WEIGHTED ENUMERATION OF SPANNING SUBGRAPHS WITH DEGREE CONSTRAINTS

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ABSTRACT. The Heilmann-Lieb Theorem on (univariate) matching polynomials states that the polynomial $\sum_k m_k(G)y^k$ has only real nonpositive zeros, in which $m_k(G)$ is the number of k-edge matchings of a graph G. There is a stronger multivariate version of this theorem. We provide a general method by which "theorems of Heilmann-Lieb type" can be proved for a wide variety of polynomials attached to the graph G. These polynomials are multivariate generating functions for spanning subgraphs of G with certain weights and constraints imposed, and the theorems specify regions in which these polynomials are nonvanishing. Such theorems have consequences for the absence of phase transitions in certain probabilistic models for spanning subgraphs of G.

1. INTRODUCTION.

Let G = (V, E) be a finite graph, possibly with loops or multiple edges. For each natural number $k \in \mathbb{N}$, let $m_k(G)$ denote the number of k-edge matchings in G. The univariate Heilmann-Lieb Theorem [4] states that all zeros of the polynomial $\mu(G; y) = \sum_k m_k(G)y^k$ lie on the negative real axis. A stronger multivariate version has variables $\mathbf{x} = \{x_v : v \in V\}$, one for each vertex, and concerns the polynomial

$$\widetilde{\mu}(G;\mathbf{x}) = \sum_{M} \mathbf{x}^{\deg(M)}$$

in which the sum is over all matchings M of G, $\deg(M) : V \to \mathbb{N}$ is the degree function of M, and for any $f : V \to \mathbb{N}$

$$\mathbf{x}^f = \prod_{v \in V} x_v^{f(v)}.$$

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The multivariate Heilmann-Lieb Theorem [4] states that if $|\arg(x_v)| < \pi/2$ for all $v \in V$ then $\tilde{\mu}(G; \mathbf{x}) \neq 0$. One sees that this implies the univariate version by means of the relation

$$\mu(G; y) = \widetilde{\mu}(G; y^{1/2}\mathbf{1})$$

(which follows from the Handshake Lemma).

The purpose of this paper is to apply some standard results from the analytic theory of complex polynomials to provide a general method by which "theorems of Heilmann-Lieb type" can easily be deduced. The multivariate Heilmann-Lieb Theorem itself appears as the simplest – and prototypical – special case of the method. Other direct applications provide multivariate extensions of previous results of the author [10], and of results of Ruelle [8, 9]. A variety of new results also appear as natural special cases.

In the remainder of this Introduction we describe the general combinatorial situation we will consider. In Section 2 we gather the necessary results from the analytic theory of complex polynomials. In Section 3 we state and prove the main theorem of the paper. Section 4 illustrates this result with several applications, including the previously known examples mentioned above. In Section 5 we explain an interpretation of the polynomials we consider as partition functions, by analogy with the Boltzmann-Gibbs formalism in statistical mechanics. Results like those in Section 4 imply that when the thermodynamic limit of the free energy exists it must be analytic in certain regions of the complex plane. As noted by Lee and Yang [5, 11], this has implications for the absence of phase transitions in these models (which enumerate spanning subgraphs subject to certain weights and constraints). A more thorough investigation of the phase structure of these models would be very interesting, but must be left for a later paper.

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The general framework we consider is that of a finite graph G = (V, E) (possibly with loops or multiple edges) and a set of weights $\lambda = \{\lambda_e : e \in E\}$ on the edges of G. These weights can for some purposes be considered as indeterminates, but will usually be taken to be complex numbers, and often will be nonnegative real numbers. (In combinatorial applications it is most natural to set all the edge-weights equal to one.) The starting point for the theory is the elementary

identity

(1.1)
$$\Omega(G, \boldsymbol{\lambda}; \mathbf{x}) = \prod_{v \in w \in E} (1 + \lambda_e x_v x_w) = \sum_{H \subseteq E} \boldsymbol{\lambda}^H \mathbf{x}^{\deg(H)}.$$

In this formula, the product is over the set of all edges $e \in E$, and the notation *vew* indicates that the ends of e are the vertices v and w(note that v = w is possible). The sum is over the set of all spanning subgraphs (V, H) of G, each of which is determined by its edge-set $H \subseteq E$. As above $\deg(H) : V \to \mathbb{N}$ is the degree function of H, and we use the shorthand notations

$$\boldsymbol{\lambda}^{H} = \prod_{e \in H} \lambda_{e}$$

and

$$\mathbf{x}^{\deg(H)} = \prod_{v \in V} x_v^{\deg(H,v)}$$

This $\Omega(G, \lambda; \mathbf{x})$ is a relatively structureless object, since it sums over all spanning subgraphs without preference. On the other hand, the product formula allows one to make very precise statements about its zero-set (as a subset of \mathbb{C}^V). To make use of this, we introduce a sequence of *activities* at each vertex $v \in V$:

(1.2)
$$\mathbf{u}^{(v)} = (u_0^{(v)}, u_1^{(v)}, ..., u_d^{(v)}) \quad (d = \deg(G, v))$$

which can be any complex numbers (usually taken to be nonnegative reals). With these activities specified, a spanning subgraph $H \subseteq E$ will be given the weight

(1.3)
$$\mathbf{u}_{\deg(H)} = \prod_{v \in V} u_{\deg(H,v)}^{(v)}$$

and we will consider the correspondingly weighted version of $\Omega(G, \lambda; \mathbf{x})$:

(1.4)
$$Z(G, \lambda, \mathbf{u}; \mathbf{x}) = \sum_{H \subseteq E} \lambda^H \mathbf{u}_{\deg(H)} \mathbf{x}^{\deg(H)}.$$

For example, if at every vertex we take $u_0 = u_1 = 1$ and $u_k = 0$ for all $k \ge 2$, then

$$\mathbf{u}_{\deg(H)} = \begin{cases} 1 & \text{if } H \text{ is a matching,} \\ 0 & \text{otherwise,} \end{cases}$$

and $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is an edge-weighted version of the multivariate matching polynomial $\tilde{\mu}(G; \mathbf{x})$ above.

The strategy in what follows is to begin with information about the zero-set of $\Omega(G, \lambda; \mathbf{x})$ and to impose conditions on the vertex activities $\mathbf{u}^{(v)}$ that are sufficient to imply similar information about the zero-set

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of $Z(G, \lambda, \mathbf{u}; \mathbf{x})$. To realize this plan, we need a few results from the analytic theory of complex polynomials.

2. Complex polynomials.

The technique we use is known as *Schur-Szegő composition*. We do not make use of the most general possible result, but for thoroughness of exposition we derive what is needed from the Grace-Szegő-Walsh Coincidence Theorem. For a more complete treatment see Sections 15 and 16 of Marden [6] and Chapters 3 and 5 of Rahman and Schmeisser [7].

Let $F(\mathbf{z})$ be a polynomial in complex variables $\mathbf{z} := \{z_v : v \in V\}$. For a subset $\mathcal{A} \subset \mathbb{C}$, we say that F is \mathcal{A} -nonvanishing if either $F \equiv 0$, or $z_v \in \mathcal{A}$ for all $v \in V$ implies that $F(\mathbf{z}) \neq 0$. In the case that $F \not\equiv 0$ we say that F is *strictly* \mathcal{A} -nonvanishing.

Lemma 2.1. Let \mathcal{A} be nonempty, connected and open. Let $F_n(\mathbf{z})$ be a sequence of strictly \mathcal{A} -nonvanishing polynomials indexed by positive integers, and assume that the limit $F(\mathbf{z}) = \lim_{n\to\infty} F_n(\mathbf{z})$ exists. Then F is \mathcal{A} -nonvanishing.

Proof. Each F_n is analytic and strictly nonvanishing on the subset \mathcal{A}^V of \mathbb{C}^V . Since these functions are polynomials, the convergence to F is uniform on compact subsets of \mathbb{C}^V . By Hurwitz's Theorem (Theorem 1.3.8 of [7]), either F is identically zero or F is nonvanishing on \mathcal{A}^V as well.

Lemma 2.2. Let \mathcal{A} be nonempty, connected and open. Let $F(\mathbf{z})$ be an \mathcal{A} -nonvanishing polynomial, and let $w \in V$. If z_w is fixed at a complex value ξ in the closure of \mathcal{A} , then the resulting polynomial in the variables $\{z_v : v \in V \setminus \{w\}\}$ is \mathcal{A} -nonvanishing.

Proof. The result is trivial if $F \equiv 0$, so assume instead that F is strictly \mathcal{A} -nonvanishing. Let $(\xi_n : n = 1, 2, ...)$ be a sequence with each $\xi_n \in \mathcal{A}$ such that $\lim_{n\to\infty} \xi_n = \xi$. Note that for all $n \geq 1$ the specialization $z_w = \xi_n$ results in a polynomial F_n that is strictly \mathcal{A} -nonvanishing in the variables $\{z_v : v \in V \setminus \{w\}\}$. The sequence $(F_n : n \geq 1)$ satisfies the hypothesis of Lemma 2.1, from which the result follows. \Box

We are concerned mostly with the following open subsets of \mathbb{C} . • For $0 < \theta \leq \pi$, the open sector

(2.1)
$$S[\theta] = \{ z \in \mathbb{C} : z \neq 0 \text{ and } |\arg(z)| < \theta \}$$

centered on the positive real axis. (For $z \neq 0$ we use the value of the argument in the range $-\pi < \arg(z) \leq \pi$.)

• For $\kappa > 0$, the open interior of a disk

(2.2)
$$\kappa \mathcal{D} := \{ z \in \mathbb{C} : |z| < \kappa \}.$$

• Also for $\kappa > 0$, the open exterior of a disk

(2.3)
$$\kappa \mathcal{E} := \{ z \in \mathbb{C} : |z| > \kappa \}.$$

When $\kappa = 1$ we more simply write just \mathcal{D} and \mathcal{E} .

A circular region in \mathbb{C} is a proper subset that is either open or closed and is bounded by either a circle or a straight line. A polynomial $F(\mathbf{z}) = F(z_1, ..., z_d)$ is multiaffine if each variable occurs at most to the first power. The polynomial $F(\mathbf{z})$ is symmetric if it is invariant under every permutation of the variables. The elementary symmetric functions of the variables $\mathbf{z} = (z_1, ..., z_d)$ are

(2.4)
$$e_j(\mathbf{z}) = \sum_{1 \le i_1 < i_2 < \dots < i_j \le d} z_{i_1} z_{i_2} \cdots z_{i_j}.$$

A multiaffine symmetric polynomial $F(z_1, ..., z_d)$ is thus a linear combination of the elementary symmetric functions $e_j(\mathbf{z})$ for $0 \le j \le d$.

Proposition 2.3 (Grace-Szegő-Walsh). Let $F(z_1, ..., z_d)$ be a multiaffine symmetric polynomial, and let \mathcal{A} be a circular region. Assume that either \mathcal{A} is convex or the degree of F is d. Then, for any values $\zeta_1, ..., \zeta_d \in \mathcal{A}$ there exists a value $\zeta \in \mathcal{A}$ such that

$$F(\zeta_1, ..., \zeta_d) = F(\zeta, ..., \zeta).$$

For a proof in the case that deg F = d, see Theorem 15.4 of [6] or Theorem 3.4.1b of [7]. The theorem also holds when deg F < d with the additional hypothesis that \mathcal{A} is convex, as explained in Theorem 2.12 of [1].

For an elaboration of the ideas of Proposition 2.4, see Lemma 5.5.4 and Theorem 5.5.5 of [7].

Proposition 2.4 (Schur-Szegő). Let $P(z) = \sum_{j} c_{j} z^{j}$ and $K(z) = \sum_{j=0}^{d} {d \choose j} u_{j} z^{j}$ be polynomials in one complex variable z, with deg $P \leq d$, and let $Q(z) = \sum_{j=0}^{d} u_{j} c_{j} z^{j}$.

(a) For any $0 \le \alpha < \pi/2$, if P(z) is $S[\pi/2]$ -nonvanishing and K(z) is $S[\pi - \alpha]$ -nonvanishing, then Q(z) is $S[\pi/2 - \alpha]$ -nonvanishing.

(b) For any $\kappa > 0$ and $\rho > 0$, if P(x) is $\rho \mathbb{D}$ -nonvanishing and K(z) is $\kappa \mathbb{D}$ -nonvanishing, then Q(z) is $\kappa \rho \mathbb{D}$ -nonvanishing.

(c) For any $\kappa > 0$ and $\rho > 0$, if P(x) is $\rho \mathcal{E}$ -nonvanishing and K(z) is $\kappa \mathcal{E}$ -nonvanishing and deg K = d, then Q(z) is $\kappa \rho \mathcal{E}$ -nonvanishing.

Proof. The conclusions are trivial if $Q \equiv 0$, so we may assume that $Q \neq 0$.

We begin by proving part (a) in the case that $K(0) \neq 0$. In this case we have

(2.5)
$$K(z) = C \prod_{i=1}^{d} (1 + \theta_i z)$$

for some complex numbers $C \neq 0$ and $\theta_1, ..., \theta_d$ such that either $\theta_i = 0$ or $|\arg(\theta_i)| \leq \alpha$ for each $1 \leq i \leq d$. Consider the *d*-th polarization of P(z): this is the multiaffine symmetric polynomial $\widetilde{P}(\mathbf{z}) = \widetilde{P}(z_1, ..., z_d)$ obtained from P(z) by replacing each monomial z^j by the normalized *j*-th elementary symmetric function $\binom{d}{j}^{-1}e_j(\mathbf{z})$. Since deg $P \leq d$, it follows that

(2.6)
$$P(z, z, ..., z) = P(z)$$

as polynomials in z. Since P(z) is $S[\pi/2]$ -nonvanishing and $S[\pi/2]$ is a circular region, it follows from (2.6) and Proposition 2.4 that $\widetilde{P}(\mathbf{z})$ is also $S[\pi/2]$ -nonvanishing. Now, consider complex numbers $\zeta_1, ..., \zeta_d \in S[\pi/2 - \alpha]$. For each $1 \leq i \leq d$, either $\theta_i \zeta_i = 0$ for all $\zeta_i \in S[\pi/2 - \alpha]$ or $|\arg(\theta_i \zeta_i)| < \pi/2$ for all $\zeta_i \in S[\pi/2 - \alpha]$. From Lemma 2.2, it follows that if $\widetilde{P}(\theta_1 z_1, ..., \theta_d z_d) \neq 0$ then $\widetilde{P}(\theta_1 \zeta_1, ..., \theta_d \zeta_d) \neq 0$ for every choice of $\zeta_1, ..., \zeta_d \in S[\pi/2 - \alpha]$. That is, it follows that $\widetilde{P}(\theta_1 z_1, ..., \theta_d z_d)$ is $S[\pi/2 - \alpha]$ -nonvanishing. A short calculation using the fact that $\binom{d}{j}u_j = Ce_j(\theta_1, ..., \theta_d)$ verifies that

(2.7)
$$Q(z) = C\widetilde{P}(\theta_1 z, ..., \theta_d z),$$

and therefore Q(z) is $S[\pi/2 - \alpha]$ -nonvanishing, as desired.

To handle the case in which K(0) = 0, let r be the multiplicity of 0 as a root of K(z) and write

(2.8)
$$K(z) = Cz^r \prod_{i=1}^{d-r} (1+\theta_i z)$$

For a positive integer N let

(2.9)
$$K_N(z) = CN^{-r}(1+Nz)^r \prod_{i=1}^{d-r} (1+\theta_i z).$$

and let $Q_N(z)$ be the polynomial in the conclusion constructed from P(z) and $K_N(z)$. By the case we have done already, each $Q_N(z)$ is $S[\pi/2 - \alpha]$ -nonvanishing. Taking the limit as $N \to \infty$, Lemma 2.1 implies that Q(z) itself is also $S[\pi/2 - \alpha]$ -nonvanishing.

The proof of part (b) is similar. Since K(z) is $\kappa \mathcal{D}$ -nonvanishing we have $K(0) \neq 0$, and so we can write K(z) as in equation (2.5) with all $|\theta_i| \leq 1/\kappa$. Again we consider the *d*-th polarization $\tilde{P}(\mathbf{z})$ of P(z). Since P(z) is $\rho \mathcal{D}$ -nonvanishing and $\rho \mathcal{D}$ is a circular region, Proposition 2.3 and equation (2.6) imply that $\tilde{P}(\mathbf{z})$ is $\rho \mathcal{D}$ -nonvanishing. It follows that $\tilde{P}(\theta_1 z_1, ..., \theta_d z_d)$ is $\kappa \rho \mathcal{D}$ -nonvanishing, and from equation (2.7) we conclude that Q(z) is $\kappa \rho \mathcal{D}$ -nonvanishing, as desired.

The proof of part (c) repeats the same pattern once more. Begin with K(z) expressed as in equation (2.8) – since K(z) is $\kappa \mathcal{E}$ -nonvanishing, each $|\theta_i| \geq 1/\kappa$. We work with the polynomials $K_N(z)$ defined in equation (2.9) with $N \geq 1/\kappa$. Since P(z) is $\rho \mathcal{E}$ -nonvanishing and $\rho \mathcal{E}$ is a circular region and deg $\tilde{P} = d$, Proposition 2.3 and equation (2.6) imply that $\tilde{P}(\mathbf{z})$ is $\rho \mathcal{E}$ -nonvanishing. It follows that

$$P(\theta_1 z_1, ..., \theta_{d-r} z_{d-r}, N z_{d-r+1}, ..., N z_d)$$

is $\kappa\rho\mathcal{E}$ -nonvanishing, and from equation (2.7) we conclude that $Q_N(z)$ is $\kappa\rho\mathcal{E}$ -nonvanishing. Taking the limit as $N \to \infty$ (using Lemma 2.1) we conclude that Q(z) is $\kappa\rho\mathcal{E}$ -nonvanishing, as desired. \Box

The polynomial Q(z) in the conclusion of Proposition 2.4 is the *Schur-Szegő composition* of P(z) and K(z).

3. The main result.

Consider a graph G = (V, E) with complex edge weights λ . We begin with some easy information about the zero-set of the polynomial $\Omega(G, \lambda; \mathbf{x})$ defined in equation (1.1).

Proposition 3.1. Let G = (V, E) be a graph with complex edge weights λ .

(a) If $\lambda_e \geq 0$ for each $e \in E$ then $\Omega(G, \lambda; \mathbf{x})$ is $S[\pi/2]$ -nonvanishing.

(a) If $\lambda_e \leq \delta$ for each $e \in E$ then $\Omega(G, \lambda; \mathbf{x})$ is $\lambda_{\max}^{-1/2} \mathcal{D}$ -nonvanishing. (b) If $|\lambda_e| \leq \lambda_{\max}$ for each $e \in E$ then $\Omega(G, \lambda; \mathbf{x})$ is $\lambda_{\max}^{-1/2} \mathcal{D}$ -nonvanishing. (c) If $|\lambda_e| \geq \lambda_{\min}$ for each $e \in E$ then $\Omega(G, \lambda; \mathbf{x})$ is $\lambda_{\min}^{-1/2} \mathcal{E}$ -nonvanishing.

Proof. In each case, each factor $1 + \lambda_e z_v z_w$ in the product form for $\Omega(G, \lambda; \mathbf{z})$ is seen to be nonvanishing in the appropriate region, from which the result follows.

Now assume that we also have a sequence of activities $\mathbf{u}^{(v)}$ at each vertex $v \in V$, as in equation (1.2). The information about these activities that we will use is recorded in the set of key polynomials

(3.1)
$$K_{v}(z) = \sum_{j=0}^{d} {\binom{d}{j}} u_{j}^{(v)} z^{j}$$

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in which $d = \deg(G, v)$. There is one key polynomial for each vertex $v \in V$.

Theorem 3.2. Let G = (V, E) be a graph, with complex edge weights λ , and with vertex activities \mathbf{u} encoded by the key polynomials $K_v(z)$ $(v \in V)$.

(a) Fix $0 \leq \alpha < \pi/2$. If $\lambda_e \geq 0$ for each $e \in E$ and $K_v(z)$ is $S[\pi - \alpha]$ -nonvanishing for each $v \in V$, then $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $S[\pi/2 - \alpha]$ -nonvanishing.

(b) Fix $\kappa > 0$ and $\lambda_{\max} > 0$. If $|\lambda_e| \leq \lambda_{\max}$ for each $e \in E$ and $K_v(z)$ is $\kappa \mathcal{D}$ -nonvanishing for each $v \in V$, then $Z(G, \boldsymbol{\lambda}, \mathbf{u}; \mathbf{x})$ is $(\kappa / \lambda_{\max}^{1/2}) \mathcal{D}$ -nonvanishing.

(c) Fix $\kappa > 0$ and $\lambda_{\min} > 0$. If $|\lambda_e| \ge \lambda_{\min}$ for each $e \in E$ and $K_v(z)$ is $\kappa \mathcal{E}$ -nonvanishing and $\deg K_v(z) = \deg(G, v)$ for each $v \in V$, then $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $(\kappa / \lambda_{\min}^{1/2}) \mathcal{E}$ -nonvanishing.

Proof. Identify the vertices V with the numbers $V = \{1, 2, ..., n\}$ arbitrarily. Define a sequence of polynomials $F_0(\mathbf{x})$, $F_1(\mathbf{x})$,..., $F_n(\mathbf{x})$ as follows. $F_0(\mathbf{x}) = \Omega(G, \boldsymbol{\lambda}; \mathbf{x})$, and for all $1 \leq v \leq n$, $F_v(\mathbf{x})$ is the Schur-Szegő composition of $F_{v-1}(\mathbf{x})$ regarded as a polynomial in the variable x_v (the other variables being absorbed into the coefficients) with $K_v(x_v)$. One sees by induction that for $0 \leq r \leq n$:

(3.2)
$$F_r(\mathbf{x}) = \sum_{H \subseteq E} \boldsymbol{\lambda}^H \left(\prod_{v=1}^r u_{\deg(H,v)}^{(v)} \right) \mathbf{x}^{\deg(H)},$$

so that $F_n(\mathbf{x}) = Z(G, \boldsymbol{\lambda}, \mathbf{u}; \mathbf{x}).$

We give the details to finish the proof of part (a) – the arguments for parts (b) and (c) are completely analogous. We prove by induction on $1 \le v \le n$ that if $(\zeta_j : 1 \le j \le n)$ are complex numbers such that • $|\arg(\zeta_j)| < \pi/2 - \alpha$ for all $1 \le j < v$, and • $|\arg(\zeta_j)| < \pi/2$ for all $v < j \le n$,

then

(3.3)
$$F_{v-1}(\zeta_1, ..., \zeta_{v-1}, x_v, \zeta_{v+1}, ..., \zeta_n)$$

is $S[\pi/2]$ -nonvanishing. The basis of induction follows from Proposition 3.1(a) and Lemma 2.2. The induction step follows from Proposition 2.4(a) and Lemma 2.2. Finally, from the statement that whenever all $\zeta_i \in S[\pi/2 - \alpha]$, then $F_{n-1}(\zeta_1, ..., \zeta_{n-1}, x_n)$ is $S[\pi/2]$ -nonvanishing, we conclude by one more application of Proposition 2.4(a) that $F_n(\mathbf{x})$ is $S[\pi/2 - \alpha]$ -nonvanishing, as desired.

The univariate specialization of Theorem 3.2 is an important consquence.

Corollary 3.3. Adopt the notation of Theorem 3.2. (a) Under the hypotheses of Theorem 3.2(a), $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $S[\pi - 2\alpha]$ -nonvanishing. (b) Under the hypotheses of Theorem 3.2(b), $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $(\kappa^2/\lambda_{\max})\mathcal{D}$ -nonvanishing. (c) Under the hypotheses of Theorem 3.2(c), $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $(\kappa^2/\lambda_{\min})\mathcal{E}$ -nonvanishing.

4. Applications.

Throughout this section, consider a graph G = (V, E) with complex edge weights $\boldsymbol{\lambda}$ and vertex activities \mathbf{u} encoded by the key polynomials $K_v(z)$ ($v \in V$).

Example 4.1 (Heilmann-Lieb [4]). Assume that all edge weights are nonnegative reals, and that at each vertex $u_0 = u_1 = 1$ and $u_k = 0$ for all $k \geq 2$. The key polynomial at a vertex of degree d in G is $K_v(z) = 1 + dz$, which is $S[\pi]$ -nonvanishing. Theorem 3.2(a) (with $\alpha = 0$) implies that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $S[\pi/2]$ -nonvanishing – this is the multivariate Heilmann-Lieb theorem. Corollary 3.3(a) implies that $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $S[\pi]$ -nonvanishing – this is the univariate Heilmann-Lieb theorem.

Example 4.2 (Wagner [10]). Assume that all edge weights are nonnegative reals, and that two functions $f, g: V \to \mathbb{N}$ are given such that $f(v) \leq g(v) \leq f(v) + 1$ for each $v \in V$. Fix the vertex activities to be

(4.1)
$$u_k^{(v)} = \begin{cases} 1 & \text{if } f(v) \le k \le g(v), \\ 0 & \text{otherwise.} \end{cases}$$

As in Example 4.1, each key $K_v(z)$ is $S[\pi]$ -nonvanishing. Theorem 3.2(a) (with $\alpha = 0$) implies that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $S[\pi/2]$ -nonvanishing – this result is new. Corollary 3.3(a) implies that $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $S[\pi]$ -nonvanishing – when $\lambda \equiv \mathbf{1}$ this is Theorem 3.3 of [10].

Example 4.3 (Ruelle [8, 9]). Assume that all edge weights are nonnegative reals, and that at each vertex $u_0 = u_2 = 1$, $u_1 = u$, and $u_k = 0$ for all $k \ge 2$. The key polynomial at a vertex of degree d in G is $K_v(z) = 1 + duz + {d \choose 2} z^2$. For $d \ge 2$, the zeros of this polynomial are at

$$z_{\pm} = \frac{-2}{d-1} \left(u \pm \sqrt{u^2 - 2 + 2/d} \right).$$

When u = 1, all the keys $K_v(z)$ are $S[3\pi/4]$ -nonvanishing, and Theorem 3.2(a) (with $\alpha = \pi/4$) implies that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $S[\pi/4]$ nonvanishing – this is new. Corollary 3.3(a) implies that $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $S[\pi/2]$ -nonvanishing – when $\lambda \equiv 1$ this is a slight weakening of Proposition 1 of [8].

If G has maximum degree Δ and $u \geq \sqrt{2-2/\Delta}$, then all the keys $K_v(z)$ are $S[\pi]$ -nonvanishing, and Theorem 3.2(a) (with $\alpha = 0$) implies that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $S[\pi/2]$ -nonvanishing – this result is new. Corollary 3.3(a) implies that $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $S[\pi]$ -nonvanishing – when $\lambda \equiv \mathbf{1}$ this is Proposition 2 of [8].

Ruelle's method produces more detailed information than ours, but only for particular choices of the vertex activities. A systematic extension of his method that handles all the cases we consider would be very interesting.

Example 4.4. Assume that all edge weights are nonnegative reals, and that two functions $f, g: V \to \mathbb{N}$ are given such that $f(v) \leq g(v) \leq f(v) + 2$ for each $v \in V$. Fix the vertex activities as in equation (4.1). Then each key $K_v(z)$ is $S[2\pi/3]$ -nonvanishing. Theorem 3.2(a) (with $\alpha = \pi/3$) implies that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $S[\pi/6]$ -nonvanishing, and Corollary 3.3(a) implies that $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $S[\pi/3]$ -nonvanishing.

Example 4.5. Assume that all edge weights are nonnegative reals, and that two functions $f, g: V \to \mathbb{N}$ are given such that $f(v) \leq g(v) \leq f(v) + 3$ for each $v \in V$. Fix the vertex activities as in equation (4.1). If every vertex of G has degree at most Δ then there is a small angle $\varepsilon > 0$ such that each key $K_v(z)$ is $S[\pi/2 + \varepsilon]$ -nonvanishing. To see this, the keys with at most three terms pose no problems (by Examples 4.2 and 4.4). A key with four terms has the form

$$K(z) = \binom{d}{f} z^{f} + \binom{d}{f+1} z^{f+1} + \binom{d}{f+2} z^{f+2} + \binom{d}{f+3} z^{f+3},$$

and the inequality

$$\binom{d}{f+1}\binom{d}{f+2} > \binom{d}{f}\binom{d}{f+3}$$

ensures that the only zero of K(z) with nonnegative real part is at the origin. Since Δ is fixed, only finitely many key polynomials need to be considered – taking the smallest positive argument of the (nonzero) zeros of these to be $\pi/2 + \varepsilon$ gives the desired angle.

Theorem 3.2(a) implies that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is $S[\varepsilon]$ -nonvanishing, and Corollary 3.3(a) implies that $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ is $S[2\varepsilon]$ -nonvanishing.

Example 4.6. In Examples 4.1 and 4.2 we concluded that the polynomial $Z(y) = Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ had only real (and nonpositive) zeros. Let $N_j = N_j(G, \lambda, \mathbf{u})$ be the coefficient of y^j in this polynomial. It is

"folklore" that if Z(y) is $S[2\pi/3]$ -nonvanishing, then

$$N_i N_k \neq 0$$
 implies that $N_j \neq 0$ for all $i \leq j \leq k$

and

$$N_j^2 \ge N_{j+1}N_{j-1}$$
 for all j .

This property (logarithmic concavity with no internal zeros) is very useful for obtaining good approximations to the sequence (N_j) (see [2, 3, 4], for example).

If all the keys $K_v(z)$ are $S[5\pi/6]$ -nonvanishing then Z(y) is $S[2\pi/3]$ nonvanishing. However, this hypothesis on the keys is unreasonably strong. Consider a key of the form

$$K(z) = \binom{d}{j-1}z^{j-1} + \binom{d}{j}z^j + \binom{d}{j+1}z^{j+1}$$

with $1 \leq j \leq d-1$, corresponding to three consecutive permissible degrees. A short calculation shows that this is $S[5\pi/6]$ -nonvanishing if and only if $2j(d-j) \leq d+2$. This happens only for the pairs (j,d) with $d \leq 4$ and j = 1 or j = d-1.

Nonetheless, I venture the following conjecture.

Conjecture 4.7. Let G = (V, E) be a finite graph, and let $f, g : V \to \mathbb{N}$ be any two functions. Fix the vertex activities \mathbf{u} as in (4.1). Then the sequence of coefficients (N_j) of $Z(G, \mathbf{1}, \mathbf{u}; y^{1/2}\mathbf{1})$ is logarithmically concave with no internal zeros.

Example 4.8. Assume that all the edge weights have unit modulus, that G is 2k-regular, and that the key at each vertex is

(4.2)
$$K(z) = 1 + \binom{2k}{k} z^k + u z^{2k}.$$

If $4u \ge {\binom{2k}{k}}^2$ then every zero of K(z) has modulus $\kappa = u^{-1/2k}$. Parts (b) and (c) of Theorem 3.2 imply that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is both $\kappa \mathcal{D}$ - and $\kappa \mathcal{E}$ -nonvanishing. Corollary 3.3 implies that every zero of $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ has modulus $u^{-1/k}$.

Example 4.9. Assume that all the edge weights have unit modulus, and that deg $K_v(z) = \text{deg}(G, v)$ and every zero of $K_v(z)$ has unit modulus, for each vertex $v \in V$. Parts (b) and (c) of Theorem 3.2 imply that $Z(G, \lambda, \mathbf{u}; \mathbf{x})$ is both \mathcal{D} - and \mathcal{E} -nonvanishing. Corollary 3.3 implies that every zero of $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ has unit modulus.

In particular, these hypotheses evidently hold if $\lambda \equiv 1$ and the key

polynomials are given by $K_v(z) = 1 + z + z^2 + \cdots + z^{\deg(G,v)}$ for each $v \in V$. Thus we conclude that every zero of

$$\sum_{H \subseteq E} \frac{y^{\#H}}{\prod_{v \in V} \binom{\deg(G,v)}{\deg(H,v)}}$$

has unit modulus.

5. Analogy with statistical mechanics.

We conclude with an interpretation of $Z(G, \lambda, \mathbf{u}; y^{1/2}\mathbf{1})$ inspired by analogy with the (canonical ensemble) partition functions in statistical mechanics. For simplicity, we restrict attention to a graph G = (V, E)that is *d*-regular, in which the edge weights $\lambda \equiv \mathbf{1}$ are all one and the activities are the same at every vertex (that is, all the key polynomials are equal). The extension to the general case is straightforward.

The "configuration space" is the set of all spanning subgraphs of G. The energy U(H) of a spanning subgraph $H \subseteq E$ depends on d + 2real parameters J and $\boldsymbol{\mu} = (\mu_0, \mu_1, ..., \mu_d)$, as follows:

(5.1)
$$U(H) = J \cdot \#H + \sum_{j=0}^{d} \mu_j \cdot \#V_j(H),$$

in which $V_j(H)$ is the set of vertices of degree j in H. The quasiphysical interpretation of this is that J is the energy of a single edge, and μ_j is the "chemical potential" energy of a vertex of degree j. With T > 0 denoting absolute temperature, and $\beta = 1/k_{\rm B}T$ where $k_{\rm B}$ is Boltzmann's constant, the *Boltzmann weight* of H is

 $e^{-\beta U(H)}$

and the *partition function* is

(5.2)
$$Z_G(\beta, J, \boldsymbol{\mu}) = \sum_{H \subseteq E} e^{-\beta U(H)}.$$

This can be interpreted as defining a family of probability measures (parameterized by β , J, and μ) on the set of all spanning subgraphs of G: a spanning subgraph $H \subseteq E$ is chosen at random with probability $e^{-\beta U(H)}/Z_G(\beta, J, \mu)$. A short computation shows that, for H chosen according to this distribution, the expected number of edges is

(5.3)
$$\langle \#H\rangle = -\frac{1}{\beta}\frac{\partial}{\partial J}\log Z_G(\beta, J, \mu)$$

and the expected number of vertices of degree j is

(5.4)
$$\langle \#V_j(H)\rangle = -\frac{1}{\beta}\frac{\partial}{\partial\mu_j}\log Z_G(\beta, J, \mu)$$

To continue with the analogy we consider a sequence of graphs G_1 , G_2 ,... that converges to an infinite, locally finite, limit graph Γ . (The precise definition of convergence is not important for this discussion – the prototypical example is that, as $n \to \infty$, the Cartesian product C_n^r of r cycles of length n should converge to the infinite graph \mathbb{Z}^r with edges of Euclidean length one.) We will further assume that the "thermodynamic limit" (Helmholtz) free energy

(5.5)
$$f_{\Gamma}(\beta, J, \boldsymbol{\mu}) = -\frac{1}{\beta} \lim_{n \to \infty} \frac{1}{\# V(G_n)} \log Z_{G_n}(\beta, J, \boldsymbol{\mu})$$

exists. As in the Lee-Yang theory [5, 11], points in the parameter space at which the free energy fails to be analytic can be interpreted as phase transitions between differing qualitative properties of a random spanning subgraph of Γ . From the form of (5.5) we see that f_{Γ} can fail to be analytic only at an accumulation point of the union of the zero-sets of all the $Z_{G_n}(\beta, J, \mu)$ $(n \geq 1)$. From the probabilistic interpretation, we are most interested in such accumulation points for which all the parameters (β, J, μ) are real.

The partition functions can be expressed as polynomials in the variables

(5.6)
$$y = e^{-\beta J}$$
 and $u_j = e^{-\beta \mu_j} \quad (0 \le j \le d).$

In fact, a tiny calculation shows that in these variables

(5.7)
$$Z_G(\beta, J, \boldsymbol{\mu}) = Z(G, \mathbf{1}, \mathbf{u}; y^{1/2} \mathbf{1})$$

with the RHS as defined in (1.4). The point y = 1 corresponds to $\beta J = 0$, which is the infinite-temperature limit. If J > 0 then y = 0 is the zero-temperature limit, and if J < 0 then $y \to +\infty$ is the zero-temperature limit. The positive real axis is thus the "physically" relevant part of the complex y-plane. If all the chemical potentials μ_j are real then all the activities u_j are positive reals. A zero activity $u_j = 0$ corresponds to an infinite chemical potential $\mu_j = +\infty$, which means that a vertex of degree j is forbidden. Notice that the activity $u_j = e^{-\beta\mu_j}$ also depends on temperature except when μ_j is $+\infty$ or 0: this is the case precisely when $u_j \in \{0, 1\}$.

In this context, Corollary 3.3 has the following immediate consequence, the proof of which is omitted.

Proposition 5.1. Let $(G_n : n \ge 1)$ be a sequence of *d*-regular graphs, and let $\beta > 0$ and $J \in \mathbb{R}$ and $\mu \in \mathbb{R}^{d+1}$ be such that the limit (5.5) exists. Form the key polynomial

$$K(z) = K(\beta, \boldsymbol{\mu}; z) = \sum_{j=0}^{d} {\binom{d}{j}} u_j z^j$$

with (u_i) as in (5.6).

(a) If there exists $\varepsilon > 0$ such that K(z) is $S[\pi/2 + \varepsilon]$ -nonvanishing then f_{Γ} is analytic at (β, J, μ) for all $J \in \mathbb{R}$.

(b) If $\kappa > 0$ is such that K(z) is $\kappa \mathbb{D}$ -nonvanishing then f_{Γ} is analytic at (β, J, μ) for all

$$J > -\frac{2}{\beta} \log \kappa.$$

(c) If $\kappa > 0$ is such that K(z) is $\kappa \mathcal{E}$ -nonvanishing and of degree d then f_{Γ} is analytic at (β, J, μ) for all

$$J < -\frac{2}{\beta}\log\kappa.$$

Finally, we revisit some of the examples of Section 4, maintaining as well the assumptions of Proposition 5.1.

Example 5.2. With the key polynomial K(z) as in Example 4.3, let $u = e^{-\beta\mu}$. If $\mu < +\infty$ (that is, if u > 0) then K(z) is $S[\pi/2 + \varepsilon]$ -nonvanishing for all $\beta \ge 0$, so that f_{Γ} is analytic at (β, J, μ) for all $J \in \mathbb{R}$. In this case there is no phase transition at any nonzero temperature. On the other hand, if $\mu = +\infty$ (that is, if u = 0) then both zeros of K(z) have modulus $\kappa = {d \choose 2}^{-1/2}$, so that f_{Γ} is analytic at (β, J, μ) for all

$$J > \frac{1}{\beta} \log \binom{d}{2}.$$

In this case there is no phase transition provided that the temperature T is sufficiently low compared to the edge energy J.

Example 5.3. With the key polynomial K(z) as in Example 4.5, K(z) is $S[\pi/2 + \varepsilon]$ -nonvanishing for all $\beta \ge 0$, so that f_{Γ} is analytic at (β, J, μ) for all $J \in \mathbb{R}$. Thus, there is never a phase transition in this model.

Example 5.4. With the key polynomial K(z) as in Example 4.8, let $u = e^{-\beta\mu}$ and d = 2k. If $\binom{2k}{k}^2 \leq 4u$ then all the zeros of K(z) have modulus $\kappa = u^{-1/2k}$ and K(z) has degree d. The only point on the positive y-axis at which f_{Γ} could fail to be analytic is at $y = u^{-1/k}$. In terms of the "physical" parameters, this says that if

(5.8)
$$-\beta\mu > 2\log\binom{2k}{k} - \log 4$$

then a phase transition can occur only at $J = -\mu/k$. The inequality (5.8) requires that $\mu < 0$ (so that vertices of degree 2k in H are energetically favoured) and that β is sufficiently large (so that the temperature is sufficiently low). If this is the case then a phase transition can occur only when the edge energy J and chemical potential μ are tuned to satisfy $J = -\mu/k$.

Example 5.5. With the key polynomial K(z) as in Example 4.9, all the zeros of K(z) have modulus one and K(z) has degree d. The only point on the positive y-axis at which f_{Γ} could fail to be analytic is at y = 1. In terms of the "physical" parameters, this says that a phase transition can occur only at $\beta J = 0$ – that is, only in the infinite temperature limit.

As these examples illustrate, Proposition 5.1 sees very little about the limit graph Γ – in fact, only the degree of Γ is relevant. (On the other hand, the existence of the limit f_{Γ} does depend on the structure of Γ .) Thus, for example, Proposition 5.1 can not tell the difference between the 3d cubical lattice and the 2d triangular grid – both graphs are regular of degree six. Of course, in truth one expects that for any given model, the free energies of these two graphs will have different phase diagrams. Accounting for more detailed structural properties of Γ remains an interesting open problem.

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