the complexity results for approximating the Ising model with external field from *e.g.* [5,7] now immediately apply to give computational complexity information for the V-polynomial when $q = 2$.

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