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New graph polynomials from the Bethe approximation of the Ising partition function

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We introduce two graph polynomials and discuss their properties. The one is a polynomial of two variables, motivated by performance analysis of the Bethe approximation of the Ising partition function. The other polynomial of one variable is obtained by its specialization. It is shown that these polynomials satisfy deletion-contraction relations and are new examples of V-function, which is introduced by Tutte (1947, Proc. Cambridge Philos. Soc. 43, 26-40). For these polynomials, we discuss interpretations of special values, and then obtain the bound on the number of sub-coregraphs, i.e., the spanning subgraphs with no vertices of degree one. It is proved that the polynomial of one variable is equal to the monomer-dimer partition function with weights parameterized by that variable. Properties of the coefficients and the possible region of zeros are also discussed for this polynomial.

1. Introduction and terminologies

1.1. Introduction

The aim of this paper is to introduce two new graph polynomials and study their properties. The first one is a two-variable polynomial denoted by $\theta_G(\beta, \gamma)$ and the second one is a one-variable polynomial denoted by $\omega_G(\beta)$, which is obtained as a specialization of θ_G.

Partition functions studied in statistical physics have been a source of various graph polynomials. For example, the partition functions of the q-state Potts model and the bivariated random-cluster model of Fortuin and Kasteleyn derive graph polynomials. They are known to be equivalent to the Tutte polynomial [4]. Another example is the monomer-dimer partition function with uniform monomer and dimer weights, which is essentially the matching polynomial [15].

The polynomial θ_G comes from the problem of computing the Ising partition function

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defined by

$$Z(G;\boldsymbol{J},\boldsymbol{h}) := \sum_{x_1,\ldots,x_N=\pm 1} \exp\Big(\sum_{\substack{e\in E\\ e=ij}} J_e x_i x_j + \sum_{i\in V} h_i x_i\Big), \tag{1.1}$$

where J_e and h_i are called coupling constants and local external fields respectively, and $G=(V,E)$ is the underlying graph. In general, the partition function is computationally intractable and the Bethe approximation is a popular method for its approximation [2]. The approximation ratio, which evaluates the performance of this method, depends on the structure of the underlying graph. Particularly, if the graph is a tree, the ratio is equal to one, i.e., the Bethe approximation gives the exact value of the partition function. In principle, the approximation becomes more difficult as the number of the nullity grows. In [30], it is shown that the ratio is described by a multivariate polynomial $\Theta_G(\boldsymbol{\beta},\boldsymbol{\gamma})$. We derive the graph polynomial $\theta_G(\beta,\gamma)$ as its two-variable version.

The polynomial $\omega_G(\beta)$ is obtained from $\theta_G(\beta,\gamma)$ by specializing $\gamma = 2\sqrt{-1}$ and eliminating a factor $(1-\beta)^{|E|-|V|}$. We will show the polynomial coincides with the monomer-dimer partition function with weights parametrized by β. Especially, for regular graphs, $\omega-$polynomials are equal to the matching polynomials up to transformations.

We discuss the properties of θ_G and ω_G from the viewpoint of graph polynomial. The most important feature of these graph polynomials is the deletion-contraction relation:

$$\theta_G(\beta,\gamma) = (1-\beta)\theta_{G\backslash e}(\beta,\gamma) + \beta\theta_{G/e}(\beta,\gamma),$$
$$\omega_G(\beta) = \omega_{G\backslash e}(\beta) + \beta\omega_{G/e}(\beta),$$

holds whenever $e\in E$ is not a loop. Note that the graph $G\backslash e$ is obtained from G by deletion of the edge e, and the graph G/e is the result of contraction of e. Furthermore, these polynomials are multiplicative:

$$\theta_{G_1\cup G_2} = \theta_{G_1}\theta_{G_2} \quad \text{and} \quad \omega_{G_1\cup G_2} = \omega_{G_1}\omega_{G_2},$$

where $G_1\cup G_2$ is the disjoint union of G_1 and G_2. Graph invariants that satisfy the deletion-contraction relation and the multiplicative law are studied by Tutte [27] in the name of V-function. Our graph polynomials θ_G and ω_G are essentially examples of V-functions.

Graph polynomials that satisfy deletion-contraction relations arise from wide range of problems [4, 11]. Most of them are known to be equivalent to the Tutte polynomial or obtained by its specialization, and thus have reduction formulae also for loops. Our new graph polynomials do not have such reduction formulae for loops and are essentially different from the Tutte polynomial.

There have been few researches on specific V-functions except for those on the Tutte polynomial. The Tutte polynomial has gathered interests due to its rich mathematical properties such as the matroid invariance and connections to links [31, 4]. These properties are not shared by general V-functions. As we will present in this paper, our new V-functions also have special properties, and thus are worth investigation.

The rest of the paper has the following structure. In Section 1.2, definitions and notations on graphs are provided. Sections 2, 3 and 4 are devoted to investigations on the θ-polynomial: the definition and basic properties of the θ-polynomial is given in Section

2, the motivation for the definition is presented in Section 3 and special values of θ_G are discussed in Section 4. Section 5 is devoted to investigations on ω_G including a study on the special value, $\beta = 1$.

1.2. Basic terminologies and definitions

Let $G = (V, E)$ be a finite graph, where V is the set of vertices and E is the set of undirected edges. In this paper, a graph means a multigraph, in which loops and multiple edges are allowed. A subset s of E is identified with the spanning subgraph (V, s) of G unless otherwise stated.

By the notation of $e = ij$ we mean that vertices i and j are the endpoints of e. The number of ends of edges connecting to a vertex i is called the *degree* of i and denoted by d_i.

The number of connected components of G is denoted by $k(G)$. The *nullity* and the *rank* of G are defined by $n(G) := |E| - |V| + k(G)$ and $r(G) := |V| - k(G)$ respectively.

For an edge $e \in E$, the graph $G \backslash e$ is obtained by deleting e and G/e is obtained by contracting e. If e is a loop, G/e is the same as $G \backslash e$. The disjoint union of graphs G_1 and G_2 is denoted by $G_1 \cup G_2$. The graph with a single vertex and n loops is called the *bouquet graph* and denoted by B_n.

For a graph G, the *core* of the graph G is given by a process of clipping vertices of degree one step by step [24]. This graph is denoted by $\mathrm{core}(G)$. For example, the core of a forest F is the graph of $k(F)$ vertices without edges. A graph G is called a *coregraph* if $G = \mathrm{core}(G)$. In other words, a graph is a coregraph if and only if the degree of each vertex is not equal to one. Note that the core of a graph is also known as the *2-core* [21] and can be generalized to the notion of the *k-core* [3, 22].

2. Two-variable graph polynomial θ

2.1. Definition

In the first place, we introduce a graph polynomial that is one of the main topics of this paper. For the definition, we define a set of polynomials $\{f_n(x)\}_{n=0}^{\infty}$ inductively by the relations

$$f_0(x) = 1, \quad f_1(x) = 0, \quad \text{and} \quad f_{n+1}(x) = x f_n(x) + f_{n-1}(x). \tag{2.1}$$

Therefore, for instance, $f_2(x) = 1, f_3(x) = x$ and so on. Note that, these polynomials are transformations of the Chebyshev polynomials of the second kind: $f_{n+2}(2\sqrt{-1}z) = (\sqrt{-1})^n U_n(z)$, where $U_n(\cos\theta) = \frac{\sin((n+1)\theta)}{\sin\theta}$.

Definition. For a given graph G,

$$\theta_G(\beta, \gamma) := \sum_{s \subset E} \beta^{|s|} \prod_{i \in V} f_{d_i(s)}(\gamma) \quad \in \mathbb{Z}[\beta, \gamma], \tag{2.2}$$

where $d_i(s)$ is the degree of the vertex i in s.

In Eq. (2.2), there is a summation over all subsets of E. Recall that an edge set s is identified with the spanning subgraph (V, s). Since $f_1(x) = 0$, the subgraph s makes a

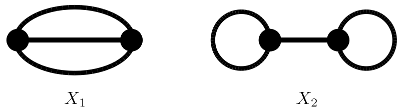

Figure 1. Graph X_1 and X_2

contribution to the summation only if s does not have a vertex of degree one. Therefore, the summation is regarded as the summation over all coregraphs of the forms (V, s); we call them *sub-coregraphs*. In relevant papers, such subgraphs are called generalized loops [8, 9] or closed subgraphs [18, 19].

The following facts are immediate from the definition.

Proposition 2.1.

(a) $\theta_{G_1 \cup G_2}(\beta, \gamma) = \theta_{G_1}(\beta, \gamma)\theta_{G_2}(\beta, \gamma)$.
(b) $\theta_{B_n}(\beta, \gamma) = \sum_{k=0}^{n} \binom{n}{k} f_{2k}(\gamma)\beta^k$.
(c) $\theta_G(\beta, \gamma) = \theta_{\mathrm{core}(G)}(\beta, \gamma)$.

Example 1. For a tree T, $\theta_T(\beta, \gamma) = 1$. For the cycle graph C_n, which has n vertices and n edges, $\theta_{C_n}(\beta, \gamma) = 1 + \beta^n$. For the complete graph K_4, $\theta_{K_4}(\beta, \gamma) = 1 + 4\beta^3 + 3\beta^4 + 6\beta^5\gamma^2 + \beta^6\gamma^4$. For the graph X_1, which is in Figure 1, $\theta_{X_1}(\beta, \gamma) = 1 + 3\beta^2 + \beta^3\gamma^2$. For the graph X_2, which is also in Figure 1, $\theta_{X_2}(\beta, \gamma) = 1 + 2\beta + \beta^2 + \beta^3\gamma^2$.

2.2. Deletion-contraction relation and expression as Tutte's V-function

2.2.1. Deletion-contraction relation We prove the most important property of the graph polynomial, θ, called a deletion-contraction relation. The following formula of $f_n(x)$ plays an important role in the proof of the relation.

Lemma 2.2. $^{\forall} n, m \in \mathbb{N}$,

$$f_{n+m-2}(x) = f_n(x)f_m(x) + f_{n-1}(x)f_{m-1}(x).$$

Proof. Easily proved by induction using Eq.(2.1). □

Theorem 2.3 (Deletion-contraction relation). *For a non-loop edge $e \in E$,*

$$\theta_G(\beta, \gamma) = (1 - \beta)\theta_{G\backslash e}(\beta, \gamma) + \beta\theta_{G/e}(\beta, \gamma).$$

Proof. Classify subgraph s in the sum of Eq. (2.2) whether s includes e or not. The former subgraph $s \ni e = ij$ yields $-\beta\theta_{G\backslash e} + \beta\theta_{G/e}$, where Lemma 2.2 is used with $n = d_i$ and $m = d_j$. The latter subgraph $s \not\ni e$ yields $\theta_{G\backslash e}$. □

2.2.2. Relation to Tutte's V-function In 1947 [27], Tutte defined a class of graph invariants called V-function. The definition is as follows.

Definition. Let $\mathcal{G}$ be the set of isomorphism classes of finite undirected graphs, with loops and multiple edges allowed. Let R be a commutative ring. A map $\mathcal{V} : \mathcal{G} \to R$ is called a *V-function* if it satisfies the following two conditions:

$$\begin{aligned} &\text{(i)} \quad \mathcal{V}(G) = \mathcal{V}(G\backslash e) + \mathcal{V}(G/e) \qquad \text{if } e \in E \text{ is not a loop,} \\ &\text{(ii)} \quad \mathcal{V}(G_1 \cup G_2) = \mathcal{V}(G_1)\mathcal{V}(G_2). \end{aligned}$$

Our graph invariant θ is essentially an example of a V-function. In the definition of V-functions, the coefficients of the deletion-contraction relation are 1, while those of θ are $(1-\beta)$ and β. However, if we modify θ to

$$\hat{\theta}_G(\beta, \gamma) := (1-\beta)^{-|E|+|V|}\beta^{-|V|}\theta_G(\beta, \gamma),$$

this is a V-function $\hat{\theta} : \mathcal{G} \to \mathbb{Z}[\beta, \gamma, \beta^{-1}, (1-\beta)^{-1}]$.

In theorem 10 of [5], Bollobás et al. have constructed non-isomorphic k-connected graphs not distinguished by deletion-contraction invariants. The result implies that these graphs have the same θ-polynomial.

2.2.3. Alternative expression of θ-polynomial By successive applications of the conditions of V-function, we can reduce the value at any graph to the values at bouquet graphs. Therefore we can say that a V-function is completely determined by its boundary condition, i.e., the values at the bouquet graphs. Conversely, Tutte shows in [27] that for an arbitrary boundary condition, there is a V-function that satisfies it. More explicitly, the V-function satisfying a boundary condition $\{\mathcal{V}(B_n)\}_{n=0}$ is given by

$$\mathcal{V}(G) = \sum_{s \subset E} \prod_{n=0} z_n^{i_n(s)}, \tag{2.3}$$

where $z_n := \sum_{j=0}^{n} \binom{n}{j}(-1)^{n+j}\mathcal{V}(B_j)$ and $i_n(s)$ is the number of connected components of the subgraph s with nullity n.

Note that another expansion, called the spanning forest expansion, of $\mathcal{V}(G)$ is found in Section 5 of [5].

In the case of θ, Eq. (2.3) derives the following expression. Though this theorem is a trivial consequence of Theorem 3.2 proved more directly later, we give a proof of Theorem 2.4 to see the relation to Eq. (2.3).

Theorem 2.4.

$$\theta_G(\beta, \gamma) = \sum_{s \subset E} \prod_{n=0} \theta_{B_n}(1, \gamma)^{i_n(s)} \beta^{|s|}(1-\beta)^{|E|-|s|}. \tag{2.4}$$

Proof. It is enough to check that

$$\hat{\theta}_G(\beta, \gamma) = \sum_{s \subset E} \prod_{n=0} \theta_{B_n}(1, \gamma)^{i_n(s)} \beta^{|s|-|V|}(1-\beta)^{|V|-|s|}. \tag{2.5}$$

By comparing the coefficients of x^k in $(1 - \frac{1-x}{1-\beta})^n = (1-\beta)^{-n}(-\beta + x)^n$, we have

$$\sum_{j=k}^{n} (-1)^{j+n} \binom{n}{j}\binom{j}{k}(1-\beta)^{-j} = \binom{n}{k}\beta^{n-k}(1-\beta)^{-n} \tag{2.6}$$

for every $0 \leq k \leq n$. Using this equality and Proposition 1.(b), we see that

$$z_n = \sum_{j=0}^{n} \binom{n}{j}(-1)^{n+j}\hat{\theta}_{B_j}(\beta,\gamma) = \theta_{B_n}(1,\gamma)\beta^{n-1}(1-\beta)^{1-n}.$$

Therefore Eq. (2.3) reduces to Eq. (2.5). □

Formulae (2.2) and (2.4) are both represented in the sum of the subsets of edges, but the terms of a subset are different. Generally, a V-function does not have a representation corresponding to Eq. (2.2); this representation is utilized in the rest of paper and makes θ-polynomial worthy of investigation among V-functions.

2.2.4. Comparison with Tutte polynomial The most famous example of a V-function is the Tutte polynomial (multiplied with a trivial factor). The *Tutte polynomial* is defined by

$$T_G(x,y) := \sum_{s \subset E} (x-1)^{r(G)-r(s)}(y-1)^{n(s)}. \tag{2.7}$$

It satisfies a deletion-contraction relation

$$T_G(x,y) = \begin{cases} xT_{G\backslash e}(x,y) & \text{if } e \text{ is a bridge,} \\ yT_{G\backslash e}(x,y) & \text{if } e \text{ is a loop,} \\ T_{G\backslash e}(x,y) + T_{G/e}(x,y) & \text{otherwise.} \end{cases}$$

It is easy to see that $\hat{T}_G(x,y) := (x-1)^{k(G)}T_G(x,y)$ is a V-function to $\mathbb{Z}[x,y]$. For bouquet graphs, $\hat{T}_{B_n}(x,y) = (x-1)y^n$. In the case of the Tutte polynomial, Eq. (2.3) derives Eq. (2.7).

Moreover, the Tutte polynomial T is known to be matroidal, i.e., if G_1 and G_2 give the same cycle matroid then $T_{G_1} = T_{G_2}$ holds [31]. Since B_{n+m} and $B_n \cup B_m$ give the same cycle matroid, the relation

$$T_{B_{n+m}} = T_{B_n}T_{B_m} \tag{2.8}$$

is a consequence of the invariance. Though $\hat{T}$ itself is not matroidal, but is matroidal and satisfies Eq. (2.8) up to the easy factor.

The V-functions $\hat{\theta}$ and $\hat{T}$ are essentially different. One intuitive understanding is that $\hat{\theta}_{B_n}$, shown in Proposition 2.1.(b), do not satisfy Eq. (2.8), even if an appropriate factor is multiplied. (If we set $\gamma = 0$, it is not the case. See Proposition 4.1.) In the following remark, we formally state the difference irrespective of transforms between (β,γ) and (x,y).

Remark. For any field K, inclusions $\phi_1 : \mathbb{Z}[\beta,\gamma,\beta^{-1},(1-\beta)^{-1}] \hookrightarrow K$, and ϕ_2 :

$\mathbb{Z}[x,y] \hookrightarrow K$, we have

$$\phi_1 \circ \hat{\theta} \neq \phi_2 \circ \hat{T}.$$

Proof. It is easy to see that $\phi_2(\hat{T}_{B_n})/\phi_2(\hat{T}_{B_0}) = \phi_2(y)^n$ and $\phi_1(\hat{\theta}_{B_n})/\phi_1(\hat{\theta}_{B_0}) = \phi_1(1-\beta)^{-n}\phi_1(\sum_{k=0}^{n}\binom{n}{k}f_{2k}(\gamma)\beta^k)$. If $\phi_1 \circ \hat{\theta} = \phi_2 \circ \hat{T}$, then $a_n := \sum_{k=0}^{n}\binom{n}{k}f_{2k}(\gamma')\beta'^k = z^n$ for some $z \in K$, where $\gamma' = \phi_1(\gamma)$ and $\beta' = \phi_1(\beta)$. The equation $a_1^2 = a_2$ gives $\gamma'^2\beta'^2 = 0$. This is a contradiction because $\beta \neq 0$ and $\gamma \neq 0$. □

3. Motivation for the definition

In this section, we explain the motivation for considering the graph polynomial θ_G, that is, the link to the Ising partition function and its Bethe approximation.

3.1. Definition of weighted graph version of θ-polynomial

We consider the multi-variable version of θ_G, attaching weights to vertices and edges of G by $\boldsymbol{\gamma} = (\gamma_i)_{i \in V}$ and $\boldsymbol{\beta} = (\beta_e)_{e \in E}$ respectively. Such a graph is called a *weighted graph.* We assume the weights are real numbers.

Definition. Let $\boldsymbol{\beta} = (\beta_e)_{e \in E}$ and $\boldsymbol{\gamma} = (\gamma_i)_{i \in V}$ be the weights of G.

$$\Theta_G(\boldsymbol{\beta}, \boldsymbol{\gamma}) := \sum_{s \subset E} \prod_{e \in s} \beta_e \prod_{i \in V} f_{d_i(s)}(\gamma_i).$$

If all vertex and edge weights are set to be the same, $\Theta_G(\boldsymbol{\beta}, \boldsymbol{\gamma})$ reduces to $\theta_G(\beta, \gamma)$. It is trivial by definition that

$$\Theta_{G_1 \cup G_2}(\boldsymbol{\beta}, \boldsymbol{\gamma}) = \Theta_{G_1}(\boldsymbol{\beta}, \boldsymbol{\gamma})\Theta_{G_2}(\boldsymbol{\beta}, \boldsymbol{\gamma}), \tag{3.1}$$

$$\Theta_{B_0}(\boldsymbol{\beta}, \boldsymbol{\gamma}) = 1, \tag{3.2}$$

$$\Theta_G(\boldsymbol{\beta}, \boldsymbol{\gamma}) = \Theta_{\mathrm{core}(G)}(\boldsymbol{\beta}, \boldsymbol{\gamma}). \tag{3.3}$$

In this definition, Θ_G is represented in the form of the edge states sum, but it is also possible to represent it in the following form of vertex state sum. This formula is important to show the link to the Bethe approximation of the Ising partition function because the partition function is also given in the form of vertex state sum.

Lemma 3.1.

$$\Theta_G(\boldsymbol{\beta}, (\xi_i - \xi_i^{-1})_{i \in V}) = \sum_{x_1, \ldots, x_N = \pm 1} \prod_{\substack{e \in E \\ e = ij}} (1 + x_i x_j \beta_e \xi_i^{-x_i} \xi_j^{-x_j}) \prod_{i \in V} \frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}}. \tag{3.4}$$

Proof. From Eq. (2.1), we can easily check by induction that

$$f_n(\xi - \xi^{-1}) = \frac{\xi^{n-1} - (-\xi)^{-n+1}}{\xi + \xi^{-1}}.$$

If we expand the product with respect to E in the right hand side of Eq. (3.4), it is equal to

$$\sum_{s\subset E}\prod_{e\in s}\beta_e\prod_{i\in V}\sum_{x_i=\pm 1}\frac{(-x_i)^{d_{i(s)}}\xi_i^{(1-d_{i(s)})x_i}}{\xi_i+\xi_i^{-1}}.$$

Then, the assertion follows immediately. □

3.2. Link to the Bethe approximation

We will explain that the value Θ_G describes the discrepancy between the true partition function of the Ising model and its Bethe approximation. More detailed discussion is found in [30].

The Bethe approximation is a method for approximating partition functions of various statistical mechanical models [2]. Here we give it in the case of the Ising partition function. Recall that the *Ising partition function* on G for given $\boldsymbol{J} = (J_e)_{e\in E}$ and $\boldsymbol{h} = (h_i)_{i\in V}$ is defined by Eq. (1.1). We write $\psi_{ij}(x_i, x_j) = \exp(J_{ij}x_ix_j)$ and $\psi_i(x_i) = \exp(h_ix_i)$.

Definition. A set of functions $\{b_e(x_i, x_j)\}_{e\in E}$ and $\{b_i(x_i)\}_{i\in V}$ is called a *belief* [33] if it satisfies

$$\sum_{x_i} b_e(x_i,x_j) = b_i(x_i) \quad \text{for all } i\in V,\ x_i\in\{\pm 1\} \text{ and } e = ij\in E, \tag{3.5}$$

$$\sum_{x_i,x_j} b_e(x_i,x_j) = 1 \quad \text{for all } e = ij\in E, \tag{3.6}$$

$$\prod_{e\in E}\frac{b_e(x_i,x_j)}{b_i(x_i)b_j(x_j)}\prod_{i\in V}b_i(x_i) \propto \prod_{e\in E}\psi_e(x_i,x_j)\prod_{i\in V}\psi_i(x_i). \tag{3.7}$$

Then the *Bethe approximation of the partition function* Z_B is defined by the proportionality constant of Eq. (3.7): $Z_B\prod_{e\in E}\frac{b_e}{b_ib_j}\prod_{i\in V}b_i = \prod_{e\in E}\psi_e\prod_{i\in V}\psi_i$.

For given $\boldsymbol{J}$ and $\boldsymbol{h}$, we can obtain a belief by an algorithm called *belief propagation* [20, 33]. In practical situations, the algorithm stops in a reasonable time. Therefore the Bethe approximation of the partition function is used in many applications [17].

We show that $\Theta_G(\boldsymbol{\beta},\boldsymbol{\gamma})$ is equal to Z/Z_B. We choose variables β_e and ξ_i to parameterize $\{b_e(x_i, x_j)\}_{e\in E}$ and $\{b_i(x_i)\}_{i\in V}$, which satisfy Eqs. (3.5) and (3.6):

$$b_e(x_i,x_j) = \frac{1}{(\xi_i+\xi_i^{-1})(\xi_j+\xi_j^{-1})}(\xi_i^{x_i}\xi_j^{x_j}+\beta_e x_ix_j),$$

$$b_i(x_i) = \frac{\xi_i^{x_i}}{\xi_i+\xi_i^{-1}}.$$

From the definition of Z_B and Lemma 3.1, we see that

$$\begin{aligned}\frac{Z}{Z_B} &= \sum_{\boldsymbol{x}} \prod_{e \in E} \frac{b_e(x_i, x_j)}{b_i(x_i) b_j(x_j)} \prod_{i \in V} b_i(x_i) \\ &= \sum_{x_1, \ldots, x_N = \pm 1} \prod_{\substack{e \in E \\ e = ij}} (1 + x_i x_j \beta_e \xi_i^{-x_i} \xi_j^{-x_j}) \prod_{i \in V} \frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}} \\ &= \Theta_G(\boldsymbol{\beta}, \boldsymbol{\gamma}),\end{aligned}$$

where $\gamma_i := \xi_i - \xi_i^{-1}$. This equation means that the approximation ratio is captured by the value of Θ_G. If the graph is a tree, we see from Eq. (3.2) and (3.3) that $\Theta_G = 1$, i.e., the Bethe approximation gives the exact value of the partition function. If the weights $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ are sufficiently small, we see that $\Theta_G \approx 1$, i.e., the Bethe approximation is a good approximation.

The definition of Θ_G implies that we can expand the approximation ratio by the sum of sub-coregraphs [8, 9, 30]. This expansion sometimes improves the approximation if we sum up some of the terms [14].

3.3. Transform of the Ising partition function

In the following, we give the explicit transform from $(\boldsymbol{\beta}, \boldsymbol{\gamma})$ to $(\boldsymbol{J}, \boldsymbol{h})$.

We can always choose $A_i, B_e, h_i^{'}, h_{e,i}$ and J_e to satisfy

$$\begin{aligned}\frac{\xi_i^{x_i}}{\xi_i + \xi_i^{-1}} &= A_i^{-1} \exp(h_i^{'} x_i), \\ 1 + x_i x_j \beta_e \xi_i^{-x_i} \xi_j^{-x_j} &= B_e^{-1} \exp(J_e x_i x_j + h_{e,i} x_i + h_{e,j} x_j).\end{aligned}$$

Therefore, setting $h_i := h_i^{'} + \sum_{e \ni i} h_{e,i}$, we have

$$Z(G; \boldsymbol{J}, \boldsymbol{h}) = \prod_{i \in V} A_i \prod_{e \in E} B_e \; \Theta_G(\boldsymbol{\beta}, (\xi_i - \xi_i^{-1})_{i \in V}). \tag{3.8}$$

This fact shows that $\Theta_G(\boldsymbol{\beta}, \boldsymbol{\gamma})$ gives the Ising partition function with $(\boldsymbol{J}, \boldsymbol{h})$, which is computed from $(\boldsymbol{\beta}, \boldsymbol{\gamma})$ as above.

If $\xi_i = 1$, or $\gamma_i = 0$ for all $i \in V$, Eq. (3.8) reduces to the well known expansion of van der Waerden [28, 31],

$$Z(G; \boldsymbol{J}, 0) = 2^{|V|} \prod_{e \in E} \cosh(J_e) \sum_{s \in \mathcal{E}} \prod_{e \in s} \tanh(J_e), \tag{3.9}$$

where $\mathcal{E}$ is the set of Eulerian subgraphs, i.e. the subgraphs in which all vertex degrees are even. This fact is deduced from $f_n(0) = 1$ if n is even and $f_n(0) = 0$ if n is odd.

It is well known by statistical physicists that Eq. (3.9) can be extended to the following expression [10]

$$Z(G; \boldsymbol{J}, \boldsymbol{h}) = 2^{|V|} \prod_{e \in E} \cosh(J_e) \sum_{s \subset E} \prod_{e \in s} \tanh(J_e) \prod_{i \in V_e(s)} \cosh(h_i) \prod_{i \in V_o(s)} \sinh(h_i), \tag{3.10}$$

where $V_e(s)$ (resp. $V_o(s)$) is the set of vertices of even (resp. odd) degree in s. Though both Eqs. (3.8) and (3.10) are extensions of Eq. (3.9) and give edge subset expansions, they are different. An obvious difference is that only the sub-coregraphs contribute to the expansion in Eq. (3.8).

Based on Eq. (3.8), we can say that the graph polynomial $\theta_G(\beta,\gamma)$ is a transformed Ising partition function with uniform coupling constants and un-uniform external fields. In contrast, a bivariate graph polynomial investigated in [1] is based on Eq. (3.10). This polynomial corresponding to the Ising partition function with uniform coupling constants and external fields. A similar type of expression is also considered in [16].

3.4. Additional remarks on the weighted graph version

In this subsection, we give additional remarks on Θ_G comparing with θ_G. The deletion-contraction relation in Theorem 2.3 is generalized to weighted graphs as follows. If the weights $(\boldsymbol{\beta},\boldsymbol{\gamma})$ on G satisfies $\gamma_i=\gamma_j$ for a non-loop edge $e=ij$, the weights on $G\backslash e$ and G/e are naturally induced and denoted by $(\boldsymbol{\beta}',\boldsymbol{\gamma}')$ and $(\boldsymbol{\beta}'',\boldsymbol{\gamma}'')$ respectively. On G/e, the weight on the new vertex, which is the fusion of i and j, is set to be γ_i. Under these conditions, we have

$$\Theta_G(\boldsymbol{\beta},\boldsymbol{\gamma})=(1-\beta_e)\Theta_{G\backslash e}(\boldsymbol{\beta}',\boldsymbol{\gamma}')+\beta_e\Theta_{G/e}(\boldsymbol{\beta}'',\boldsymbol{\gamma}''), \tag{3.11}$$

which is proved in the same way as Theorem 2.3.

If we set all vertex weights γ_i to be equal, the generalization of Theorem 2.4 holds. We write $\Theta_G(\boldsymbol{\beta},(\gamma_i=\gamma)_{i\in V})$ by $\Theta_G(\boldsymbol{\beta},\gamma)$ for simplicity.

Theorem 3.2.

$$\Theta_G(\boldsymbol{\beta},\gamma)=\sum_{s\subset E}\prod_{n=0}\theta_{B_n}(1,\gamma)^{i_n(s)}\prod_{e\in s}\beta_e\prod_{e\in E\backslash s}(1-\beta_e). \tag{3.12}$$

Proof. In this proof, the right hand side of Eq. (3.12) is denoted by $\tilde{\Theta}_G(\boldsymbol{\beta},\gamma)$. First, we check that Θ_G and $\tilde{\Theta}_G$ are equal at the bouquet graphs.

$$\begin{aligned}\tilde{\Theta}_{B_n}(\boldsymbol{\beta},\gamma)&=\sum_{s\subset E}\theta_{B_{|s|}}(1,\gamma)\prod_{e\in s}\beta_e\prod_{e\in E\backslash s}(1-\beta_e)\\&=\sum_{s\subset E}\sum_{k=0}^{|s|}\binom{|s|}{k}f_{2k}(\gamma)\prod_{e\in s}\beta_e\sum_{t\subset E\backslash s}\prod_{e\in t}(-\beta_e)\\&=\sum_{u\subset E}\sum_{s\subset u}\sum_{k=0}^{|s|}\binom{|s|}{k}f_{2k}(\gamma)(-1)^{|u|-|s|}\prod_{e\in u}\beta_e\\&=\sum_{u\subset E}\sum_{l=0}^{|u|}\sum_{k=0}^{l}\binom{|u|}{l}\binom{l}{k}f_{2k}(\gamma)(-1)^{|u|-l}\prod_{e\in u}\beta_e.\end{aligned}$$

Using the equality $\sum_{j=k}^{n}\binom{n}{j}\binom{j}{k}(-1)^{n+j}=\delta_{n,k}$, which is obtained at $\beta=0$ of Eq. (2.6), we have

$$\tilde{\Theta}_{B_n}(\boldsymbol{\beta},\gamma)=\sum_{u\subset E}f_{2|u|}(\gamma)\prod_{e\in u}\beta_e=\Theta_{B_n}(\boldsymbol{\beta},\gamma).$$

Secondly, we see that $\tilde{\Theta}_G(\boldsymbol{\beta},\gamma)$ satisfies the deletion-contraction relation

$$\tilde{\Theta}_G(\boldsymbol{\beta},\gamma) = (1-\beta_e)\tilde{\Theta}_{G\setminus e}(\boldsymbol{\beta}',\gamma) + \beta_e\tilde{\Theta}_{G/e}(\boldsymbol{\beta}'',\gamma)$$

for all non-loop edges e, because the subsets including e amount to $\beta_e\tilde{\Theta}_{G/e}(\boldsymbol{\beta},\gamma)$ and the other subsets amount to $(1-\beta_e)\tilde{\Theta}_{G\setminus e}(\boldsymbol{\beta},\gamma)$.

Applying this form of deletion-contraction relations to both Θ_G and $\tilde{\Theta}_G$, we can reduce the values at G to those of disjoint unions of bouquet graphs. Therefore we conclude that $\tilde{\Theta}_G = \Theta_G$. □

A *coloured* graph is a graph with a map from the edges to a set of colours. If it is the set of real numbers, the term weighted is preferred. We can generalize the definition of V-functions to coloured graphs by allowing the coefficients of the deletion-contraction relation dependent on colours. Since $\Theta_G(\boldsymbol{\beta},\gamma)$ satisfies Eqs. (3.1) and (3.11), it is a V-function of (edge) weighted graphs. A similar expansion to Theorem 3.2 holds for any coloured V-function because the proof only uses Eqs. (3.1) and (3.11).

Regarding the Tutte polynomial, there have been a lot of works on the extensions to edge weighted or coloured versions. In [6], the "universal" Tutte polynomial is constructed on coloured graphs, generalizing the ordinary Tutte polynomial as far as possible. The "universal" Tutte polynomial derives other extensions of the Tutte polynomial such as the dichromatic polynomial for edge weighted graphs given by Traldi [26] and the *random-cluster model* by Fortuin and Kasteleyn [12].

Our extension, $\Theta_G(\boldsymbol{\beta},\gamma)$, for weighted graphs resembles the random-cluster model defined by

$$R_G(\boldsymbol{\beta},\kappa) = \sum_{s\subset E}\kappa^{k(s)}\prod_{e\in s}\beta_e\prod_{e\in E\setminus s}(1-\beta_e)$$

because of Eq. (3.12). The random-cluster model satisfies a deletion-contraction relation of the form

$$R_G(\boldsymbol{\beta},\kappa) = (1-\beta_e)R_{G\setminus e}(\boldsymbol{\beta}',\kappa) + \beta_e R_{G/e}(\boldsymbol{\beta}'',\kappa) \quad \text{for all } e\in E.$$

Note that this relation holds for loops in contrast to $\Theta_G(\boldsymbol{\beta},\gamma)$ as $R_G(\boldsymbol{\beta},\kappa)$ is an extension of the Tutte polynomial. This difference comes from that of the coefficients of subgraphs s: $\kappa^{k(s)}$ and $\prod\theta_{B_n}(1,\gamma)^{i_n(s)}$.

4. Further properties of θ and its implications

4.1. Special values

4.1.1. $\gamma = 0$ case As suggested in Section 2.2.4, if we set $\gamma=0$, the polynomial $\theta_G(\beta,0)$ is included in the Tutte polynomial.

Proposition 4.1.

$$\theta_G(\beta,0) = (1-\beta)^{n(G)}\beta^{r(G)}T_G\Big(\frac{1}{\beta},\frac{1+\beta}{1-\beta}\Big).$$

Proof. From Proposition 2.1.(b) and $f_{2k}(0) = 1$, we have

$$\hat{\theta}_{B_n}(\beta, 0) = (1-\beta)^{1-n}\beta^{-1}\sum_{k=0}^{n}\binom{n}{k}\beta^k = (1-\beta)^{1-n}\beta^{-1}(1+\beta)^n.$$

We also have $\hat{T}_{B_n}(\frac{1}{\beta}, \frac{1+\beta}{1-\beta}) = (\beta^{-1}-1)(\frac{1+\beta}{1-\beta})^n$. Therefore $\hat{\theta}_{B_n}(\beta, 0) = \hat{T}_{B_n}(\frac{1}{\beta}, \frac{1+\beta}{1-\beta})$. Since V-functions are determined by the values at the bouquet graphs, $\hat{\theta}_G(\beta, 0) = \hat{T}_G(\frac{1}{\beta}, \frac{1+\beta}{1-\beta})$ holds for any graph G. □

This result is natural from the view point of the Ising partition function. The Tutte polynomial is equivalent to the partition function of the q-Potts model [4]; if we set $q = 2$, it becomes the Ising partition function (with uniform coupling constants J and without external fields). In terms of the Tutte polynomial, such points correspond to the parameters $(x, y) = (\frac{1}{\beta}, \frac{1+\beta}{1-\beta})$, and thus $T_G(\frac{1}{\beta}, \frac{1+\beta}{1-\beta})$ is the Ising partition function of that type in essence. On the other hand, as discussed in Section 3.3, $\theta_G(\beta, 0)$ is also equal to the Ising partition function of that type essentially. Therefore they must be equal up to some easy factor.

We can say that the Tutte polynomial is an extension of the Ising partition function (with uniform coupling constants and without external fields) to the q-state model while the θ-polynomial is an extension of it to a model with specific forms of local external fields.

4.1.2. $\beta = 1$ case At $\beta = 1$, $\theta_G(1, \gamma)$ is determined by the nullity and the number of the connected components of the graph.

Lemma 4.2. *For a connected graph G,*

$$\theta_G(1, \xi - \xi^{-1}) = \xi^{1-n(G)}(\xi + \xi^{-1})^{n(G)-1} + \xi^{n(G)-1}(\xi + \xi^{-1})^{n(G)-1} \tag{4.1}$$

Proof. We use the right hand side of Lemma 3.1, which gives an alternative representation of θ_G. If $x_i \neq x_j$, then $1 + x_i x_j \xi^{-x_i}\xi^{-x_j} = 0$. Thus only two terms of $x_1 = \cdots = x_N = 1$ and $x_1 = \cdots = x_N = -1$ contribute to the sum, because G is connected. □

If $\xi = \frac{1+\sqrt{5}}{2}$, then $\xi - \xi^{-1} = 1$. From Eq. (4.1), we see that

$$\theta_G(1, 1) = \left(\frac{5-\sqrt{5}}{2}\right)^{n(G)-1} + \left(\frac{5+\sqrt{5}}{2}\right)^{n(G)-1}. \tag{4.2}$$

Setting $\xi = 1$, we also deduce from Eq. (4.1) that

$$\theta_G(1, 0) = 2^{n(G)}. \tag{4.3}$$

4.2. Number of sub-coregraphs

4.2.1. Bounds For a given graph G, let $\mathcal{C}(G) := \{s; s \subset E, (V, s) \text{ is a coregraph.}\}$ be the set of sub-coregraphs of G. In the following theorem, the values (4.2) and (4.3) are used to bound the number of sub-coregraphs.

Though the following upper bound is proved in [30], here we present the both proofs of the bounds for completeness.

Theorem 4.3. *For a connected graph G,*

$$2^{n(G)} \leq |\mathcal{C}(G)| \leq \left(\frac{5-\sqrt{5}}{2}\right)^{n(G)-1} + \left(\frac{5+\sqrt{5}}{2}\right)^{n(G)-1}. \tag{4.4}$$

The lower bound is attained if and only if $\mathrm{core}(G)$ *is a subdivision of a bouquet graph, and the upper bound is attained if and only if* $\mathrm{core}(G)$ *is a subdivision of a 3-regular graph or G is a tree.*

Note that a *subdivision* of a graph G is a graph that is obtained by adding vertices of degree 2 on edges.

Proof. It is enough to consider the case that G is a coregraph and does not have vertices of degree 2, because the operations of taking core and subdivision do not change the nullity and the set of sub-coregraphs essentially.

From the definition Eq. (2.2), we can write

$$\theta_G(1, \gamma) = \sum_{s \in \mathcal{C}} w(s; \gamma),$$

where $w(s; \gamma) = \prod_{i \in V} f_{d_i(s)}(\gamma)$. For all $s \in \mathcal{C}$, we claim that

$$w(s; 0) \leq 1 \leq w(s; 1). \tag{4.5}$$

The left inequality of Eq. (4.5) is immediate from the fact that $f_n(0) = 1$ if n is even and $f_n(0) = 0$ if n is odd. The equality holds if and only if all vertices have even degree in s. Since $f_n(1) > 1$ for all $n > 4$ and $f_2(1) = f_3(1) = 1$, we have $w(s; 1) \geq 1$. The equality holds if and only if $d_i(s) \leq 3$ for all $i \in V$. Then the inequalities in Eq. (4.4) are proved. The upper bound is attained if and only if G is a 3-regular graph or the B_0. For the equality condition of the lower bound, it is enough to prove the following claim.

Claim. Let G be a connected graph, and assume that the degree of every vertex is at least 3 and $d_i(s)$ is even for every $i \in V$ and $s \in \mathcal{C}$. Then G is a bouquet graph.

If G is not a bouquet graph, there is a non-loop edge $e = i_0 j_0$. Then E and $E \setminus e$ are sub-coregraphs of G. Thus $d_{i_0}(E)$ or $d_{i_0}(E \setminus e) = d_{i_0}(E) - 1$ is odd. This is a contradiction. □

4.2.2. Number of sub-coregraphs in 3-regular graphs If the core of a graph is a subdivision of a 3-regular graph, we obtain more information on the number of specific types of sub-coregraphs.

We can rewrite Lemma 4.2 as follows.

Lemma 4.4. *Let G be connected and not a tree. Then we have*

$$\theta_G(1,\gamma) = \sum_{l=0}^{n(G)-1} C_{n(G),l}\gamma^{2l},$$

where $C_{n,l} := \sum_{k=l+1}^{n} \binom{n}{k}\binom{k+l-1}{2l}$ for $1 \leq l \leq n-1$ and $C_{n,0} := 2^n$.

Proof. First we note that for $k \geq 1$,

$$f_{2k}(\gamma) = \sum_{l=0}^{k-1} \binom{k+l-1}{2l}\gamma^{2l} \quad \text{and} \quad f_{2k+1}(\gamma) = \sum_{l=0}^{k-1} \binom{k+l}{2l+1}\gamma^{2l+1}.$$

This is easily proved inductively using Eq. (2.1). Then Lemma 4.2 derives

$$\begin{aligned}\theta_G(1,\gamma) = \theta_{B_{n(G)}}(1,\gamma) &= \sum_{k=1}^{n(G)} \binom{n(G)}{k} f_{2k}(\gamma) + f_0(\gamma) \\ &= \sum_{l=0}^{n(G)-1} \sum_{k=l+1}^{n(G)} \binom{n(G)}{k}\binom{k+l-1}{2l}\gamma^{2l} + 1 \\ &= \sum_{l=0}^{n(G)-1} C_{n(G),l}\gamma^{2l}.\end{aligned}$$

□

Theorem 4.5. *Let G be a connected graph and not a tree. If every vertex of the* core(G) *has the degree at most 3, then*

$$C_{n(G),l} = |\{s \in \mathcal{C}(G); s \textit{ has } 2l \textit{ vertices of degree 3.}\}|$$

for $0 \leq l \leq n(G) - 1$.

Proof. For a sub-coregraph s, $\prod_{i\in V} f_{d_i(s)}(\gamma) = \gamma^{2l}$ if and only if s has $2l$ vertices of degree 3. □

5. One-variable graph polynomial ω

In this section we define the second graph polynomial ω by setting $\gamma = 2\sqrt{-1}$. It is easy to check that $f_n(2\sqrt{-1}) = (\sqrt{-1})^n(1-n)$, using Eq. (2.1). Therefore

$$\theta_G(\beta, 2\sqrt{-1}) = \sum_{s\subset E} (-\beta)^{|s|} \prod_{i\in V} (1 - d_i(s)). \tag{5.1}$$

An interesting point of this specialization is the relation to the monomer-dimer partition function with specific form of monomer-dimer weights, as described in Section 5.2.

5.1. Definition and basic properties

From Eq. (4.1), $\theta_G(1, 2\sqrt{-1}) = 0$ unless all the nullities of connected components of G are less than 2. The following theorem asserts that $\theta_G(\beta, 2\sqrt{-1})$ can be divided by $(1-\beta)^{|E|-|V|}$. We define ω_G by dividing that factor.

Theorem 5.1.

$$\omega_G(\beta) := \frac{\theta_G(\beta, 2\sqrt{-1})}{(1-\beta)^{|E|-|V|}} \quad \in \mathbb{Z}[\beta].$$

In Eq. (5.1), $\theta_G(\beta, 2\sqrt{-1})$ is given in the summation over all sub-coregraphs and each term is not necessarily divisible by $(1-\beta)^{|E|-|V|}$, but if we use the representation in Theorem 2.4, each summand is divisible by the factor as we show in the following theorem. Theorem 5.1 is a trivial consequence of Theorem 5.2.

Theorem 5.2.

$$\omega_G(\beta) = \sum_{s \subset E} \beta^{|s|} \prod_{n=0} h_n(\beta)^{i_n(s)},$$

where $h_0(\beta) := (1-\beta)$, $h_1(\beta) := 2$ and $h_n(\beta) := 0$ for $n \geq 2$.

Proof. From (b) of Proposition 2.1 and $f_m(2\sqrt{-1}) = (\sqrt{-1})^m(1-m)$, we have

$$\theta_{B_n}(1, 2\sqrt{-1}) = \sum_{k=0}^{n} \binom{n}{k} (-1)^k (1-2k) = \begin{cases} 1 & \text{if } n = 0 \\ 2 & \text{if } n = 1 \\ 0 & \text{if } n \geq 2. \end{cases}$$

Theorem 2.4 gives

$$\begin{aligned} \omega_G(\beta) &= \sum_{s \subset E} \prod_{n=0} \theta_{B_n}(1, 2\sqrt{-1})^{i_n(s)} \beta^{|s|} (1-\beta)^{|V|-|s|} \\ &= \sum_{s \subset E} \prod_{n=0} [(1-\beta)^{1-n} \theta_{B_n}(1, 2\sqrt{-1})]^{i_n(s)} \beta^{|s|}. \end{aligned}$$

Then the assertion is proved. □

Example 2.

For a tree T, $\omega_T(\beta) = 1-\beta$. For the cycle graph C_n, $\omega_{C_n}(\beta) = 1+\beta^n$. For the complete graph K_4, $\omega_{K_4}(\beta) = 1+2\beta+3\beta^2+8\beta^3+16\beta^4$. For graphs in Figure 1, $\omega_{X_1}(\beta) = 1+\beta+4\beta^2$ and $\omega_{X_2}(\beta) = 1+3\beta+4\beta^2$.

We list basic properties of ω below.

Proposition 5.3.

(a) $\omega_{G_1 \cup G_2}(\beta) = \omega_{G_1}(\beta)\omega_{G_2}(\beta)$.
(b) $\omega_G(\beta) = \omega_{G \setminus e}(\beta) + \beta\omega_{G/e}(\beta)$ *if $e \in E$ is not a loop.*
(c) $\omega_{B_n}(\beta) = 1 + (2n-1)\beta$.
(d) $\omega_G(\beta) = \omega_{\mathrm{core}(G)}(\beta)$.
(e) *$\omega_G(\beta)$ is a polynomial of degree $|V_{\mathrm{core}(G)}|$. The leading coefficient is $\prod_{i \in V_{\mathrm{core}(G)}}(d_i - 1)$ and the constant term is 1.*
(f) *Let $G^{(m)}$ be the graph obtained by subdividing each edge to m edges. Then,*

$$\omega_{G^{(m)}}(\beta) = (1 + \beta + \cdots + \beta^{m-1})^{|E|-|V|}\omega_G(\beta^m).$$

Proof. The assertions (a-e) are easy. (f) is proved by $|E_G| - |V_G| = |E_{G^{(m)}}| - |V_{G^{(m)}}|$ and $\theta_{G^{(m)}}(\beta, 2\sqrt{-1}) = \theta_G(\beta^m, 2\sqrt{-1})$. □

Proposition 5.4. *If G does not have connected components of nullity 0, then the coefficients of $\omega_G(\beta)$ are non-negative.*

Proof. We prove the assertion by induction on the number of edges. Assume that every connected component is not a tree. If G has only one edge, then $G = B_1$ and the coefficients are non-negative. Let G have $M(\geq 2)$ edges and assume that the assertion holds for the graphs with at most $M - 1$ edges. It is enough to consider the case that G is a connected coregraph because of Proposition 5.3.(a) and (d). If all edges of G are loops, $G = B_n$ for some $n \geq 2$ and the coefficients are non-negative. If $G = C_M$, the coefficients are also non negative as in Example 2. Otherwise, we reduce ω_G to graphs with nullity not less than 1 by an application of the deletion-contraction relation and see that the coefficients of $\omega_{G\setminus e}$ and $\omega_{G/e}$ are both non-negative. □

5.2. Relation to monomer-dimer partition function

In the next theorem, we prove that the polynomial $\omega_G(\beta)$ is the monomer-dimer partition function with specific form of weights.

A *matching* of G is a set of edges such that any edges do not occupy a same vertex. It is also called a *dimer arrangement* in statistical physics [15]. We use both terminologies. The number of edges in a matching $\mathbf{D}$ is denoted by $|\mathbf{D}|$. If a matching $\mathbf{D}$ consists of k edges, then it is called a *k-matching*. The vertices covered by the edges in $\mathbf{D}$ are denoted by $[\mathbf{D}]$. The set of all matchings of G are denoted by $\mathcal{D}$.

The monomer-dimer partition function with edge weights $\boldsymbol{\mu} = (\mu_e)_{e \in E}$ and vertex weights $\boldsymbol{\lambda} = (\lambda_i)_{i \in V}$ is defined as

$$\Xi_G(\boldsymbol{\mu}, \boldsymbol{\lambda}) := \sum_{\mathbf{D} \in \mathcal{D}} \prod_{e \in \mathbf{D}} \mu_e \prod_{i \in V \setminus [\mathbf{D}]} \lambda_i.$$

We write $\Xi_G(\mu, \boldsymbol{\lambda})$ if all weights μ_e are set to be the same μ.

Theorem 5.5. *Let $\lambda_i := 1 + (d_i - 1)\beta$, then*

$$\omega_G(\beta) = \Xi_G(-\beta, \boldsymbol{\lambda}).$$

Proof. We show that $\Xi_G(-\beta, \boldsymbol{\lambda})$ satisfies the deletion-contraction relation and the boundary condition of the form in Proposition 5.3.(c). For the bouquet graph B_n, $\mathbf{D} = \phi$ is the only possible dimer arrangement, and thus

$$\Xi_{B_n}(-\beta, \boldsymbol{\lambda}) = 1 + (2n-1)\beta = \omega_{B_n}(\beta).$$

For a non-loop edge $e = i_0 j_0$, we show that the deletion-contraction relation is satisfied. A dimer arrangement $\mathbf{D} \in \mathcal{D}$ is classified into the following five types: (a) $\mathbf{D}$ includes e, (b) $\mathbf{D}$ does not include e and $\mathbf{D}$ covers both i_0 and j_0, (c) $\mathbf{D}$ covers i_0 while does not cover j_0, (d) $\mathbf{D}$ covers j_0 while does not cover i_0, (e) $\mathbf{D}$ covers neither i_0 nor j_0. According to this classification, $\Xi_G(-\beta, \boldsymbol{\lambda})$ is a sum of the five terms A, B, C, D and E. We see that

$$\begin{aligned}
C &= \sum_{\substack{\mathbf{D} \in \mathcal{D} \\ [\mathbf{D}] \ni i_0, [\mathbf{D}] \not\ni j_0}} (-\beta)^{|\mathbf{D}|} \prod_{i \in V \setminus [\mathbf{D}]} \lambda_i \\
&= \sum_{\substack{\mathbf{D} \in \mathcal{D} \\ [\mathbf{D}] \ni i_0, [\mathbf{D}] \not\ni j_0}} (-\beta)^{|\mathbf{D}|} (1 + (d_{j_0} - 2)\beta) \prod_{\substack{i \in V \setminus [\mathbf{D}] \\ i \neq j_0}} \lambda_i \\
&\qquad + \beta \sum_{\substack{\mathbf{D} \in \mathcal{D} \\ [\mathbf{D}] \ni i_0, [\mathbf{D}] \not\ni j_0}} (-\beta)^{|\mathbf{D}|} \prod_{\substack{i \in V \setminus [\mathbf{D}] \\ i \neq j_0}} \lambda_i \\
&=: C_1 + \beta C_2.
\end{aligned}$$

In the same way, $D = D_1 + \beta D_2$. Similarly,

$$\begin{aligned}
E &= \sum_{\substack{\mathbf{D} \in \mathcal{D} \\ [\mathbf{D}] \not\ni i_0, [\mathbf{D}] \not\ni j_0}} (-\beta)^{|\mathbf{D}|} \lambda_{i_0} \lambda_{j_0} \prod_{\substack{i \in V \setminus [\mathbf{D}] \\ i \neq i_0, j_0}} \lambda_i \\
&= \sum_{\substack{\mathbf{D} \in \mathcal{D} \\ [\mathbf{D}] \not\ni i_0, [\mathbf{D}] \not\ni j_0}} (-\beta)^{|\mathbf{D}|} (1 + (d_{i_0} - 2)\beta)(1 + (d_{j_0} - 2)\beta) \prod_{\substack{i \in V \setminus [\mathbf{D}] \\ i \neq i_0, j_0}} \lambda_i \\
&+ \beta \sum_{\substack{\mathbf{D} \in \mathcal{D} \\ [\mathbf{D}] \not\ni i_0, [\mathbf{D}] \not\ni j_0}} (-\beta)^{|\mathbf{D}|} (2 + (d_{i_0} + d_{j_0} - 3)\beta) \prod_{\substack{i \in V \setminus [\mathbf{D}] \\ i \neq i_0, j_0}} \lambda_i \\
&=: E_1 + \beta E_2.
\end{aligned}$$

We can straightforwardly check that

$$\Xi_{G \setminus e}(-\beta, \boldsymbol{\lambda}') = B + C_1 + D_1 + E_1$$

and

$$\beta \Xi_{G/e}(-\beta, \boldsymbol{\lambda}'') = A + \beta C_2 + \beta D_2 + \beta E_2, \tag{5.2}$$

where $\boldsymbol{\lambda}'$ and $\boldsymbol{\lambda}''$ are defined by the degrees of $G \setminus e$ and G/e respectively. Note that $C_2 + D_2$ in Eq. (5.2) corresponds to dimer arrangements in G/e that cover the new vertex formed by the contraction. This shows the deletion-contraction relation. □

Let $p_G(k)$ be the number of k-matchings of G. The *matching polynomial* α_G is defined by

$$\alpha_G(x) = \sum_{k=0}^{\lfloor \frac{|V|}{2} \rfloor} (-1)^k p_G(k) x^{|V|-2k}.$$

The matching polynomial is essentially the monomer-dimer partition function with uniform weights; if we set all vertex weights λ and all edge weights μ respectively, we have

$$\Xi_G(\mu, \lambda) = \alpha_G\Big(\frac{\lambda}{\sqrt{-\mu}}\Big)\sqrt{-\mu}^{|V|}.$$

Therefore, for a $(q+1)$-regular graph G, Theorem 5.5 implies

$$\omega_G(u^2) = \alpha_G\Big(\frac{1}{u} + qu\Big)u^{|V|}. \tag{5.3}$$

In [18], Nagle derives a sub-coregraph expansion of the monomer-dimer partition function with uniform weights, or matching polynomials, on regular graphs. With a transform of variables, his expansion theorem is essentially equivalent to Eq. (5.3); Theorem 5.5 gives an extension of the expansion to non-regular graphs.

As an immediate consequence of Eq. (5.3), we remark on the symmetry of the coefficients of ω_G for regular graphs.

Corollary 5.6. *Let G be a $(q+1)-$regular graph $(q \geq 1)$ with N vertices and w_k be the k-th coefficient of $\omega_G(\beta)$. Then we have*

$$w_{N-k} = w_k q^{N-2k} \qquad \text{for } 0 \leq k \leq N.$$

5.3. Zeros of $\omega_G(\beta)$

Physicists are interested in the complex zeros of partition functions, because it restrict occurrence of phase transitions, i.e., discontinuity of physical quantities with respect to parameters such as temperature. In the limit of infinite size of graphs, analyticity of the scaled log partition function on a complex domain is guaranteed if there are no zeros in the domain and some additional conditions hold. (See [32, 23].) For the monomer-dimer partition function, Heilman and Lieb [15] show the following result.

Theorem 5.7 ([15] Theorem 4.6). *If $\mu_e \geq 0$ for all $e \in E$ and $\mathrm{Re}(\lambda_j) > 0$ for all $j \in V$ then $\Xi_G(\boldsymbol{\mu}, \boldsymbol{\lambda}) \neq 0$. The same statement is true if $\mathrm{Re}(\lambda_j) < 0$ for all $j \in V$.*

Since our polynomial $\omega_G(\beta)$ is a monomer-dimer partition function, we obtain a bound of the region of complex zeros.

Corollary 5.8. *Let G be a graph and let d_m and d_M be the minimum and maximum degree in $\mathrm{core}(G)$ respectively and assume that $d_m \geq 2$. If $\beta \in \mathbb{C}$ satisfies $\omega_G(\beta) = 0$, then*

$$\frac{1}{d_M - 1} \leq |\beta| \leq \frac{1}{d_m - 1}.$$

Proof. Without loss of generality, we assume that G is a coregraph. Let $\beta = |\beta|\mathrm{e}^{i\theta}$ satisfy $\omega_G(\beta) = 0$, where $0 \le \theta < 2\pi$ and i is the imaginary unit. Since $\omega_G(0) = 1$ and the coefficients of $\omega_G(\beta)$ is not negative from Proposition 5.4, we have $\beta \neq 0$ and $\theta \neq 0$. We see that

$$\omega_G(\beta) = \Xi_G(-\beta, \boldsymbol{\lambda}) = \Xi_G(|\beta|, i\mathrm{e}^{-i\theta/2}\boldsymbol{\lambda})(i\mathrm{e}^{-i\theta/2})^{-|V|},$$

where $\lambda_j = 1 + (d_j - 1)\beta$, and $\mathrm{Re}(i\mathrm{e}^{-i\theta/2}\lambda_j) = (1 - (d_j - 1)|\beta|)\sin\frac{\theta}{2}$. From Theorem 5.7, the assertion follows. □

Especially, if the graph is a $(q+1)$-regular graph, the roots are on the circle of radius $1/q$, which is also directly seen by Eq. (5.3) combining the famous result on the roots of matching polynomials [15]: the zeros of matching polynomials are on the real interval $(-2\sqrt{q}, 2\sqrt{q})$.

5.4. Determinant sum formula

Let $\mathcal{T} := \{C \subset E; d_i(C) = 0 \text{ or } 2 \text{ for all } i \in V\}$ be the set of unions of vertex-disjoint cycles. In this subsection, an element $C \in \mathcal{T}$ is identified with the subgraph (V_C, C), where $V_C := \{i \in V; d_i(C) \neq 0\}$. A graph $G \setminus C$ is given by deleting all the vertices in V_C and the edges of G that are incident with them.

The aim of this subsection is Theorem 5.9, in which we represent ω_G as a sum of determinants. This theorem is similar to the expansion of the matching polynomial by characteristic polynomials [13];

$$\alpha_G(x) = \sum_{C \in \mathcal{T}} 2^{k(C)} \det[xI - A_{G\setminus C}], \tag{5.4}$$

where $A_{G\setminus C}$ is the adjacency matrix of $G \setminus C$ and $k(C)$ is the number of connected components of C.

Theorem 5.9.

$$\omega_G(u^2) = \sum_{C \in \mathcal{T}} 2^{k(C)} \det\left([I - uA_G + u^2(D_G - I)]\Big|_{G\setminus C} \right) u^{|C|}, \tag{5.5}$$

where D_G is the degree matrix defined by $(D_G)_{i,j} := d_i\delta_{i,j}$ and $\cdot\big|_{G\setminus C}$ denotes the restriction to the principal minor indexed by the vertices of $G \setminus C$.

Proof. For the proof, we use the result of Chernyak and Chertkov [7]. For given weights $\boldsymbol{\mu} = (\mu_e)_{e\in E}$ and $\boldsymbol{\lambda} = (\lambda_i)_{i\in V}$, a $|V| \times |V|$ matrix H is defined by

$$H := \mathrm{diag}(\boldsymbol{\lambda}) - \sum_{e\in E} \sqrt{-\mu_e} A_e,$$

where $A_e = E_{i,j} + E_{j,i}$ for $e = ij$ and $E_{i,j}$ is the matrix base. In our notation, their result implies

$$\Xi_G(\boldsymbol{\mu}, \boldsymbol{\lambda}) = \sum_{C \in \mathcal{T}} 2^{k(C)} \det H|_{G\setminus C} \prod_{e\in C} \sqrt{-\mu_e}.$$

If we set $\lambda_i = 1 + (d_i - 1)u^2$ and $\sqrt{-\mu_e} = u$, then the assertion follows. □

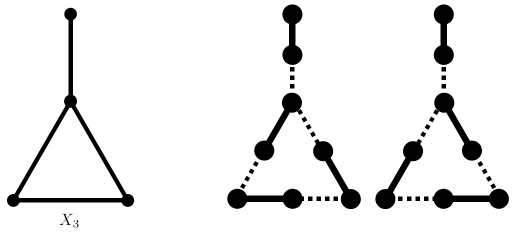

Figure 2. Graph X_3 and possible arrangements on $X_3^{(2)}$.

For regular graphs, Eqs. (5.4) and (5.5) are equivalent because of Eq. (5.3).

The matrix $(I - uA_G + u^2(D_G - I))$ is well known for its appearance in the Ihara formula of the graph zeta function [25]. The result in [29] shows that the Bethe free energy and the graph zeta function are intimately related though mathematical connections between the result and Theorem 5.9 are unknown.

5.5. Values at $\beta = 1$

The value of $\omega_G(1)$ is interpreted as the number of a set constructed from G. For the following theorem, recall that $G^{(2)}$ is obtained by adding a vertex on each edge in $G = (V, E)$. The vertices of $G^{(2)} := (V^{(2)}, E^{(2)})$ are classified into V_O and V_A, where V_O is the original vertices and V_A is the ones newly added, respectively. The set of matchings on $G^{(2)}$ is denoted by $\mathcal{D}_{G^{(2)}}$.

Theorem 5.10.

$$\omega_G(1) = |\{\mathbf{D} \in \mathcal{D}_{G^{(2)}}; [\mathbf{D}] \supset V_O\}|.$$

Proof. From Theorem 5.2, we have

$$\omega_G(1) = \sum_{\substack{s \subset E, s = G_1 \cup \cdots \cup G_{k(s)} \\ n(G_j)=1 \text{ for } j=1\ldots k(s)}} 2^{k(s)}, \tag{5.6}$$

where G_j is a connected component of (V, s). We construct a map F from $\{\mathbf{D} \in \mathcal{D}_{G^{(2)}}; [\mathbf{D}] \supset V_O\}$ to $s \subset E$ as

$$F(\mathbf{D}) := \{e \in E; \text{ the half of } e \text{ is covered by an edge in } \mathbf{D}\}.$$

Then the nullity of each connected component of $F(\mathbf{D})$ is 1 and $|F^{-1}(s)| = 2^{k(s)}$. $\square$

Example 3. For the graph X_3 in Figure 2, $\omega_{X_3}(1) = \omega_{C_3}(1) = 2$. The corresponding arrangements are also shown in Figure 2.

In the end, we remark on the relations between the results on $\omega_G(1)$ obtained in this paper. From Proposition 5.3, $\omega_G(1)$ satisfies

$$\omega_G(1) = \omega_{G \backslash e}(1) + \omega_{G/e}(1) \quad \text{if } e \in E \text{ is not a loop.}$$

This relation can be directly observed from the interpretation of Theorem 5.10. Theorem 5.5 gives

$$\omega_G(1) = \sum_{\mathbf{D} \in \mathcal{D}} (-1)^{|\mathbf{D}|} \prod_{i \in V \setminus [\mathbf{D}]} d_i,$$

which can be proved from Theorem 5.10 with the inclusion-exclusion principle. Theorem 5.9 gives

$$\omega_G(1) = \sum_{C \in \mathcal{T}} 2^{k(C)} \det \left[D_G - A_G \right] \Big|_{G \setminus C}.$$

We can directly prove this formula from Theorem 5.10 using a kind of matrix-tree theorem.

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